MPC-548
November 20, 2017

Project Title

Development of Models for the Prediction of Shear Strength of Swelling Clays

University

North Dakota State University

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Research Needs

Accurate prediction of the shear strength of swelling clays is critical for the design of roads, railway infrastructure, foundations, embankments, slopes, canals, erosion control, retaining walls, etc. The damage caused by swelling clays to the U.S. infrastructure is estimated to be of the order of about $13 billion per year (2009)[1]. Swelling clays are found in various parts of the United States (Fig. 1)[2] and the world. In Fig. 1, the red and blue colored regions contain soils with high swelling potential and orange, and green colored regions contain soils with moderate to low swelling potential. Portions of North and South Dakota contain soils that have high swelling potential. Overestimation of strength parameters can lead to failures and underestimation can lead to significant increase in the cost of the project. Shear strength of soils with high swelling clay content can vary from high values when swelling is restrained to significant degradation in strength or even complete loss of strength due to swelling. The change in shear strength can also be seasonal. Fundamental strength parameters that define strength

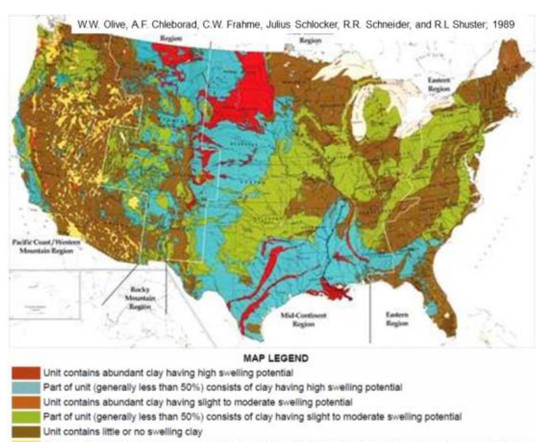

Fig. 1. Swelling Clays Map of US[2]

properties of soils are related to a variety of factors that include soil type, microstructural characteristics, fluid properties, mineralogy, saturation, etc. Reliable predictive tools that can accurately predict the shear strength of swelling clays are lacking. Our prior work on clays demonstrates the key role of molecular interactions on the evolution of microstructure and the macroscopic properties such as permeability, consolidation, and swelling pressure[3].

This is a continuing funding request for year 2 and year 3 funding. The earlier proposal contained tasks for all three years. The previous proposal has been modified to include tasks accomplished in year 1 and the tasks to be accomplished in year 2 and 3. The research needs and year 2 and year 3 research tasks and methodology included here are from our previous proposal.

Research Objectives

1. Construction of multiscale computational simulations test-beds for swelling clays to evaluate the role of molecular interactions and microstructure to macroscale shear strength properties of swelling clays.
2. Development of experimental techniques to evaluate the swelling clay-fluid interactions and mechanical properties at various length scales: molecular scale to macroscale.

The proposed plan is shown in Fig. 2. Bridging the molecular interactions to the evolution of microstructure and bridging both molecular interactions and microstructure to the mechanics of the swelling clays will provide powerful predictive capabilities and develop a clear understanding of underlying mechanisms that lead to shear strength properties of swelling clays.

Research Methods

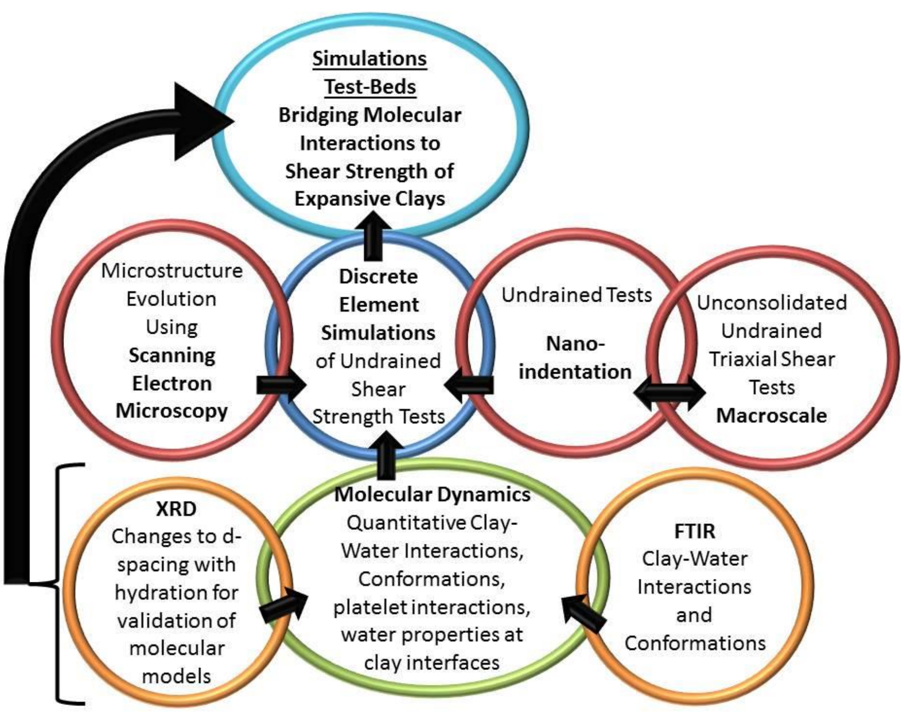

Figure 2. Schematic showing the integration of experimental and modeling tasks proposed and a general path towards achieving the project goal.

