OPEN GEOMECHANICS

Review History for "In situ X-ray CT imaging of transient water retention experiments with cyclic drainage and imbibition"

Marius Milatz, Edward Andò, Gioacchino Viaggiani & Serge Mora *2022*

Summary

The paper was sent to two reviewers — Dr. Mohmad Mohsin Thakur (Reviewer A) and Dr. Max Wiebicke (Reviewer B). The reviewers remained anonymous during the entire review process and the authors were anonymous for the reviewers. After the reviewing process was complete, both reviewers agreed to disclose their identity. In Review Round 1, the reviewers provided a series of comments for the authors and required a revision of the manuscript. In Review Round 2, the reviewers recommended the manuscript for publication.

Reply to the reviewer comments after first review from May 19th, 2022

We thank the editor and all reviewers for their work and their valuable comments to improve our manuscript. In this document, all reviewer comments have been numbered and are typeset in black colour, while our responses are added in blue print. In the revised manuscript all changes are also highlighted in blue print colour. Discussions, not occurring in the manuscript, are highlighted in green print colour.

Reviewer A:

The authors present an interesting experimental approach to investigate the spatial distribution of fluids in partially saturated sands under cyclic wetting and drying paths. The authors automated experimental procedure via Raspberry pi computer using python scripting which can be useful to study various wetting and drying paths in a timely fashion in conjunction with CT imaging. Overall, the manuscript is well written and should be considered for the publication in Open Geomechanics.

The reviewer has some concerns and suggestions that should be addressed by the authors.

1. The authors measured different capillary state variables from pore scale data. The question that remains unanswered is, "Can we define a unique function of capillary variables to describe water retention curve comprehensively"? Currently, water retention curve is expressed as a function of capillary pressure and degree of saturation which is non-unique. However, with additional capillary variables, there is a possibility of defining a unique capillary retention function. The authors should consider this in reference to the additional capillary variables that were measured in this study.

We thank the reviewer for the positive critical view and advice on the capillary state variables. As the "concept of capillary state variables" based on microscopic data is still an open question, its application to the description of the water retention curve as well as to effective or suction stress yet needs to be proven which should be done in further future work. Nevertheless, the reviewer is right in proposing to include thoughts on uniqueness of functional relationships of those variables and the role they play for the water retention curve. If we are not mistaken, the idea that the water retention curve is not purely a function of capillary pressure and degree of saturation and that hysteresis originates from only considering the WRC by plotting the dependence of degree of saturation on matric suction is based on the works with theoretical thermodynamics background of Hassanizadeh and Gray, e. g., Hassanizadeh and Gray (1990; 1993).

We will include their work in the references along with a discussion on the uniqueness of the WRC regarding "capillary state variables" as proposed by the reviewer. Also based on the work by Porter et al. (2009) from the group of Prof. Dorthe Wildenschild at Oregon State University, there is evidence that unique surfaces are obtained, when plotting air-water interfacial area vs. degree of saturation AND matric suction or capillary pressure.

Motivated by the reviewer's comment, we had a look at the available data for the tested Hamburg Sand: Based on our data (measured macroscopic matric suction, degree of saturation and interfacial areas in a central cubic subvolume of CT data), we can show that apparently a "state surface" for air-water interfacial area (Fig. 1 in this document and new Fig. 35 in the revised manuscript) but also for solid-water interfacial area and the contact lines (not shown here) is obtained, when those capillary state variables are each plotted vs. degree of saturation and matric suction, confirming the results of Porter et al. (2009). This is a promising finding, showing that the capillary state variables are obviously related to capillary pressure and degree of saturation, yielding an apparently unique WRC-surface in which the hysteretic behaviour is taking place. However, more research is required, especially in finding a unique function for a comprehensive description of the water retention curve as discussed by the reviewer.

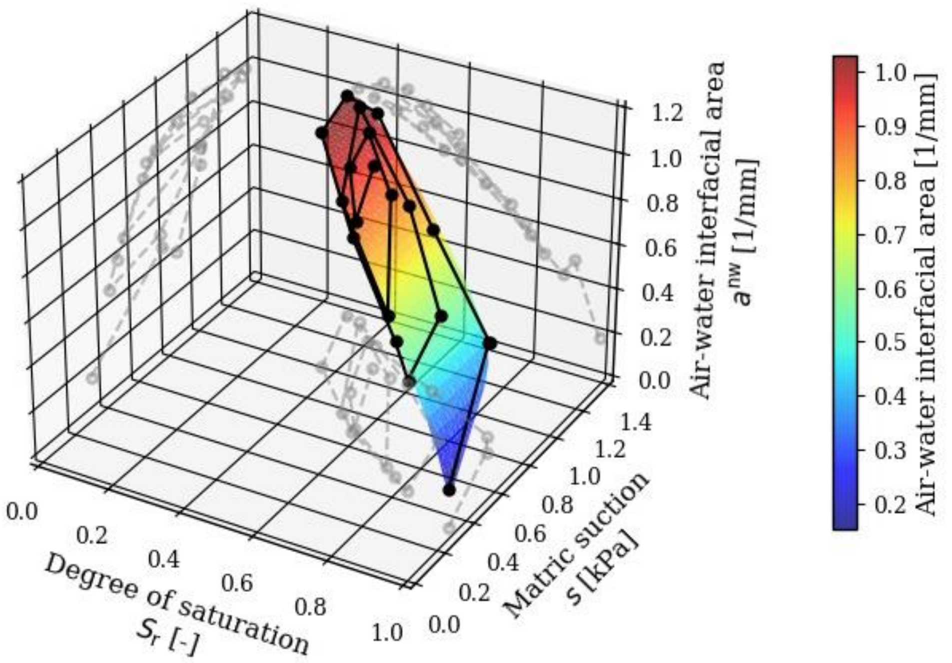

Fig. 1: 3D plot of air-water interfacial area vs. degree of saturation and matric suction (the suction measurements after each scan are selected) based on data from the *in situ* CT experiments, including the projections of all inter-relationships (grey) and a 3D surface fitted to the data points to highlight the position of the data in a plane with good approximation.

