A White Paper on:
Research Challenges Involving Coupled Flows and Processes in Geotechnical Engineering

by
Charles D. Shackelford[1]

BACKGROUND

Conduction Phenomena
Conduction phenomena refers to the combination of direct and coupled flow phenomena associated with the transfer of fluids, chemicals (solutes), electrical current, and heat through porous media (e.g., soils or rocks) due to hydraulic, chemical, electrical, and thermal gradients, as summarized in Table 1. The direct conduction phenomena represent flows that are linearly related to the corresponding driving force (gradient) as represented by Darcy's, Fick's, Ohm's and Fourier's laws. The indirect or coupled flow phenomena represents flows of one type due to driving forces or gradient of another type. For example, fluid flow can result not only from a hydraulic gradient, but also from chemical, electrical, and thermal gradients, the latter three processes commonly being referred to as chemico-osmosis, electro-osmosis, and thermos-osmosis, respectively[2].

Table 1. Direct and Indirect (Coupled) Conduction (Flow) Phenomena[3,4,5]

Flow, *J*	**Driving Force or Gradient, *X***			
	Hydraulic	**Chemical (Concentration)**	**Electrical (Voltage)**	**Thermal (Temperature)**
Fluid	Hydraulic Conduction (Darcy's law)	Chemico-Osmosis	Electro-Osmosis	Thermo-Osmosis
Solute	Streaming Current (Advection), or Ultrafiltration	Diffusion (Fick's law)	Electrophoresis	Thermal Diffusion (Soret Effect)
Current	Streaming Current (Rouss Effect)	Sedimentation Current	Electrical Conduction (Ohm's law)	Thermo-Electricity (Seebeck Effect)
Heat	Thermal Filtration or Isothermal Heat Transfer	Dufour Effect	Peltier Effect	Thermal Conduction (Fourier's law)

Coupled Processes
In some cases, direct and/or indirect flows associated with the aforementioned conduction phenomena occur simultaneously. For example, solute (e.g., aqueous miscible chemical) migration through porous media involves both advection in accordance with Darcy's law and diffusion in accordance with Fick's law. Advection tends to dominate solute migration in high permeability porous media (e.g., coarse grained soils such as aquifers), whereas diffusion tends to dominate solute migration in low permeability

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[1] Professor and Head, Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO 80523-1372; E: shackel@engr.colostate.edu
[2] Medved, I. and Černy, R. (2013). "Osmosis in porous media: A review of recent studies." Microporous and Mesoporous Materials, 170, 299-317.
[3] de Marsily, G. (1986). Quantitative Hydrogeology, Academic Press, Inc., Orlando, FL.
[4] Mitchell, J.K. (1991). "Conduction phenomena: from theory to geotechnical practice." Géotechnique, 41(3), 299-340.
[5] Mitchell, J.K. (1993). *Fundamentals of Soil Behavior*, 2nd Edition, John Wiley & Sons, Inc. New York.

porous media (e.g., aquitards and clay barriers for waste containment).

An example of direct and indirect flows occurring simultaneously is electrokinetics, whereby a voltage gradient is applied across electrodes (anode and cathode) inserted into contaminated fine-grained soils for the purpose of removing the contaminants (i.e., remediation). In this case, three primary processes are known to contribute to electrokinetics, viz. diffusion, electro-osmosis, and ion migration (electrophoresis), although diffusion generally is negligible relative to electro-osmosis and ion migration has been shown to be more significant relative to electro-osmosis[6].

Finally, both direct and indirect conduction phenomena may be coupled with other processes, such as mechanical deformation of porous media[7] (e.g., consolidation of contaminated soft sediments), chemical reactions (e.g., ion exchange, precipitation), and biological reactions (e.g., bioclogging, microbial mediated precipitation). Physico-chemical interactions between migrating solutes and the host porous medium, commonly referred to as compatibility, also can significantly affect both direct and indirect conduction phenomena, particularly in high activity clays such as sodium bentonites[8,9].

