TWO SIDES OF A COIN:

A CRITICAL REVIEW, AND MATHEMATICAL AND PHENOMENOLOGICAL STUDY OF WHAT WE CALL HYDRO-MECHANICAL COUPLING

J.M.HUYGHE*, E. NIKOOEE†, T. SWEIJEN† AND S. MAJID HASSANIZADEH†

*Department of Mechanical Engineering, TU Eindhoven, The Netherlands

e-mail: j.m.r.huyghe@tue.nl

† Earth Sciences Department, Utrecht University, The Netherlands

E-mail: e.nikooee@uu.nl, T.Sweijen@uu.nl, s.m.hassanizadeh@uu.nl

Key words: Unsaturated soils, Coupled phenomena, Capillary-pressure saturation curve, Discrete Element Modeling (DEM), Two phase flow

Abstract. In this paper a brief and critical review of the current literature on hydro-mechanical coupling is presented. Furthermore, an enhanced discrete element model is used to investigate the mutual relationship of soil water retention curve and suction stress curves and how the two are affected as a result of change in the initial porosity of the soil sample. The model revealed the suction stress values in wetting were less affected as in drying branch as a result of the change in the initial porosity of the soil sample.

1 INTRODUCTION

Unsaturated soil is a complex medium composed of different phases and interfaces. The volume fraction of different phases influences the overall macroscopic behavior of unsaturated soil. On the other hand the porous network of unsaturated soil changes under external loading and is stress level dependent. Therefore, the volume fraction of different phases changes with the stress level and accordingly the topology, connectivity of the porous network, and fluid paths change. This means the mechanical behavior of system is saturation dependent and the hydraulic behaviour of the system is stress level dependent. This has been referred to as hydro-mechanical coupling in the literature of unsaturated soil mechanics. There are various studies in the literature which investigate each of these phenomena alone and independently and the connection of the two is not comprehensively looked into [1]. The soil water retention curves for deformable porous media have been explored by various researchers [e.g., 2-4] and the dependency of stress measures on the saturation level has been investigated in some others [5]. However, these two phenomena are mutually inter-related and it is also of practical importance to look into saturation dependent stress measures and stress dependent retention properties in a single framework, and not only that, different micro scale and macro scale phenomena are also worth being investigated from this perspective. In this study, a thorough and critical review of current literature on the hydro-mechanical coupling is presented and different phenomenological and mathematical aspects of hydro-mechanical coupling are discussed.

2 A BRIEF AND CRITICAL DISCUSSION OF THE LITERATURE

Noting the points raised in the introduction section, one will find the following two issues have faced less attention in the current literature:

1. Is there any mathematical, and or physical framework to demonstrate the mutual relationship discussed above? In other words, such coupled behavior which can be empirically and intuitively understood and is widely acknowledged among researchers, should also be established and demonstrated via a mathematical and/or physical approach. The benefit of any further elaboration on this is better understanding of such coupling and arriving at the better options to incorporate it in the current constitutive models and computational tools instead of the ad hoc, heuristic and empirical ways of proposing equations for it.

2. One of the important factors influencing the hydro-mechanical coupling is the internal structure of the porous medium (i.e., the porous structure of the medium). In other words, the effect of stress level on the hydraulic behaviour of the porous media can be different for different porous network structures. It can vary in different porous media with various porous networks (in networks with mono-modal or bimodal pore size distribution, dissimilar pore shapes, different distribution of pores and throats, and coordination number distributions (or porous network connectivity). This means a pore and/or grain scale study of the coupled phenomena is important to shed light into such coupling. We hereafter refer to this part as phenomenological study as with such a tool we can better study different processes and physical effects associated with the coupled phenomena.

This paper briefly reports some of the recent works of the authors on these two important aspects of coupled phenomena in unsaturated poromechanics. In the following section, we first quickly illustrate how such mutual relationship is expected to exist due to the inherent mathematical symmetry in the unsaturated system. Afterwards, the DEM approach which is employed by the authors to look at hydro-mechanical behaviour of unsaturated soils is introduced. Finally concluding remarks are given and further research directions are discussed.