Research tasks accomplished in Year 1:

1. Preparation and saturation of Na-montmorillonite clay samples in the controlled uniaxial swelling (CUS) cell for macroscale and nanoindentation testing, electron microscopy imaging, and spectroscopy.
2. Atomistic models of Na-montmorillonite clay with various dimensions were constructed. Molecular dynamics (MD) simulations of clay-fluid interactions, with different polarity fluids.
3. Development of mathematical relationships from MD simulations and FTIR/XRD experiments that relate interlayer water content to change in d-spacing, binding interaction energy between clay sheets versus interlayer water content and speed of flow of water molecules into the clay interlayer. These relationships will be used in the DEM models.
4. Development of procedures and parameters for conducting nanoindentation experiments on clays and preliminary results from nanoindentation experiments on dry clays. A 3D printed device was designed and fabricated to allow for conducting nanoindentation tests on compacted and undisturbed clay samples.

Computational Multiscale Modeling

- Molecular Modeling and Simulations
    - Conformation of water molecules, interaction energies, density and mechanical properties in the close proximity and away from clay surfaces. – Clay platelet sizes of 8, 18, 32, 72 and 144 unit cells (21Å to 110Å) will be inserted in water/fluid boxes, and simulations run for 5 to 100ns for conformation equilibrium. The conformation of the fluid molecules will be calculated. The H-bond bridging between the fluid molecules will be mapped. Interaction energies and the density of the water with distance will be calculated to evaluate bound water thickness. The mechanical properties of water in the proximity and away from the clay surface will be found by applying constant velocity or forces to single or cluster of molecules.
    - Platelet-platelet interactions and the role of molecular bridging – Platelets with water molecules in between and varying distances between platelets (with different orientations) will be analyzed using SMD. We will evaluate the interactions between the platelets, the interactions between water molecules and ions and platelets, as the platelets move away from each other, and calculate the stress-displacement response (3.5 A° to about 100 A°)[23]. The effect of model size will be evaluated and extrapolated to a size range of real platelets obtained from atomic force microscopy[30] and SEM.
- Original Plan: Discrete Element Modeling: Bridging Molecular Response And Microstructure And Role On Mechanics Of Swelling Clays
    - A discrete element model that incorporates particle subdivision, developed by PIs for swelling clays[19] will be used. The interlayer fluid flow rate will be initially evaluated from experiments[30] and later from solvation modeling[31]. A hierarchical multiscale approach that will introduce interlayer interactions, interparticle variables such as particle-particle interactions, mechanical properties of the fluid at varying distances from clay surfaces, the stress-displacement relationship

between platelets as they approach (varying orientations), cation concentration, etc. into the DEM. DEM models of the expansive clays mimicking experimental swelling, used for undrained shear tests and nanoindentation tests, will be constructed and experimental shear and nanoindentation tests simulated to evaluate the mechanical response with swelling. Particle by particle analysis will be conducted and related back to molecular scale deformation behavior and relate clay fluid molecular interactions to the mechanical response of swelling clay with swelling.

- New Plan: All atomistic modeling of clay aggregates: The discrete element modeling would attempt to model the interaction between the swelling clay particles. The swelling clay particles (also called clay aggregates) are dynamic, unlike conventional soil particles. The internal forces within the particles change when hydrated, leading to changes in particle sizes and mechanics of the particle. We had hypothesized that the clay tactoid (which is a single stack of about 10 clay sheets approximately 10nm tall) would be able to capture the particle breakdown. Our experiments show that even after particle breakdown, the size of the particle is significantly larger than 10 nm, suggesting that there are additional factors that play a role in particle dynamics. We would need to simulate dry and hydrated all atomistic models of clay aggregate to model the clay particle dynamics accurately. A clay aggregate consists of several clay tactoids with various orientations. The models will simulate interactions within each tactoid and interactions between tactoids at various hydration conditions. Specifically, we will be comparing binding energies within the aggregate to discern the mechanism of particle breakdown. These simulations would accurately capture the dynamics within the swelling clay particle, leading to the development of a robust clay particle model that can capture the clay particle dynamics and mechanics and would be essential for developing accurate discrete element models for swelling clays that would be carried out in a separate study in the future. Since it has been shown in the prior work and the current work, the important role of particle breakdown on the engineering properties including strength, it is essential that the particle breakdown be accurately evaluated and modeled before implementation in discrete element models of swelling clays. We plan to accomplish this task in the summer of 2022.