Relevance of Coupled Flows and Processes to Geotechnical Engineering

Mitchell (1991)[4] summarized the relevance of the 12 coupled (indirect) flows shown in Table 1 to soil-water systems. Examples of the relevance to Geotechnical Engineering were provided for seven of these 12 coupled flows,, viz., thermo-, electro-, and chemico-osmosis, isothermal heat transfer, streaming current both in terms of hydraulically driven electrical current and hydraulic driven ion (solute) migration (i.e., advection), and electrophoresis (e.g., ion migration). Of the remaining five coupled flows, the relevance of three, viz., thermal-electricity (Seebeck effect), diffusion/membrane potentials, and thermal diffusion of electrolytes (Soret effect), was somewhat uncertain, whereas electrically and chemically driven heat flow (i.e., Peltier and Dufour effects, respectively) were considered to likely be irrelevant, although these last two flows had not been studied to any significant extent at that time.

Nowadays, direct and coupled flows are particularly relevant to two sub-disciplines of Geotechnical Engineering, i.e., Environmental Geotechnics and Energy Geotechnics. For example, advection, diffusion, chemico-osmosis, thermos-osmosis, and thermal diffusion of electrolytes (e.g., radionuclides) are relevant to applications involving the use of engineered clay barriers for chemical containment, such a municipal and hazardous solid wastes, liquid (e.g., petroleum) storage facilities, both low-level and high-level radioactive wastes, and carbon sequestration (i.e., long-term storage of carbon dioxide or other forms of carbon generated for the purpose mitigating anthropogenic climate change). As previously noted, diffusion, electro-osmosis and electrophoresis (ion migration) are relevant flows for electrokinetic remediation. Finally, thermal conduction is relevant to geothermal piles that serve both as foundations for buildings and as heat exchangers used to store and extract heat from the subsurface, whereas the production of electrical power via geothermal reservoirs involves consideration of fluid and heat flows through porous media (soils and rocks) coupled with mechanical and chemical processes, commonly referred to as coupled thermal-hydrological-mechanical-chemical (THMC) processes, under unsaturated conditions[10].

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[6] Acar, Y.B., and Alshawabkeh, A.N. (1993). "Principles of electrokinetic remediation." Environmental Science and Technology, 27(13), 2638-2647.

[7] Bai, M. and Elsworth, D. (2000). Coupled Processes in Subsurface Deformation, Flow, and Transport. ASCE Press, Reston, VA.

[8] Shackelford, C.D, Benson, C.H., Katsumi, T., Edil, T.B., and Lin, L. (2000). "Evaluating the hydraulic conductivity of GCLs permeated with non-standard liquids." *Geotextiles and Geomembranes*, 18(2-4), 133-161.

[9] Shackelford, C.D. and Lee, J.-M. (2003). "The destructive role of diffusion on clay membrane behavior." *Clays and Clay Minerals*, 51(2), 187-197.

[10] Xiong, Y., Fakcharoenphol, P., Winterfeld, P., Zhang, R., and Wu, Y.-S. (2013). "Coupled geomechanical and reactive geochemical model for fluid and heat flow: Application for enhanced geothermal reservoir." Society of Petroleum Engineers, paper SPE 165982.

CHALLENGES FOR RESEARCH ON COUPLED FLOWS AND PROCESSES

A number of research challenges involving coupled flows and processes in Geotechnical Engineering need to be addressed in the coming decades. The premise for each of these research challenges follows.

- Experimental versus Theoretical Research: In the field of physics, theoretical physicists have been decades if not centuries ahead of the experimental physicists. A classic example of this observation is Albert Einstein's field equations for the Theory of General Relativity, which were postulated in November of 1915. Although the Theory of General Relativity now forms the basis for our current understanding of the interaction of space, time, and gravity, which is used to explain the expansion of the Universe, the motion of the planets, and the existence of black holes, some postulates of this Theory, such as the existence of gravity waves, still remain to be proven experimentally[11].

  In some cases, the theories describing coupled flows and coupled processes for applications relevant to Geotechnical Engineering similarly seem to be far ahead of the experimental evidence in support of these theories (e.g., the application of coupled THMC processes for radioactive waste containment). Therefore, the challenge is to provide experimental evidence in support of existing theory.