3 A MATHEMATICAL VIEW POINT: INHERENT SYMMETRY

Let W be a strain energy function which represents the free energy of the deformable unsaturated medium per a unit initial volume of it. Huyghe et al. (2015) have revealed that the following results can be obtained through a systematic formulation of the thermodynamics of such media [6]:

$$\boldsymbol{\sigma}_{eff} = \frac{1}{J}\boldsymbol{F}.\frac{\partial W}{\partial \boldsymbol{E}}.\boldsymbol{F}^{c} \tag{1}$$

$$\mathrm{P_C} = -\rho_i^w \frac{\partial W}{\partial \mathrm{R}^w} \tag{2}$$

In Equation 1, $\boldsymbol{\sigma_{eff}}$is the so-called effective stress tensor. $\mathbf{E}$ specifies the Green strain, and J denotes the Jacobian of the deformation gradient tensor (**F**).

In Equation 2, $\mathrm{P_c}$ is capillary pressure which is the pressure difference between air and water. ρ_i^w stands for the intrinsic density of the wetting fluid and $\mathrm{R^w}$ is Lagrangian apparent density of wetting fluid. These two equations are two of the most important equations which can define mechanics and hydraulics of the unsaturated mixture. Having a look at the symmetry involved in the following equation:

$$\frac{\partial W}{\partial \mathrm{R}^w \partial \boldsymbol{E}} = \frac{\partial W}{\partial \boldsymbol{E} \partial \mathrm{R}^w} \tag{3}$$

If we note that the left hand side is connected to the deformation effect on the values of capillary pressure and the right hand side is the effect of change of saturation on effective stress relationship, then this equation and the symmetry involved there basically states from an energetic view point these two phenomena are mutually interrelated. In fact such relationship can be used to establish a formulation for the effective stress in unsaturated soil which is fully discussed in Huyghe et al. (2015) and interested reader can refer to that [6].

We now add two other important equations to the set of equations presented above. The soil water retention curve (SWRC), defined as follows:

$$\mathrm{P_C} = \mathrm{F}(\mathrm{S^W}) \tag{4}$$

It is worth mentioning that the F function (appearing in Equation 4) could be directly thermodynamically/ mathematically obtained, if the exact form of dependencies of W (mixture strain energy) was known. In the absence of such knowledge, the numerical and experimental approaches are utilized to get insights on the form of F function. Therefore the F function is usually determined empirically, most well-known forms of it are Brooks-Corey (BC), Van Genuchten (VG), Fredlund and Xing (FX) [7-9] but of course it can also be obtained from modeling tools such as discrete element model provided that the model can hydraulically represent the unsaturated soil well enough to give results which are within a reasonable/acceptable range of accuracy. For this purpose, calibration of the model with experimental data at the first stage is pursuit. In general, the pore and grain characteristics of the model and the medium (and their degree of similarity) can be considered as two most influential factors in arriving at a proper estimation of SWRC. Geometry of the grain and the intra and inter-aggregate porosities are also of importance.

Not surprisingly there is the same problem with the effective stress defined in Equation (1) based on the strain energy function of the mixture which leaves us with the option of empirical equation for it (of course the effective stress formulation can still be obtained through a thermodynamic framework but we need to either assume some dependences for strain energy function or for the soil water retention relationship and plug it into the Equation (1) or (2), respectively). This is of course subject of a separate study (see for instance Huyghe et al. 2015). For the current study, let us consider one of the most famous empirical equations for the effective stress in unsaturated soils, known as Bishop Equation [10]:

$$\boldsymbol{\sigma_{eff}} = \boldsymbol{\sigma} - p^a \boldsymbol{I} + \chi(p^a - p^w)\boldsymbol{I} \tag{5}$$

where $\boldsymbol{\sigma}$ is total stress. Hereafter, the first term on the right hand side (the difference between total stress and pore air pressure) is called net stress. p^w and p^a are wetting phase and nonwetting phase pressures, respectively (in our case, water and air). χ is the so-called effective stress parameter.