We have added the following to the revised manuscript:

"Based on thermodynamics considerations, Hassanizadeh and Gray (1990) and Hassanizadeh and Gray (1993) argue that the hysteresis effect might be due to only considering the WRC as a functional relationship between degree of saturation and capillary pressure without taking a dependence on interfaces into account. By considering the air-water interfacial area as an additional state variable, it was shown based on experimental data and simulations that representative state surfaces can be obtained in the space, see Porter et al. (2009). This would confirm the theoretical thermodynamical considerations about the hysteresis of the WRC, but it is still not clear how a unique functional relationship for the WRC based on the named and maybe even other variables can be established."

Furthermore, Fig. 1 has been added to the Appendix (as a new Fig. 35 with side information on the fitted surface) with a short discussion in the results section:

“Meaning of interfacial capillary state variables regarding a unique WRC

If we plot the degree of saturation and air-water interfacial area derived from the extracted subvolume of CT data together with matric suction measured after each CT scan, we can establish a unique relationship in the form of a 3D surface, expressing a^{nw} as a function of S_r and s as shown in Fig. 35 in the Appendix. The function $a^{nw} = f(S_r, s)$, fitted to the 3D data points, is a quartic polynomial surface function, intended only to suggest that the data can be fitted well by a 3D surface. On the way to a unique relationship for the WRC based on capillary state variables, this corroborates the theoretical considerations of Hassanizadeh and Gray (1990, 1993), suggesting that the view of the WRC as a functional relationship between S_r and s is incomplete. It also confirms the findings by Porter et al (2009) who also found a similar state surface for a glass bead packing.

Although not shown here, similar dependencies and surface approximations can also be found for the solid-water interfacial area and for the specific contact line. This highlights that the capillary state variables are deeply connected to degree of saturation and capillary pressure with the hysteresis phenomenon occurring in a kind of ``state surface".”

Finally, we have added the following statement to the Conclusion and Outlook section:

“Including the measured capillary state variables in hydro-mechanical considerations, could also improve our understanding of the functional dependencies behind the WRC. As proposed by Hassanizadeh and Gray (1990, 1993), the interfacial properties could also be relevant to the hysteresis in the WRC. Based on the data presented in this study, it could be shown that the air-water interfacial area evolves in a 3D surface, when plotted vs. degree of saturation and matric suction. Although not presented in this contribution, the same holds true for the solid-water interfacial area and the specific length of contact line.”

Additional literature added to the references:

Hassanizadeh MS, Gray WG (1990): Mechanics and thermodynamics of multiphase flow in porous media including interphase boundaries. *Advances in Water Resources* 13(4), pp. 169–86.

Hassanizadeh M S, Gray W G (1993): Thermodynamic basis of capillary pressure in porous media. *Water Resources Research* 29(10), pp. 3389–3405.

Porter, M. L., Schaap, M. G., and D. Wildenschild (2009): Lattice-Boltzmann simulations of the capillary pressure-saturation-interfacial area relationship of porous media. *Advances in Water Resources* 32, pp. 1632–1640, doi: 10.1016/j.advwatres.2009.08.009.

2. The authors used rudimentary approach to determine contact angles. Determination of contact angle from 2d images can result in errors and is prone to subjective bias due to manual procedure. The current state of art technique involves determining contact angles automatically from 3D images. The author may refer to Al Ratrout et al. 2017

AlRatrout, Ahmed, et al. "Automatic measurement of contact angle in pore-space images." *Advances in Water Resources*109 (2017): 158-169.

The reviewer’s hint on further works on contact angle detection is very helpful. It is true that the manual measurement of contact angles may contain errors and lack of objectivity to some extent. We have added a reference to the proposed paper and included the idea of automatic contact angle measurement in the revised manuscript as follows:

"Contact angles were measured manually by Andrew et al. (2014) and by Manahiloh and Meehan (2017). An automatic approach to contact angle measurement based on algorithmic processing of multiphase image data was presented by AlRatrout et al. (2017)."

It is true that the manual measurement procedure includes sources of bias and error and that it is time-consuming and only results in a limited number of measurements, however, properly done, the manual procedure yields similar results as the automatic approach as shown by Al Ratrout et al. (2017). Furthermore, in our case, we have tried to link the individual measurements to specific hydraulic steps and to measurements of the corresponding radius of curvature for the same meniscus for which the contact angles have been measured. This approach is desirable if these variables are supposed to be related to each other.

As our data will be shared with the research community, other measurement techniques for the detection of contact angles can be applied in the future to complement our work.

3. Quiet often erroneously, surface tension and interfacial tension are used interchangeably in unsaturated soils. This has been addressed by Blunt (2017) in the first page of his book.

Blunt, Martin J. *Multiphase flow in permeable media: A pore-scale perspective*. Cambridge university press, 2017.

"Surface tension is the energy per unit area of a surface between a fluid or solid and its vapour in thermodynamic equilibrium, with no other components present"

'Interfacial energy is the energy per unit area of the surface between the phases"

In unsaturated sands, air and water phases consist of mixtures of chemical components, the correct expression describing water retention behavior should include interfacial tension rather than surface tension.

We thank the reviewer for the concerns on the terminology. It is right that under natural and even under lab conditions, the mixture consisting of sand, water, and air might not be as chemically pure as we idealise it to be. Furthermore, thermodynamic equilibrium might not be valid in most cases in soil mechanical experiments. In the revised manuscript, we have highlighted the difference between "surface tension" and "interfacial tension" and now adopt the more general terminology using "interfacial tension" based on Blunt (2017) as proposed by the reviewer. The following has been added to the revised manuscript:

"These forces originate from the interfacial tension γ, also known as surface tension for thermodynamic equilibrium and chemically pure fluids (Blunt, 2017), inside the air-water interfacial area of the menisci and represent a contribution to effective stress in the unsaturated state."

Further occurrences of the term "surface tension" have been changed to "interfacial tension" in the revised manuscript.

Additional literature added to the references:

Blunt, M. J. (2017): Multiphase Flow in Permeable Media: A Pore-Scale Perspective. Cambridge University Press, doi: 10.1017/9781316145098.

4. Although authors have discussed some of the causes of hysteresis in Section 1.1. It would be useful to discuss other main causes of hysteresis for completeness such as widely known ink bottle effect which is attributed to non-uniform pore size distributions in soils.