- Fundamental versus Applied Research: Although all research in Geotechnical Engineering should be related to an application, fundamental based research focusing on mechanisms is necessary for accurate, long-term prediction of the performance of engineered systems, e.g., engineered barriers used for LLRW and HLRW containment where the design lives are 1,000 and 10,000 yr, respectively. Although comprehending such long time periods can be difficult, there is relatively recent, tangible evidence that consideration of such long time frames is relevant. For example, the current impact of anthropogenic climate change can be traced to the onset of the industrial revolution, which started circa 1760 to ~ 1820, or about 195 to 255 years ago[12]. Second, several 1,000-yr precipitation events were associated with the flooding that occurred at several locations along the front range of the Rocky Mountains in Colorado in September of 2013, referred to as the *2013 Colorado Front Range Flood*[13]. Clearly, our ability to predict system performance over such large time scales will be accurate only if the models being used for this purpose are based on fundamental mechanisms, and all such fundamental mechanisms are included in the model, including time-dependent changes in material properties.

  For example, as previously noted, relatively recent research has shown that bentonite based containment barriers can exhibit chemico-osmosis, which is derived from the ability of the bentonite to behave as a semipermeable membrane resulting in solute restriction. Such solute restriction, also referred to as anion exclusion, also has been recognized to exist in highly compacted bentonite buffers (dry densities ranging from 1.8 to 2.0 Mg/m^3 (112 to 125 pcf)) used for HLRW containment. However, chemico-osmosis often is ignored in the models used to predict the long-term performance of these buffers, and solute exclusion often is treated in an empirical, rather than fundamental, manner in terms of the migration of radionuclides. Thus, the challenge is to conduct fundamental based research focused on mechanisms that take into account time-dependent changes in material properties over long time frames.

- Laboratory- versus Field-Scale Research: Fundamental studies typically are conducted under controlled conditions in the laboratory. For example, the vast majority of experimental research pertaining to coupled flow processes has been conducted in the laboratory using relatively small-scale specimens and homogeneous soils, such as the processed clays (e.g., kaolin, bentonite) and mixtures of sands with processed clays. While these studies do provide a basis for fundamental behavior, the

[11] http://www.bbc.com/news/science-environment-34815668
[12] https://en.wikipedia.org/wiki/Industrial_Revolution
[13] https://en.wikipedia.org/wiki/2013_Colorado_floods

justification for upscaling the results of these studies to the field scale often is problematic, due in part to complexity of the conditions that can occur at larger scales (e.g., boundary and initial conditions, heterogeneities in the materials). This reality suggests the need for long-term, large-scale field laboratories as recommended by Mitchell et al. (2007).[14] Several such field-scale research facilities exist around the world related to deep disposal of HLRW in argillaceous deposits, such as the Hades Underground Research Laboratory (URL) located in Boom Clay formation in Belgium, The Meuse/Haute Marne URL in France, and the Mont Terri URL located in the Opalinus Clay formation in Switzerland. However, no such similar laboratories exists in the USA. Therefore, the challenge is to develop capabilities that allow for an evaluation of performance at more realistic field scales.

- Saturated versus Unsaturated Research: The bulk of experimental studies on coupled flows and processes have been conducted under saturated soil conditions. Although the assumption of saturated soil conditions may be appropriate in some case and/or conservative in other cases, the assumption of saturated soil conditions frequently has been made for convenience, i.e., because measurement of the governing parameters under unsaturated conditions is more problematic than measurement under saturated soil conditions.

For example, a recent study evaluated the effect of the degree of water saturation, *S*, on the existence and magnitude of semipermeable membrane behavior in sodium homo-ionized bentonite[15,16]. As hypothesized on the basis of classic diffuse double layer theory, the magnitude of the solute restriction increased with decreasing *S*. However, due to long testing durations (~ 1 yr) and the complexity and limitations of the testing equipment, the lowest *S* evaluated was limited to 79 %. Since many problems faced in Geotechnical Engineering occur under unsaturated soil conditions (e.g., water-balance covers for waste containment, subsurface contaminant migration in the vadose zone, etc.), a challenge is to extend our understanding of the existence, magnitude, and relevance of couple flows and processes under unsaturated soil conditions.