Experiments

- Macroscale testing of Na-montmorillonite samples: Clay samples obtained from the clay repository will be swollen to 0%, 25%,50%, 75%, and 100% in the controlled uniaxial swelling (CUS) cell[32]. Unconsolidated undrained triaxial tests (ASTM D 2850) will be conducted to obtain undrained shear strength versus swelling relationship. Undisturbed samples will be obtained for nanoindentation, FTIR, and microscopy. Clay samples maintained at RH[33] from 0-100% will be used for determination of bound-water thickness.
- Characterization: Nanoindentation on wet clay samples. 1) *Rapid Test:* Nanoindentation under rapid displacement rate indentation to obtain the nanoscale undrained shear strength of the clay with swelling and compared with discrete element simulations. FTIR insitu spectroscopy will be used to (1) Identify the nature of water (structure) on clay surfaces, (2) To evaluate the limiting water thickness beyond which clay fluid interactions do not change, and (3) 2D resolved FTIR with water loss as perturbation to

evaluate change in nature of water and thickness of adsorbed water, and compared with conformations from MD. Cryo-Scanning Electron Microscopy will be used to capture the evolving microstructure of clay with swelling. XRD experiments will be conducted in a constant humidity device to obtain changes to d-spacing for verification of MD models by comparing computed d-spacing to experiments.

Expected Outcomes

The major outcome of this basic research will be a multiscale computational framework for swelling clays to evaluate the mechanical response of swelling clay to external loading. The models incorporate the molecular scale clay-fluid interactions and the evolution of microstructure during swelling, the two critical factors that influence the mechanical properties of swelling clays. These simulation testbeds will provide insight into the key mechanisms that affect the mechanics of swelling clays during swelling. The innovative experiments and experimental techniques developed in this research would not only serve as model development and verification tools but also could lead to the introduction of new experimental techniques for swelling clays.

Relevance to Strategic Goals

This research will elucidate the key mechanisms that influence the shear strength of expansive (swelling) clays, which are responsible for significant damage to transportation infrastructure. The computational modeling work along with the understanding of the key mechanisms will help improve prediction capabilities of the strength of swelling clays and contribute towards the more reliable design of transportation infrastructure in swelling clay areas. This research fits well with the themes, “state of good repair” of transportation infrastructure.

Educational Benefits

Two doctoral students will work on this research project and portions of the research work conducted will go towards their dissertation. The students and PIs will present seminars at NDSU and present papers at meetings and conferences for wider dissemination of results to students, researchers and professionals. The students will also author journal and conference manuscripts. Research results will be incorporated in the advanced soil mechanics course in the department of civil and environmental engineering.

Tech Transfer

The research results will be presented at meetings, conferences and seminars where researchers, professionals and practitioners in the field participate. The results will also be published in peer reviewed journals that are read by researchers, professionals and practitioners in the field. The PIs will develop educational modules for presenting results at seminars targeting practitioners. The PI has in the past offered workshops across cities in ND in the past through T-square center to professionals on topics of geosynthetics. The workshops were well attended. The research results will also be highlighted via websites. The results will also be reported in the quarterly and other reports requested by MPC.

Work Plan

1. Molecular Scale Modeling
2. Experimental Tasks
3. All Atomistic Modeling of Clay Aggregates Reports
4. Seminars/Presentations
5. Journal/Conference Papers

The total duration of the project is 24 months. The first 18 months will be spent towards molecular dynamics and steered molecular dynamics simulations, analysis of data, interpretation of results and publication of results. The experimental tasks include macroscale testing, nanoscale testing and characterization using spectroscopy and electron microscopy and would take 18 months to accomplish. This will include data analysis and interpretations and publication. The discrete element modeling tasks will be executed over the entire duration of 24 months and will include code development, simulations, data analysis, interpretation and publication. Reports will be prepared on a quarterly basis with a final report at the end of the project. Seminars and conference presentations will be made atleast annually. Journal and conference papers will be submitted annually.

Task	**Months**			
	1-6	7-12	13-18	19-24
Molecular Modeling				
Experimental tasks				
Discrete Element Modeling				
Reports		12		24
Seminar/Presentation		12		24
Journal/Conference Papers	***Conference and Journal Papers***			

Project Cost

Total Project Costs: $200,000
MPC Funds Requested: $100,000
Matching Funds: $100,000
Source of Matching Funds: Civil & Environmental Engineering

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