The reviewer's comment on the sources of hysteresis is much acknowledged. Further known phenomena responsible for hydraulic hysteresis are now addressed in the revised manuscript as follows:

We have added the paper by Haines (1930), noticing hysteresis for the very first time, in the following sentence:

"When a consecutive imbibition process takes place, a different macroscopic hydraulic path in the s-S_r space is measured, leading to the hysteresis effect of the macroscopic water retention curve that was described for the first time by Haines (1930)."

As the ink-bottle effect might be relevant to the tested soil with its different pore sizes, we have also added this effect to the literature review in the revised manuscript:

"A further known source of hysteresis is the non-uniform pore size distribution in many soils. With the help of a pore space model that resembles to an ink-bottle, idealising a non-uniform pore space with small pore necks and larger pore bodies, different degrees of saturation for drainage and imbibition at the same matric suction can be explained. Due to the higher suction required to empty a water filled pore by air entering through a small pore neck compared to the lower suction required to fill a pore through its larger pore body, higher degrees of saturation are encountered on drainage paths compared to imbibition paths. This source of hysteresis in porous media due to the individual contributions of different pore sizes is usually referred to as the "ink-bottle effect" (Haines, 1930)."

Additional literature added to the references:

Haines, W. B. (1930). Studies in the physical properties of soil: V. The hysteresis effect in capillary properties and the modes of moisture distribution associated therewith. *Journal of Agricultural Science*, 20, pp. 97–116.

5. Neutron imaging has been proposed to investigate fluid flow in unsaturated geomaterials as it provides high attenuation contrast between air and water phase. For instance, Tengattini et al. 2021 provided a comprehensive review on advantages of using neutron imaging for fluid flow in geomechanics problems. Thakur et al. 2021 used Neutron imaging to study fluid flow in rounded and angular sand. The current manuscript used X-ray CT imaging without any tracers to visualize air and water phase. The authors should include a discussion on how to effectively image air and water phase without any tracers using X-ray CT imaging. The suggested references below or other references which authors may consider appropriate may be included in reference to neutron imaging for unsaturated sands.

   Tengattini, Alessandro, et al. "Neutron imaging for geomechanics: A review." *Geomechanics for Energy and the Environment* 27 (2021): 100206.

Thakur, Mohmad Mohsin, et al. "Pore space and fluid phase characterization in round and angular partially saturated sands using radiation-based tomography and persistent homology." *Transport in Porous Media* 137.1 (2021): 131-155.

We thank the reviewer for this advice. Due to own measurements using the neutron source at the Institut Laue-Langevin in Grenoble, we are aware of the advantages of neutron tomography to achieve good contrast of the water phase in hydraulic flow experiments. We have added the papers by Kim et al. (2013) and Tengattini et al. (2021), focusing on neutron imaging, to the references.

As we did not want the water properties to be changed, we chose not to use dopants or tracers in the experiments. However, without tracers, we have to rely on good contrast based on the X-ray imaging settings, e. g. by means of choosing the energy properly to optimise absorption and we have to use filters in image processing and special segmentation tools as outlined in the manuscript to achieve a good phase segmentation. In the revised manuscript, we have added additional thoughts on contrast enhancement by different techniques, such as tracers and other radiation sources as follows:

"In order to achieve good contrast in images of multiphase materials, different techniques can be applied. In addition to image processing methods used after image acquisition, such as de-noising and filtering, the image contrast can already be enhanced during imaging by special experimental and imaging techniques. For a better contrast of water, dopants such as iodine, can be added, increasing its density and therefore contrast in X-ray images (Wildenschild et al., 2002; Wildenschild et al., 2005). Furthermore, the X-ray energy can be set in a way to cause the maximum absorption which is characteristic of the applied dopant. Especially when using synchrotron-based imaging, propagation-based phase contrast in conjunction with phase retrieval algorithms can be considered to enhance the contrast at phase boundaries for media with different refraction indices. Finally, neutron radiation can be applied on a stand-alone basis or combined with X-rays (Kim et al., 2013). In contrast to X-rays, neutrons are mainly attenuated by atomic nuclei and allow to achieve strong contrast for hydrogen-containing materials which is very useful for the imaging of water in geomaterials (Tengattini et al., 2021)"

Additional literature added to the references:

Kim, F. H., D. Penumadu, J. Gregor, and N. Kardjilov (2013): High-Resolution Neutron and X-Ray Imaging of Granular Materials. *Journal of Geotechnical and Geoenvironmental Engineering*, 139. doi: 10.1061/(ASCE)GT.1943-5606.0000809.

Wildenschild, D., J. W. Hopmans, C. M. P. Vaz, M. L. Rivers, D. Rikard, and B. S. B. Christensen (2002): Using X-ray computed tomography in hydrology: systems, resolutions, and limitations. *Journal of Hydrology* 267, pp. 285–297. doi: 10.1016/S0022-1694(02)00157-9.

Wildenschild, D., J. W. Hopmans, A. J. R. Kent, and M. L. Rivers (2005): Quantitative analysis of flow processes in a sand using synchrotron-based x-ray microtomography. *Vadose Zone Journal* 4(1), pp. 112–126. doi: 10.2113/4.1.112.

Tengattini, A., N. Lenoir, E. Andò, and G. Viggiani (2021): Neutron imaging for geomechanics: A review. *Geomechanics for Energy and the Environment* 27. doi: 10.1016/j.gete.2020.100206.

6. As the local pore is desaturated, water films may exist as thin layers on solid surface of grains because of the hydrophilic nature of the sand grains. These thin layers can be

submicron in size which is typically beyond the resolution of CT imaging equipment. Please discuss this in relation to solid-water interfacial area and air-water interfacial area determined in this study.

Although the tested sand seems not to be perfectly wetting based on measured contact angles, thin water films might exist on the grain surfaces. However, we have no evidence for or against thin wetting layers covering the grain surfaces. It is true that we cannot resolve such thin wetted regions with the applied technique. In the revised version of the manuscript, we have included the reviewer's concern as follows:

"The solid- and air-water interfacial areas have been measured based on the available phase segmentation relying on the image resolution at a voxel size of 10 µm. It must be noted that potential thin liquid layers on the solid grain surfaces as a basis for film flow as discussed in some studies, e. g., Tuller et al. (1999) and Tuller and Or (2001), can't be resolved at this resolution and therefore are not considered in the determination of the interfacial areas."