The difference between the effective stress and net stress has been coined by Lu and Likos as suction stress [11].

Lu et al. (2010) proposed the following equation for the suction stress [12]:

$$\boldsymbol{SS} = \boldsymbol{\sigma_{eff}} - (\boldsymbol{\sigma} - p^a \boldsymbol{I}) = S^e(p^a - p^w)\boldsymbol{I} \tag{6}$$

where $\boldsymbol{S^e}$ is the effective degree of saturation. Here, we have changed their formulation regarding the sign convention and we have also rewritten it in a tensorial format.

Therefore, one straight forward way to look into the coupled phenomena and mutual relationship stated by Equation 3 is first investigating the effect of stress level on the soil water retention curve. The values of effective saturation at each capillary pressure can then be employed to look into the effect of stress level or deformation on the stress measures of the medium (effective stress or suction stress). This can be done by investigating the suction stress at different stress levels or porosity levels, or investigating it, at least (in a most simple way), at different initial porosities. For this purpose experimental data or numerical models can be employed. Numerical models have this merit that they are not as time consuming as the experimental tests and a better control on the physical factors can be achieved but on the other hand, at the present, there are lots of simplifying assumptions involved in the numerical modeling. That said, due to considerable merits of the numerical model, we have focused on a numerical model (discrete element model) here.

One can notice the mathematical analysis presented above did not elaborate on the hysteresis phenomenon (i.e., the difference in the soil water retention curves in drying and wetting as well as the other hydraulic paths). However, a possible approach to account for the hysteresis phenomenon is considering different parameters for Equation (4) for different hydraulic paths. Nonetheless, in order to consider the effect of deformation, similar hydraulic paths would need to be compared at different states of stress (or measures of deformation). The numerical simulation presented in this study, thus, includes the variation of suction stress for both drying and wetting at different porosity values.

In what follows a modeling tool (discrete element technique) which is capable of capturing the main features of unsaturated porous media is employed to model the two sides of hydro-mechanical coupling. As we are in the preliminary stages of this research, the study presented here is limited to first model the effect of different initial porosities on the soil water retention curve and then to investigate the suction stress values at different levels of capillary pressure for different values of initial porosity (for drying and wetting branches). Therefore, in the current study basically the change of initial porosity has been considered as a measure of stress level and then drying and wetting paths have been modeled. This means highly collapsible soils and/or highly swelling soils are not subject of this study. In order to have a precise model to study them, the instantaneous change of porosity as a result of suction change needs to be accounted for.

4 THE PHENOMENOLOGICAL STUDY: DISCRETE ELEMENT MODELING OF THE COUPLED PHENOMENA

The phenomenological study contains two parts. First simulating the soil water retention curves using a Discrete Element Method (DEM). The discrete elements model is calibrated to be utilized as a virtual laboratory. It is then employed to obtain the soil water retention curve for different initial porosities of the same soil type to account for the effect of stress level. To study the other direction of this mutual relationship (the effect of change of porosity on soil water retention curve and then consequently on the effective stress state of the medium), the suction stress curves under different porosities are obtained using the results of DEM.

The simulation of SWRCs are done in two subsequent stages. First a packing was generated in particle model Yade-DEM, and second the SWRC was determined by an implemented quasi-static two-phase flow module.

Particle model Yade-DEM is based on the Discrete Element Method (DEM), where particles are considered as discrete elements. Each particle is simulated as an elastic sphere. At a contact between two particles a force is calculated which is a consequence of elasticity, this is calculated using the physical based Hertz-Mindlin mechanics. The elastic force at a contact between two particles is given by [13]:

$$f_n = -k_n \delta_n{}^{3/2} \tag{7}$$

f_n is the inter-particle force at a contact, δ_n is the normal displacement. k_n is the contact stiffness in the normal direction and is given by:

$$k_n = \frac{4}{3} E^* \sqrt{R^*} \tag{8}$$

Where $E^* = \left(\frac{1-\nu_1{}^2}{E_1} + \frac{1-\nu_2{}^2}{E_2}\right)^{-1}$, representing the average of Young's moduli of the two particles, R^* is the reduced radius and given by $R^* = \frac{R_1 R_2}{R_1 + R_2}$