- Abiotic versus Biotic Research. Biological activity can play a major role in affecting coupled flow processes. For example, in the aforementioned study on the effect of *S* on semipermeable membrane behavior,[14] aerobic biological activity was shown to affect the measurement of the chemico-osmotic pressure under unsaturated soil conditions to an extent that the addition of a biocide to the circulating chemical solutions was required in order to eliminate the biological effect. Also, electrokinetics has been proposed as a method to induce biodegradation of contaminants in clays via either bioaugmentation, whereby specific non-indigenous microbes are used to degrade susceptible contaminants, or biostimulation, whereby nutrients are injected to stimulate biodegradation by indigenous microbes[17,18]. However, due to the complexity associated with biological processes, the inclusion biological activity can significantly complicate research. Therefore, our ability to conduct relevant research related to the effects of biology on coupled flows and processes remains a significant research challenge.

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[14] Mitchell, J.K., Alvarez-Cohen, L., Atekwana, E.S., Burns, S.E., Gilbert, R.B., Kavazanjian, Jr., E., O'Riordan, W.H., Rowe, R.K., Shackelford, C.D., Sharma, H.D., and Yesiller, N. (2007). *Assessment of the Performance of Engineered Waste Containment Barriers*. The National Academies Press, 500 Fifth Street, N.W., Washington, DC 20001.

[15] Sample-Lord, K.M. and Shackelford, C.D. (2014). "Membrane behavior of unsaturated bentonite barriers." *Geo-Congress 2014: Geo-Characterization and Modeling for Sustainability*, M. Abu-Farsakh, X. Yu, and L.R. Hoyos, Eds., Geotechnical Special Publication 234, ASCE, Reston, VA, 1900-1909.

[16] Sample-Lord, K.M. (2014). Membrane Behavior and Diffusion in Unsaturated Sodium Bentonite. PhD Dissertation, Colorado State University, Fort Collins, CO.

[17] Alshawabkeh, A. N., and Maillacheruvu, K. 2001. Electrochemical and Biogeochemical Interactions Under DC Electric Fields. Chapter 4, *Physicochemical Groundwater Remediation*, Smith, J. A. and Burns, S. E. (Eds), Kluwer Academic/Plenum Publishers, New York, 73-90.

[18] Shackelford, C.D. (2005). "Environmental issues in geotechnical engineering." *16th International Conference on Soil Mechanics and Geotechnical Engineering*, Osaka, Japan, Sept. 12-16, 2005, Millpress, Rotterdam, The Netherlands, Vol. 1, 95-122.

A Few Emerging Issues to Understand the Processes in Geomaterials

Xiong (Bill) Yu, M. ASCE

Professor, Department of Civil Engineering, Case Western Reserve University, 10900 Euclid Avenue, Bingham 206, Cleveland, Ohio 44106, xxy21@case.edu, 216-368-6247

ABSTRACT: This white paper discusses a few important aspects of soil mechanics relevant to the enhanced understanding of its associated coupled multiphysics process as well as coupled continuous and discontinuous process. New experimental methods are needed to augment/supersede the existing experimental techniques; they will provide a cohort of fundamental parameters intrinsic of soil behaviors. Computational tools based on the enriched knowledge of the fundamentals will offer new insights to the solution of many historical or emerging geotechnical issues. The concerned progresses in experiment and simulation will fortify the foundation of soil mechanics. The educational needs to raise the latitude of geotechnical profession are briefly discussed.

INTRODUCTION

This white paper summarizes the author's observation on a few important fundamental issues relevant to the further advancement of soil mechanics. These include 1) understanding the fundamental variables underlying the coupled multiphysics processes in geomaterials, 2) describing the continuous and discontinuous processes in the geomaterials; 3) incorporating the effects of the structural randomness of geomaterials to its physical process. The origin of these problems and the impacts of solving these problems are discussed. Progresses in these fields have the possibility to catalyze advancement in various domains of geotechnical practice and research. The educational needs to prepare competent new generation of geotechnical engineers are also discussed.