Additional literature added to the references:

Tuller M., Or, D., and L. M. Dudley (1999): Adsorption and capillary condensation in porous media: Liquid retention and interfacial configurations in angular pores. *Water Resources Research* 35(7), pp. 1949–1964.

Tuller M., and D. Or (2001): Hydraulic conductivity of variably saturated porous media: Film and corner flow in angular pore space. *Water Resources Research* 37(5), pp. 1257–1276.

7. The following references are highly relevant to the topic discussed in the manuscript and may be considered by the authors

Manahiloh, Kalehiwot Nega, and Christopher L. Meehan. "Determining the soil water characteristic curve and interfacial contact angle from microstructural analysis of X-ray CT images." *Journal of Geotechnical and Geoenvironmental Engineering* 143.8 (2017): 04017034.

Mohsin Thakur, Mohmad, Dayakar Penumadu, and Constantin Bauer. "Capillary suction measurements in granular materials and direct numerical simulations using X-ray computed tomography microstructure." *Journal of Geotechnical and Geoenvironmental Engineering* 146.1 (2020): 04019121

We thank the reviewer for the hint to these interesting publications that we have now added to the state-of-the art section and bibliography of the revised manuscript.

8. Typo: When plotted the local degree of , on page 18

The typo has been corrected.

Recommendation: Revisions Required

Reviewer B:

This manuscript presents the application of x-ray CT to one cyclic water retention experiment on sand. A range of image analysis techniques were used and developed to describe the interaction of the three phases. The techniques as well as the results are described well. Furthermore, several couplings between microscopic states and the macroscopically measured water retention curve are presented and provide insight that can be used for the consititutive modelling/effective stress formulations of unsaturated granular materials in the future. Furthermore, the results of this study are available in an open access archive. The images are also available there, but embargoed until 1st of October. I could access them from the archive with the permission of (most probably the first author) Marius Milatz.

The work carried out here is an original and important contribution to the field of the mechanics of unsaturated granular materials. I definitely recommend it for publication, but have some remarks that might be considered before publication. For the future, it would be helpful for reviewers to add line numbers to manuscripts.

General comments:

1. page 7, right column, last paragraph: how did you label the clusters? Did you perform an additional segmentation to split clusters or did you label them based on the connectivity of the phases? I always have troubles understanding an individual cluster of water or air in 3D when the complete pore network in connected. So I would guess that close to S_r=1 you only have a single water label and some air labels and vice versa close to S_r=0? Especially, after inspecting scan 3, I wonder the labelling looks like, e.g. on a vertical slice. On a vertical slice through the centre (x-z plane) it was hard for me to identify many clusters without applying any restriction at e.g. pore throats. Could you maybe add a sketch to visualise the problem? I think that would help to understand how the approach works and what to expect as a visual result.

We thank the reviewer for the interest in our work and the constructive critical remarks. The labelling of water and air clusters is done based on connectivity of phases in the segmented or trinarised images only containing solid, water and air. Each connected cluster is assigned a unique label in the software Avizo using the "labelling module". A connectivity of voxels is detected if voxel based volumes share at least one common vertex, i. e., a voxel corner node. An example of connected and unconnected voxels is given in Fig. 2 of this document. In 3D, a single voxel can have a maximum of 26 neighbouring voxels based on the vertex connectivity definition used here. For the water and air phase, the connectivity definition leads to independent voxel clusters that are assigned individual labels. Example slices for illustration through the air and water clusters are shown in Fig. 3 of this document.

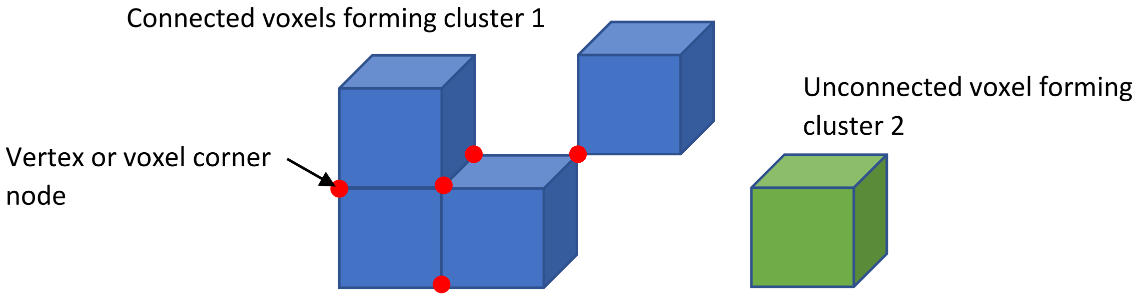

Fig. 2: Sketch illustrating the voxel connectivity definition used here.

The reviewer is right, that initially, there is rather only a single large water cluster close to S_r = 1. During drainage, the cluster is reduced and splits into smaller isolated clusters as air enters the pores. Regarding the air phase, it is vice versa with air clusters or air ganglia forming upon drainage. However, the images also contain noise which leads to the detection of additional very small clusters which are probably not physical.