For each particle all forces arising from contacts, gravity, and boundary conditions are summed and transferred to particle motions (using Newton's second law). Using Yade-DEM, a packing of 4000 spheres was randomly generated with the particle size distribution for Hostun sand [14]. The particles were packed by an all-round stress, before a vertical confinement was applied. The vertical net-stress was increased until a target porosity was achieved, this was 0.39 [14]. For the inter-particle friction we used that of Labenne sand (17°) and a Poisson ratio of 0.5 [15]. The particle stiffness was set at 1MPa. However as we used porosity as a measure for state-of-stress, the exact particle stiffness is not required to arrive at a certain initial porosity, as the confining stress would capture the exact state-of-stress.

After the target porosity was achieved, an implemented quasi-static two-phase flow algorithm was used to obtain points on the SWRC for both drainage and imbibition. First the pore geometry was meshed into tetrahedra using Delauney triangulation [16]. Each tetrahedron represents one pore-unit and has at each corner one particle. The resulting network of pore-units was used to simulate the SWRC experiments. The top of the box generated in Yade-DEM represented an air reservoir and had an air-pressure (P^a) and at the bottom a water reservoir with a water pressure (P^w). As mentioned before, the capillary pressure is defined as $P_C = P^a - P^w$. The water saturation in each pore-unit was either one or zero (i.e., small partial water volumes in pore units were considered negligible). Initially the packing was saturated with water. At the pore-scale the capillary pressure was used to establish whether air will invade during drainage or water during imbibition, using the following criteria. Drainage: the invasion criterion was based on the entry pressure (P_e) associated with the smallest transect in between two pore units. Air invaded if $P_c > P_e$. Imbibition: the invasion criterion was based on the critical pressure (P) corresponding to the largest curvature found inside a pore-unit, which is that of an inscribed sphere and was calculated following [17]. Water invaded if $P_c < P_e$. For each invasion of a pore-unit the connectivity of both water and air phase with their reservoirs was checked, if a residual phase was present invasion of that pore-unit did not occur.

5 RESULTS AND DISCUSSION: SIMULATED SWRCS AND SSCCS FOR HOSTUN SANDS

Most granular materials do not contain perfect spherical particles. Therefore, a slightly more angular material, sand, is tested. Lins and Schanz (2005) have studied the soil-water retention curve in Hostun dune sand, at a porosity of 0.39 [14] The results (Fig. 1) indicate that the capillary pressure for both drainage and imbibition is in good agreement with the experimental data. We simulated spherical particles in contrast to sand, which typically is more angular, although the effect of particle angularity on SWRC is limited [18]. During drainage, the irreducible water saturation in angular sands can be present in pendular rings, corners, and as disconnected blobs, from which the later one is only accounted for in these simulations. During imbibition corner flow can strongly influence snap-off, thus affecting the amount of disconnected air blobs. To improve the magnitude of residual air saturation and the irreducible water saturation, effects of angularity such as corner flow, should be accounted for. Our above-mentioned relatively basic simulation of imbibition does, however, still capture the main effects.

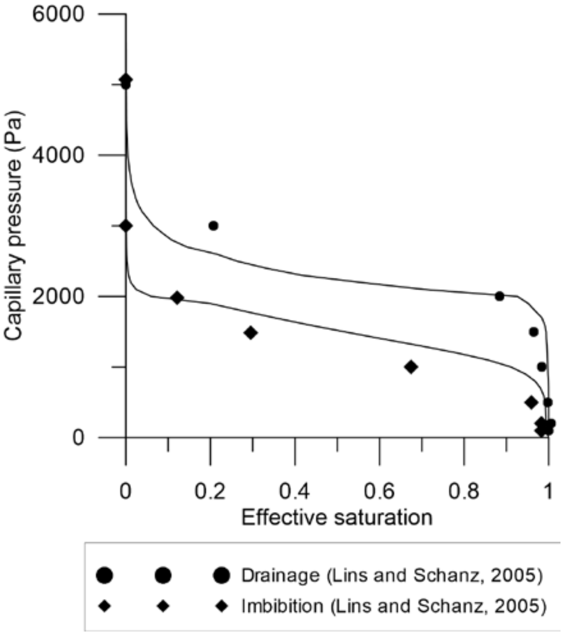

Fig. 1: Capillary-pressure saturation behavior for Hostun sand, with a porosity of 0.39. Experimental data by Lins and Schanz (2005), and model results by quasi-static two-phase flow within Yade-DEM.