UNDERSTANDING THE FUNDAMENTAL VARIABLES UNDERLYING THE COUPLED MULTIPHYSICS PROCESS IN GEOMATERIALS

Geomaterials, with their porous nature, are subjected to multiphysics processes. The pore structure and interfacial interactions within their pore space facilitate the transport of energy and mass. By nature, description of the processes in geomaterials has to involve the coupling of multiple fields including those of thermal, hydraulic, chemical, biological, and mechanical nature. The conventional geotechnical practice primarily focused on the individualized mechanical or hydraulic process under the assumption of an isothermal material system, which typically renders satisfactory approximation of the real processes occurring in the physical realm. However, emerging geotechnical practice such as energy piles, underground thermal energy storage, unconventional gas exploration, permafrost responses to the climate change, etc. requires a more holistic look into the coupled processes occurring in the pore space of geomaterials. Figure 1 illustrate an example of the coupled processes involved with the frozen soil subjected to thermal excitation (freezing or thawing), which couples the thermos-hydro-mechanical processes.

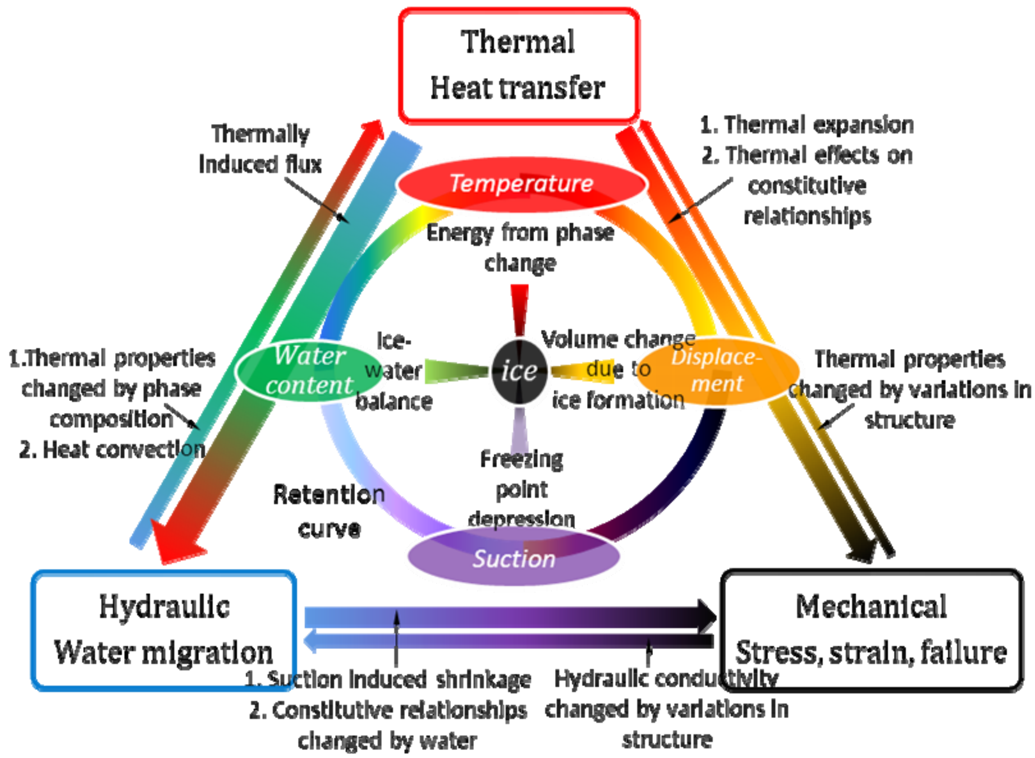

FIG. 1. Schematic of coupled thermal-hydro-mechanical processes in frozen soil (Liu and Yu 2011).

Research in this area requires the development and application of new tools that allow to study the topological characteristics of geomaterials (such as 3D micro-/nano-CT), the surface and interface behaviors in relation to the topological pore structure, imaging the flow behaviors in pore space (such as by uMRI), etc. In the author's opinion, there are needs to identify the most intrinsic physico-chemical properties governing the macroscopic coupled behaviors in the geomaterial system. Such properties can be characterized at the fundamental scale as well as application scales; the goal of such set of properties are to describe the physico-chemical interactions of fluid phase with the pore structure. The author believes that the physico-chemical energy of the porous system at the interface together with the topological characteristics of the pore space are the most intrinsic quantities relevant to study of the coupled processes in soils. Practical measurement technologies for these parameters are necessary to augment what is available in the existing soil mechanics lab.