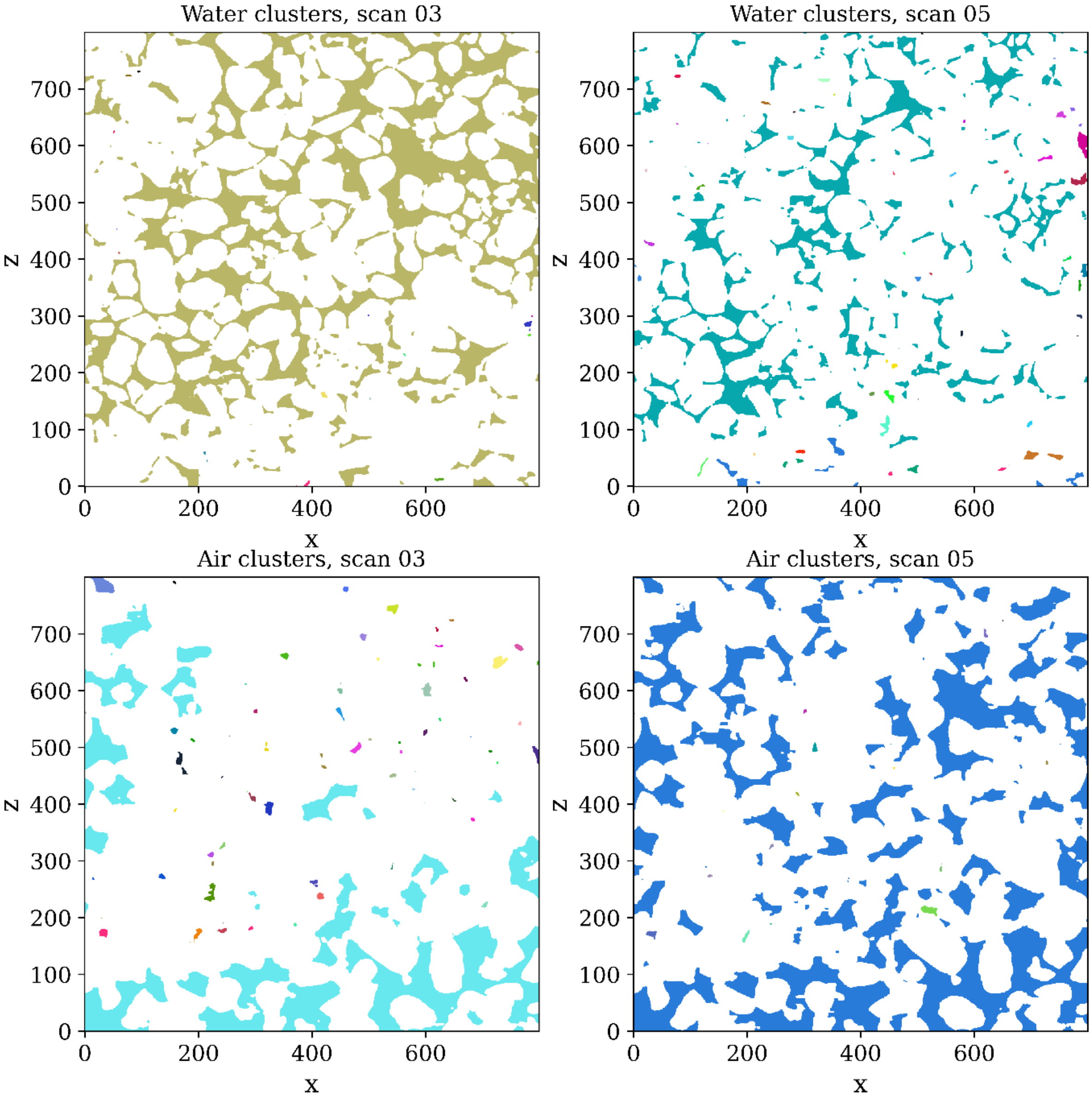

Fig. 3: Vertical slices through a cubic subvolume with edge lengths of 800 px centred in the x-z plane showing the labelled air and water clusters after scan 03 and scan 05 on a primary drainage path.

We have addressed the reviewer’s comments in the revised manuscript as follows to make the procedures more clear:

“With the help of *labelling*, the air and water clusters inside the experimental data (the central cubic subvolume of 800×800×800 px is evaluated) can be separated in order to analyse their behaviour with regard to macroscopic degree of saturation and suction during different hydraulic steps. The labelling is computed in Avizo based on connectivity. An individual cluster is defined as the assembly of connected voxels sharing at least one common vertex (voxel corner node) with their neighbouring voxels."

2. page 8, left column, 2nd paragraph: when you measure the interfacial areas you use a triangulation of the surface connecting the two phases. Do you have any idea of how accurate this triangulation is considering your spatial resolution? The question of accuracy is generally important, but not mentioned in this manuscript. It starts with the measurement of the phases and can be posed to every image analysis step. It's fine for this pioneering work to not study it in details. But if you have any idea on the metrology, it would be great to include it in the paper or cite papers if it was already touched upon somewhere else.

Accuracy is of course an important point addressed by the reviewer and we have tried to improve this open aspect in the revised manuscript. It is true that the quality of the triangular surface meshes generated on voxelised and segmented 3D data will determine the interfacial area measurements. In the steps of data evaluation, we applied two different surface meshing settings – using the default settings vs. the settings with the highest extent of fineness – which indeed resulted in different interfacial area measurements which can be refined based on the meshing settings. The choice of meshing settings will affect the computation efforts, but lead to increased accuracy of the meshes. We have finally decided to apply the best possible settings leading to the finest resolution of the surface meshes in order not to miss small geometric structures of the interfacial areas.

In Avizo, the selected settings for the control of the surface meshes include: (1) an option to optimise or compact (Avizo-terminology: "compactify") the extracted meshes in a post-processing approach, (2) the option to adjust coordinates to lie exactly on the nearest boundary face of the bounding box including the surface, and (3) a constrained smoothing procedure, ensuring thin regions not to vanish at the lowest possible smoothing extent (a smoothing extent value between 1 and 9 can be selected, with 1 selected for the calculation of interfacial properties here). Based on the Avizo 2019.3 documentation, these settings yielded the best surface approximation, while at the same time reducing the risk of missing surface information. The presented interfacial properties have been extracted with these optimal meshing settings. As compared to a surface generation with the default settings without "compactifying" the mesh and with a medium constrained smoothing extent (the default smoothing extent value is 5), the finally selected optimal settings resulted in an average increase of 25 % of the air-water interfacial area and of 9 % of the solid-water interfacial area, which probably accounts for fine surface structures being missed when the default meshing settings are used. It should be the task of future studies to further assess the accuracy and also the effect of different input voxel sizes on the accuracy of surface measurements based on this methodology.