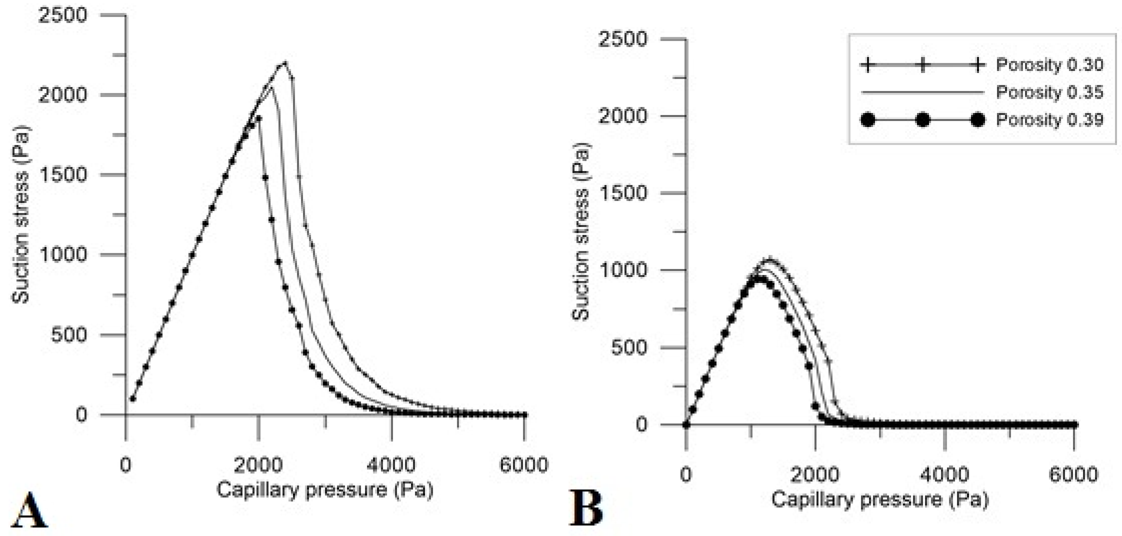

Fig 2: Suction stress as function of capillary pressure for Hostun sand at different porosities A) drainage and B) imbibition.

To investigate the hysteresis and stress level effects on suction stress, the capillary pressure - saturation curve of Huston sand at a porosity of 0.39 (Fig. 1) is transferred to suction stress – capillary pressure curve for drainage (Fig. 2A) and imbibition (Fig. 2B).

It is apparent that larger states of suction stresses are found during drainage than imbibition. The effect of porosity on suction stress is investigated by decreasing the porosity from 0.39 to 0.35 and 0.30. Simulations indicate that a decrease in porosity causes an increase in suction stress, as pore sizes become smaller. Such effects are more pronounced in the drying curves as compared to the imbibition ones. That can root in the fact that throat radii control the drying process and they are more easily affected by a change in the porosity and/or an increase in the stress level than the radii of pores. The radii of pores control the imbibition and therefore, imbibition branches of suction stress are not affected as much as drying branches as a result of porosity change.

6 CONCLUDING REMARKS

- Critical evaluation of the literature showed the mutual relationship between stress level effects on the capillary pressure and effective stress measure has not yet been well studied in the literature. To better investigate such mutual interrelationship, some insights based on mathematical symmetry were presented. This issue has extensively and comprehensively been explained in a forthcoming publication of the authors [6].
- A discrete element model was employed to elucidate how such mutual relationship holds. In particular, we investigated the effect of deformation (change in the initial porosity of the soil sample) on the suction stress and soil water retention curve in both drying and wetting paths. The utilized discrete element model was first calibrated with soil water retention data of one of the samples and was then used to predict the effect of porosity change on the suction stress and soil water retention curves.