The soil water characteristic curve (SWCC). The concept of soil water characteristic curve (SWCC) has conventionally been used to describe the variation of the system status of energy with the variation of water in the pore space. It is the lumped demonstration of the interfacial energy at the interfaces between air-liquid-solid as well as the effects of pore geometry. It remains as one of the most fundamental properties.

The internal contact angle. The internal contact angle, which is an extension of a popular technology in soil physics and chemical engineering that measures the interfacial energy among air-liquid-solid interface, provides the lumped measurement of the interfacial energy status in light of the characteristics of pore space.

The pore size distribution. It describes the topological characteristics of the soil pore space, including the distribution of pore size as well as their spatial arrangement. It is a geometric property determined by the arrangement of soil grains. The confinement by the pore space leads to distinctive interactions with the fluid phase.

The SWCC, internal contact angle, and pore size distribution provide redundancy in terms of capturing the fundamental physico-chemical interactions in geomaterials. Geotechnical laboratory procedures that captures combination of any two of these three properties provide complete parameters required to describe the interphase interactions with the pore space of soils. Therefore, development of practical measurement technologies that covers the full range of such parameters will be a major driving force to advance the theory and practice application involving coupled processes.

DESCRIBING THE CONTINOUS AND DISCONTINOUS PROCESSES

Geomaterials are discontinuous systems of solid grains organized with unique spatial arrangements. Interactions of the constituent grains underlies the observed macroscopic mechanical behaviors of geomaterials. Compared with its discrete solid counterpart, the fluid phase behaves more as a continuous homogenous phase. Interactions between fluid and solid grain in the dynamic sense is complex and involves the coupling of continuous and discontinuous processes. Holistically description of such interactions, while challenging, provides important insight on engineering phenomena such as soil liquefaction, soil erosion, debris flow, etc.

Computational modeling tools are available to simulate the behaviors of discrete material systems, such as DEM, SPH, and other Meshless Method; tools are also available to treat and simulate material phases as continuous materials such as FEM, FVM, CFD etc. All of these computational tools describe the conservation principles with different perspectives and extent of approximation. The combination of the continuous and discontinuous models provides an opportunity to understand the mechanism of the interphase interactions and how they determine the observed physical behaviors (i.e., prediction of the angle of repose of sand particles under water, Fig. 2). The advantage of coupling continuous and discontinuous approach is that it only requires to prescribe the most fundamental physical laws, without the needs of complex heuristic constitutive relationships (as seen in the DEM, which allows to describe the soil mechanical behaviors without the need of complex constitutive relations) while minimize the computational requirements (an advantage of FEM compared with DEM). Therefore, this allows to set the focus of research on the most basic interactions between continuous and discontinuous components. For example, the conventional concept of drag force, which was originally formulated in the hydraulic engineering, might need to be revisit. The challenge on the computational power remain to be addressed via advancing the efficiency of computational algorithm.

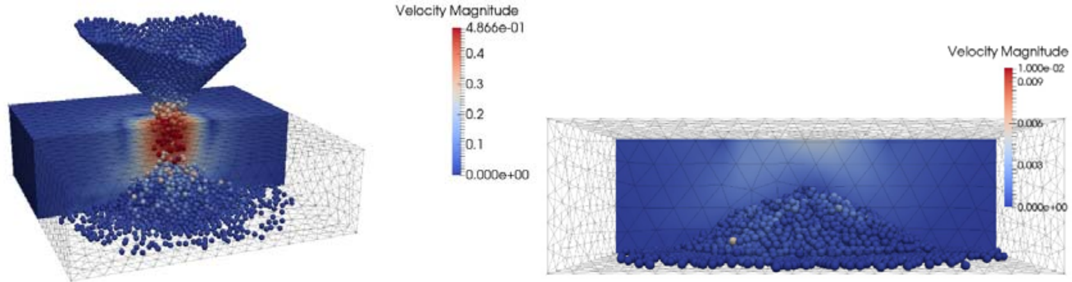

FIG 2. Angle of repose via coupled continuous and discrete model (Guo and Yu 2015)