In the revised manuscript we have added the following information on the generation of triangulated surfaces and derivation of interfacial areas:

"For this purpose, the interfaces of different phases are detected and approximated by a triangulated surface mesh using the Avizo software. In Avizo, the selected settings for the control of the surface meshes include (1) an option to optimise or compact (Avizo-terminology: "compactify") the extracted meshes in a post-processing approach, (2) the option to adjust coordinates to lie exactly on the nearest boundary face of the bounding box including the surface, and (3) a constrained smoothing procedure, ensuring thin regions not to vanish at the lowest possible smoothing extent. The presented interfacial areas have been computed with these optimal settings yielding the highest possible accuracy. As compared to a surface generation with the default settings without “compactifying” the mesh and with a medium constrained smoothing extent, the selected settings at the highest possible accuracy of surface approximation resulted in an average increase of 25 % of the air-water interfacial area and of 9 % of the solid-water interfacial area, which probably accounts for fine surface structures being missed or smoothed out when the default meshing settings are used. It should be the task of future studies to further assess the accuracy and also the effect of different input voxel sizes on the accuracy of interfacial area measurements based on this methodology.”

3. page 9, left column: You run your pore-based analysis on tetrahedral elements connecting grain centres. How representative are such pores in your sample? Despite the problem of defining individual pores in 3D, I assume that you have quite a number of larger pores that cannot be described by linking 4 grain centres. In scan 3 I could identify lots of pores, that I intuitively would rather see as being "bounded" by 6-10 grains. If this thought is correct: could you add an image from your data set as visualisation, possibly where this assumption is correct and where it fails?

This is an interesting and important point. The generation of a mesh of tetrahedra of course represents a discretisation and therefore approximation of the pore space allowing to work with structuring elements, e. g., for the computation of a “pore saturation”. In the following plots presented in Fig. 4 and Fig. 5, a central slice showing the Euclidean distance map of the pore space from a cubic subvolume is overlain with a 3D representation of the tetrahedron mesh which is cut in the same plane as the 2D slice. This visualisation allows to evaluate the discretisation of pores based on the presented approach. Large pores can be identified by a large Euclidian distance and the corresponding red intensity based on the heat map. In Fig. 5 of this document, three red circles labelled A–C highlight different cases for the approximation of pores by 3D tetrahedra. While case A represents a nearly ideal case, where a pore in between three neighbouring grains is well captured by the triangular cross section of the related tetrahedron, case B shows a case where a larger pore is split into different corresponding tetrahedral elements, and case C also shows a case, where a pore is missed because the 3D mesh includes an inner hole where no tretrahedra were placed during meshing. Summing up, it seems that the approach encloses individual pores well by a single tetrahedral element if the pore is only surrounded by a few (ideally 4 grain neighbours). If there are more neighbours surrounding a larger pore, the pore is typically captured by more than one tetrahedral element. Despite these approximations of pores and also weaknesses in the approach, e. g., due to inner voids in the mesh, the results of the pore characterisation are still believed to be representative as there is a large number of tetrahedral elements included in the evaluation (in this case the mesh consists of more than 46,000 tetrahedra, yielding the same number of pore volumes based on the corresponding included “pore voxels”). Further future studies should evaluate and quantify the accuracy of the approach for different granular materials, e. g., ideal sphere packings compared to arbitrarily shaped grains.

In the revised manuscript, we have added the following discussion on the tetrahedral mesh used for characterising pores:

“Note that the characterisation of pores by tetrahedral elements linking the grain centres represents a discrete approximation which might capture a “regular pore”, i. e., a pore in between only four neighbouring grains, better than a pore enclosed by a multitude of neighbouring grains. In the latter case, the pore will be represented by more than one tetrahedral element, i. e., it will be discretised. Further future studies should evaluate and quantify the accuracy of the approach for different granular materials, e. g., ideal sphere packings compared to arbitrarily shaped grains.”

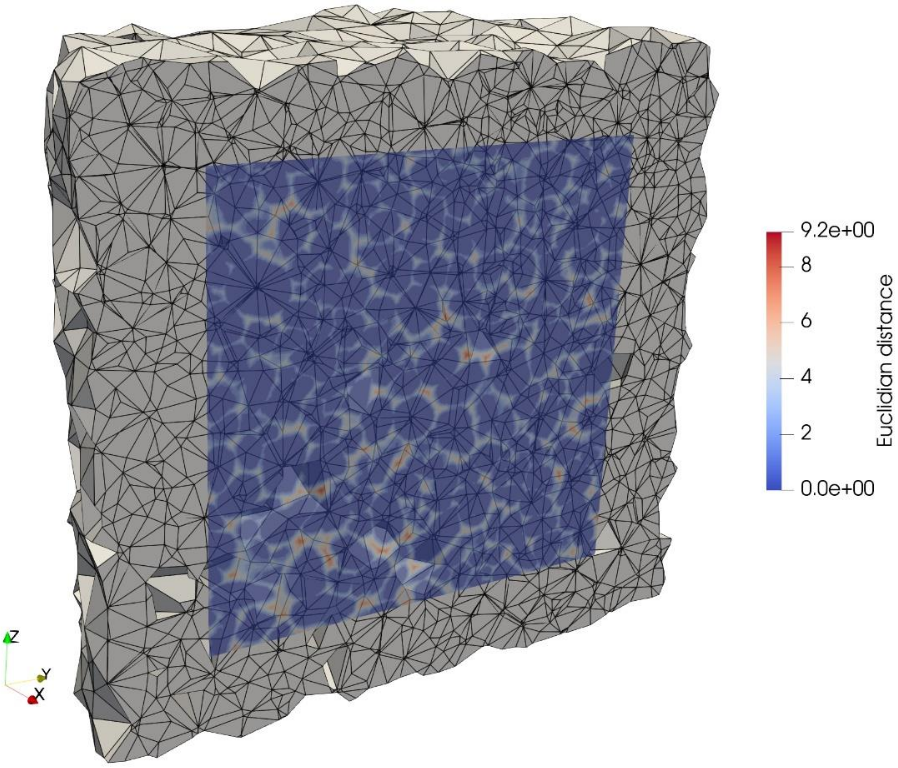

Fig. 4: Overlay plot showing a 2D slice with the results of an Euclidian distance map computation on the pore space and a cut through a 3D tetrahedron mesh linking the grain centres.