ACKNOWLEDGEMENT

The research of Thomas Sweijen has been made possible thanks to grant 12538 of the Technology Foundation STW, the technological branch of the Netherlands Organization of Scientific Research NWO, and the Ministry of Economic Affairs. The second author would like to thank the European Research Council (ERC) and the Department of Earth Sciences of Utrecht University for hosting and financing his research as a Post-Doctoral Researcher. We sincerely acknowledge the valuable intellectual contributions of our best friend and colleague, Dr. Chareyre of Grenoble Institute of Technology who is the YADE project leader. Without his help, this study could not reach the current state.

REFERENCES

[1] Mašín, D. Predicting the dependency of a degree of saturation on void ratio and suction using effective stress principle for unsaturated soils. *International Journal for Numerical and Analytical Methods in Geomechanics* (2010) **34(**1):73-90.

[2] Tarantino, A. A water retention model for deformable soils. *Géotechnique*, (2009) **59** (9): 751 – 762.

[3] Nuth, M. and Laloui L. Advances in modelling hysteretic water retention curve in deformable soils. *Computers and Geotechnics* (2008) **35**(6): 835-844.

[4] Mbonimpa, M., Aubertin, M., Maqsoud, A., and Bussière B. Predictive Model for the Water Retention Curve of Deformable Clayey Soils. *J. Geotech. Geoenviron. Eng.* (2006)**132**(9):1121–1132.

[5] Nuth, M. and Laloui. L. Effective stress concept in unsaturated soils: clarification and validation of a unified framework, *International Journal for Numerical and Analytical Methods in Geomechanics*, (2008) **32**(7):771-801.

[6] Huyghe, J., Nikooee, E., Hassanizadeh, S. Majid. A thermodynamical analysis of deforming unsaturated media, *Trasnport in porous media,* to be submitted soon, (2015).

[7] Brooks, R. H. and Corey, A. T. Hydraulic Properties of Porous Media. Hydrology Paper No. 3. Colorado State University, Fort Collins, CO, (1964).

[8] Van Genuchten, M. T. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil science society of America journal* (1980) **44**(5): 892-898.

[9] Fredlund, D. G., and Xing, A., and Huang, S. Predicting the permeability function for unsaturated soils using the soil-water characteristic curve. *Canadian Geotechnical Journal* (1994) **31** (4): 533-546.

[10] Bishop, A. W. The effective stress principle. *Teknisk Ukeblad* (1959) **39**: 859-863.

[11] Lu, N., and Likos, W.J. *Unsaturated soil mechanics*. J. Wiley, (2004).

[12] Lu, N., Godt, J.w., and Wu, D.T. A closed-form equation for effective stress in unsaturated soil. *Water Resources Researc*h (2010), **46**(5).

[13] Johnson KL. *Contact mechanics*. Cambridge university press; (1987).

[14] Lins Y, Schanz T. Determination of hydro-mechanical properties of sand. In: *Unsaturated soils: Experimental studie*s. Springer (2005):15-32.

[15] Belheine N, Plassiard J, Donzé F, Darve F, Seridi A. Numerical simulation of drained triaxial test using 3D discrete element modeling. *Comput Geotech*. (2009)**36**(1):320-331.

[16] Chareyre B, Cortis A, Catalano E, Barthélemy E. Pore-scale modeling of viscous flow and induced forces in dense sphere packings. *Transp Porous Media*. (2012)**94**(2):595-615.

[17] MacKay A. To find the largest sphere which can be inscribed between four others. *Acta Crystallographica Section A: Crystal Physics, Diffraction, Theoretical and General Crystallography*. (1973)**29**(3):308-309.

[18] Torskaya T, Shabro V, Torres-Verdín C, Salazar-Tio R, Revil A. Grain shape effects on permeability, formation factor, and capillary pressure from pore-scale modeling. *Transp Porous Media*. (2014) **102**(1):71-90.