THE EFFECTS OF RANDOMNESS OF GEOMATERIALS ON THE PHYSICAL PROCESSES

The computational models of traditional soil mechanics tend to treat soil as a continuous homogeneous system. Such assumptions describe the macroscopic behaviors of soils; they, however, are insufficient to describe the processes related to the microstructure of soils. These include important engineering issues such as crack initialization in light of soil skeleton, the internal stresses on the soil skeleton due to swelling of fluid phases, the non-uniform pore water pressure during earthquake, among many others. The inherent randomness has to be accounted for at the element level or at the geological scales. The random FEM, which establishes the FEM model based on the random grain fields, combines the advantages of DEM in describing the structural characteristics and the computational efficiency of FEM. By defining the behaviors of individual phase (mechanical, thermal, hydraulic, etc.), the global behaviors can be predicted without the use of complex constitutive relations. This allows to study the mass and thermal transport processes originating from the fundamental microstructure characteristics (Fig. 2).

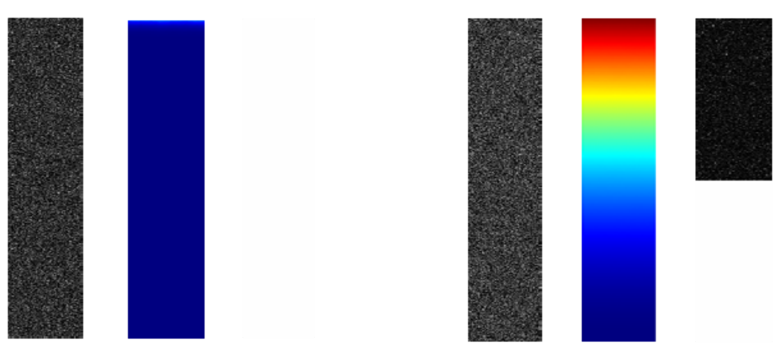

FIG 3. Microstructure based model for the thawing soil (phase distribution,

temperature, suction) a) complete frozen; b) 50% thawing (Dong and Yu 2015)

EDUCATIONAL NEEDS

The existing geotechnical engineering curricula does not adequately prepare our students to be receptive to advanced geotechnical concepts and methods. Most course coverage are still limited to the empirical framework established from practice, which while provide important technical support to the profession, has become a constraint on the further development of soil mechanics. There lacks exploration of the sound science and mechanics underlying the heuristic formula widely used for practice. Further advancement of geotechnical engineering requires to training a new generation of engineers with strong knowledge in mechanics, interfacial physico-chemistry, computational methods, and advanced experimental skills. There are room to revising the existing geotechnical engineering curricula to bring up the profession to a higher level.

CONCLUSIONS

This white paper summarizes the author's observation on a few important fundamental issues relevant to the further advancement of soil mechanics. These include 1) understanding the fundamental variables underlying the coupled multiphysics processes in geomaterials, 2) describing the continuous and discontinuous processes in the geomaterials; 3) incorporating the effects of the structural randomness of geomaterials to its physical process. It also discussed the educational needs to prepare competent new generation of geotechnical engineers.

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REFERENCES

1. Liu, Z. and Yu, X. (2011). Coupled Thermo-Hydro-Mechanical Model for Porous Materials under Frost Action: Theory and Implementation, *ACTA Geotechnica*, Volume 6, Issue 2, pp51-65.

2. Guo, Y. and Yu, X. (2015). Mechanism of Soil Erodibility Using Coupled Computational Fluid Dynamics and Discrete Element Method Model, the TRB 95th Annual Meeting Compendium of Papers, January 11-15, Washington DC.

3. Dong, S. and Yu, X. (2015). Experimental Characterization and Microstructure Based Random FEM Simulation of Freezing and Thawing Effects on Soils, the TRB 95th Annual Meeting Compendium of Papers, January 11-15, Washington DC.