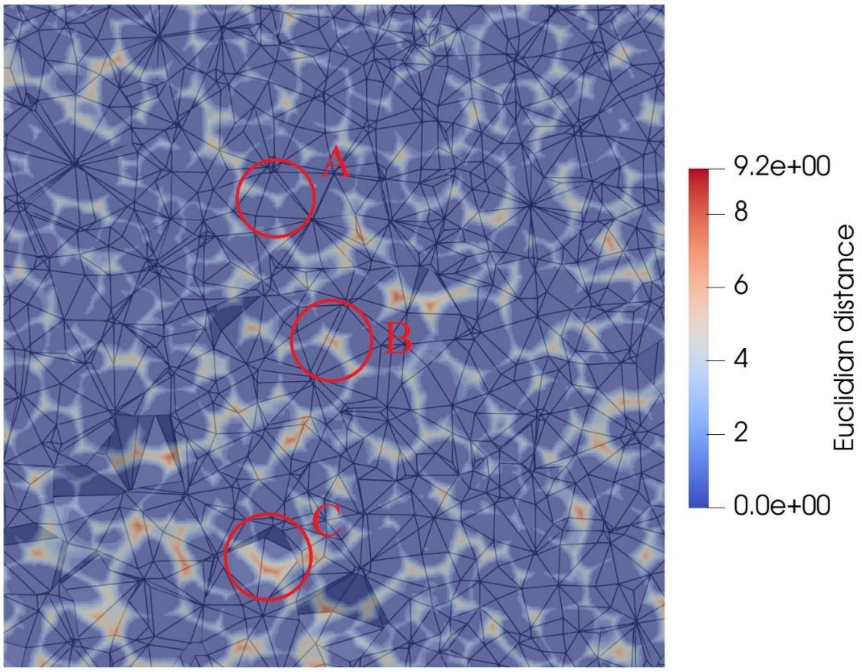

Fig. 5: Plane view of the heat map of Euclidian distance characterising the pore sizes overlain with the cut through the 3D tetrahedral mesh. The red circles highlight different exemplary cases of pore classification. Note that the different tetrahedra are cut in different angles, yielding either triangles or quadrangles according to their representation in the 2D plane.

4. I feel like images in the appendix should only serve as a further explanation and not for the actual analysis. This applies for example to the problem of 3D histograms (page 14). This is just my personal feeling, so no need to change that if you feel that it is reasonable.

We understand this logic. It was not a simple choice to put the figures into the Appendix as they are part of the results. You are right. However, for a better readability of the paper, we prefer having the larger histogram plots rather in the Appendix than inside the running text.

5. page 18, right column, discussion on the macroscopic suction vs the capillary pressure calculated from the mean curvature. You explain the difference between the two mainly by the accuracy of measuring the radii. There is, however, a difference between the macroscopic (measured on the boundary) and the intrinsic suction, see e.g. Y. Jiang, I. Einav, M. Liu, JMPS (2017) https://doi.org/10.1016/j.jmps.2016.11.018 What you measure with your microscopic measurements would be connected to the intrinsic suction, if I understand that correctly. So, the two of them do not need to identical for your measurements to be justified.

We thank the reviewer for this comment. The differentiation between measured suction and instrinsic suction based on thermodynamic considerations according to Jiang et al. (2017) might represent a reason for differences between suction values. However, in the work of Jiang et al. (2017), the intrinsic suction based on exemplary soil is typically higher than the measured suction. In our case, based on the measurements, the measured suction is higher, which is most probably due to the reasons discussed in the paper. Nevertheless, we will add the reference to the paper manuscript as well as an additional discussion as follows:

"Although maybe not applicable here, Jiang et al. (2017) explain differences between a 'measured suction' and an 'intrinsic suction' inside the soil based on theoretical thermodynamic considerations. According to their results, the intrinsic suction deviates from the measured suction and can be much higher than the measured suction. Interestingly, this is not the case based on our measurements where the suction calculated from interfacial curvatures is lower than the suction measured macroscopically."

Additional literature added to the manuscript:

Jiang, Y., Einav, I., and M. Liu (2017): A thermodynamic treatment of partially saturated soils revealing the structure of effective stress. *Journal of the Mechanics and Physics of Solids* 100, pp. 131–146, doi: 10.1016/j.jmps.2016.11.018.

Specific comments:

1. Table 1: the font size is cosiderably larger than that of the text. Please change it to a reasonable size comparable to the text.

The font size has been adjusted.

2. page 4, right column, last paragraph: previous studies. please cite more than one of you mention studies in plural.

The sentence has been modified in agreement with the cited single study.

3. page 6, left column, 3rd paragraph: first sentence is pretty long and only explains in great detail at which states the scans are acquired, which is obvious from the figure. You can considerably shorten this, but it's not necessary.

The sentence is long, but it also contains information on the kind of paths that are sequentially applied by naming them according to the terminology of hydraulic history of the WRC. We think that this is important information. A primary drainage path should be distinguished from a main drainage path and from scanning paths. Nevertheless, in the revised manuscript, the sentence has been split in order to shorten it a bit:

“Starting from the water-saturated initial state, 5 hydraulic steps on the primary drainage path were applied. They were followed by 4 steps on a 1st scanning imbibition path, 3 steps on a main imbibition or 1st drainage scanning path (after air entrapment), 2 steps on a 2nd imbibition scanning path, 2 steps on a 2nd drainage scanning path, 2 steps on a 3rd imbibition scanning path, and one last step on a 3rd drainage imbibition path.”

4. you use and mention the software "Avizo" several times. Please add a citation with the version of the software that you used.

A citation has been added including the used version Avizo 2019.3

5. page 7, right column, 2nd paragraph: first sentence is very long (7 lines). It could help readability to split it into two.

The long sentence has been split into two.

6. page 7, right column, 2nd paragraph: you mention boundary effect and show them in terms of the two vertical boundaries. Did you also study any boundary effects that might arise in the radial direction in order to choose the subvolume?

The lateral boundary conditions have not been studied here, however, they might lead to different hydraulic permeability as compared to the bulk material due to preferential flow paths. The centred cubic subvolume has been optimised to capture a large specimen volume at a given edge length, however, also excluding possible boundary effects in lateral direction close to the walls of the acrylic flow cell.

In the revised manuscript, we have added the following information regarding boundary effects:

“From the phase distribution boundary effects can be noticed especially for the air and water phase at the specimen bottom and top. The central cubic subvolume of 800 px × 800 px × 800 px has been selected in a location free of boundary effects representing the bulk of the specimen also excluding the lateral boundaries close to the walls of the flow cell.”

7. Figure 6: could you maybe use a higher resolution of the images? I was wondering when reading the text whether that is the pixel size that you use for the image analysis, but after accessing the images through TORE I saw that you resolution is much higher. I was also wondering whether the water layer on the top left quarter of the labelled image belongs to the water phase. But from the raw CT images it seems that it's the membrane/boundary of the specimen. Although it plays no role in your analysis (as you use smaller windows), I would remove it for clarity.

Due to file size limitations when uploading the pdf of the manuscript for review in OGEO, we had to reduce its size. Therefore, some figures have apparently also been reduced in quality. In the full size pdf, the figure quality should be much better.

The blue ring labelled as water is part of the flow cell wall and not meaningful for the analyses run on the subvolume. Following the reviewer's advice, it has been removed for clarity in the revised manuscript.

8. page 8, left column, last paragraph: in the first long sentence you explain what the contact line consists of, etc, but it is unclear what it actually represents. It gets clear in the following sentences, but for the reading flow it would be better, to start with what it represents and follow with how you measure it.

To make its meaning clear prior to a description of the measurement, we have restructured the sentence about the contact line in the revised manuscript:

"A further geometric measure of capillary action is the contact line representing the location shared by all present phases where interfacial tension is transferred to the solid grains. It is measured in the central cubic subvolume as a 3D path, consisting of nodes and line segments, the length of which can be measured to calculate the specific length of the contact line per unit volume."

9. page 10, left column, first sentence: If I understand this correct, it would not be "during" the hydraulic steps but in between them or during the image aquisition.

That's right. We thank the reviewer for this remark. We have changed the sentence to "During image acquisition…"

10. page 10, right column, last paragraph: what do you mean by "... further branches to the sides"? top/bottom or radial? I can't see radial in these graphs.

In order to clarify the observation based on Fig. 12 and 13 showing the phase distributions, we have added information to the text as follows:

"Focusing on the air distribution, this behaviour corresponds well to the sudden break through of an air channel from specimen top to bottom that further branches laterally to the sides in the lower zone of the pore volume during primary drainage, which has already been observed in the reconstructed image sequences shown in Fig. 12 and Fig. 13 for the step in between $S_r = 0.86$ and $S_r = 0.76$."

11. Figure 14: could you indicate on the scale where we have a change of drainage/imbibition? This would help to see immediately when the loading is reversed.

Black bars indicating the experimental steps after which a change in flow direction takes place have been added to the colourbar in the legend of Fig. 14. This information has also been added to the figure caption.

12. page 14, right column, last paragraph: please cite the recent mathematical approaches.

The corresponding citations regarding the meaning of interfaces for effective stress and for the water retention behaviour have been added.

13. Figure 25: The fit and the relationship of radius of curvature and contact angle are not very convincing. Might this be due to it being 2D measurements of a 3D problem?

The data in Fig. 25 indeed show a lot of spread or outliers which is to some extent likely based on the inhomogeneity of wettability in sands, however requiring further studies. Furthermore, as mentioned in the paper, there is a lower bound for the measurement of radii of curvature due to image resolution limits, and also contact angles are manually measured at a limited accuracy of a few degrees. Despite the spread, it is interesting to keep the figure because the trend of increasing radius of curvature with increasing contact angle is logical if, for instance, a meniscus in a capillary tube with varying radii of curvature and resulting contact angles is considered.

We have addressed the reviewer's concern in the revised manuscript by adding a discussion as follows:

"Although the presented data show a lot of spread with regard to the measured radii of curvature and related contact angles, a certain trend between both measures can be found: with increasing contact angle, also the radius of curvature increases both for drainage and imbibition which is a plausible relationship if, for instance, one thinks of the geometric relationship of an ideal meniscus inside a capillary tube with varying contact angles and related radii of curvature."

14. Figure 26: It would be good to indicate clearer what is a macroscopic measurement (start and end) and what is calculated from the micro. measurements (the mean) either in the legend or the caption of the figure.

Many thanks for this valuable comment. We have changed the caption of the figure to make the meaning of plotted data clearer:

"Evolution of capillary pressure, calculated from interfacial tension γ and 2D mean curvature $1/R_1$ (lone grey circles and blue squares and corresponding mean value indicated by black squares linked by a black line), compared to matric suction before and after a CT scan measured on a macroscopic level (indicated by circles and squares linked by dashed lines) for all drainage and imbibition steps."

15. page 20, last line: please cite the different authors.

The corresponding citations have been added.

16. page 21, left column, second paragraph: what do you mean as evidence for hydro-mechanical coupling? Was experimental evidence missing before?

With "experimental evidence for hydro-mechanical coupling", we refer to evidence for the link between changing effective stress and the resulting grain movements in unsaturated soils due to changes in the capillary state (saturation and suction). This evidence was not missing, but is in our eyes rare because changes in effective stress typically can't be measured directly. In order to avoid misunderstandings, we have changed and simplified the sentence as follows:

“As potential experimental evidence for a changing suction stress during drainage and imbibition which is typically hard to measure directly, a “breathing” of the grain skeleton leading to a small reversible and cyclic change in void ratio could be observed showing a decrease in void ratio upon drainage and suction build up and an increase of void ratio upon imbibition and suction reduction.”

Typos:

1. page 3, left column, line 2: "divided"

The typo has been corrected.

2. page 20, right column, next-to-last line: "lengths"

The typo has been corrected.

Recommendation: Revisions Required

Review Round 2

Reviewer A (Mohmad Mohsin Thakur)

The authors have carefully addressed the concerns raised in the first round of the review. I recommend the publication of the paper. The discussion provided in the review response can also be helpful to curious readers, thanks to the Open Geomechanics journal for appending the review history to the paper.

Recommendation: Accept Submission

Reviewer B (Max Wiebicke)

All the comments on the initial manuscript have been adressed very thoroughly and the changes to the manuscript are appreciated from my side. I thank the authors for the careful explanations – that also helped me in my understanding of some specific problems.

Recommendation: Accept Submission