MPC-506
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Project Title:
Reliable Prediction of Shear Strength of Swelling Clays

University:
North Dakota State University

Principal Investigators:
Dr. Dinesh R. Katti, P.E., (NDSU), Interim Chair and Jordan A. Engberg Presidential Professor, Department of Civil & Environmental, dinesh.katti@ndsu.edu, (701) 231-7245

Dr. Kalpana S. Katti, (NDSU), University Distinguished Professor, Department of Civil & Environmental, kalpana.katti@ndsu.edu, (701) 231-9504

Research Needs:
Accurate prediction of the shear strength of swelling clays is extremely important 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 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[4].

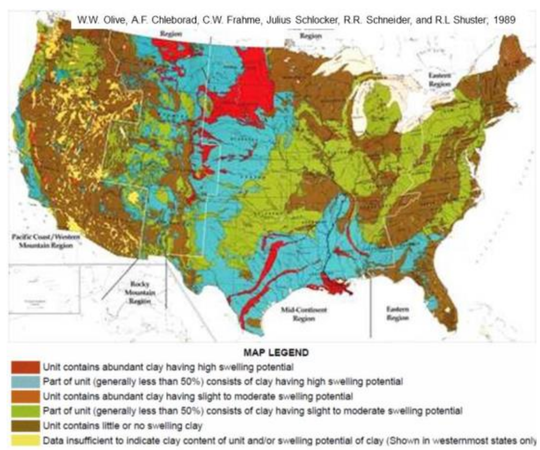

Fig. 1. Swelling Clays Map of US

Research Objectives:
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 in swelling clays.

Specific objectives are,

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.

Research Methods: **RESEACH TASKS AND METHODOLOGY (Figure 2)**

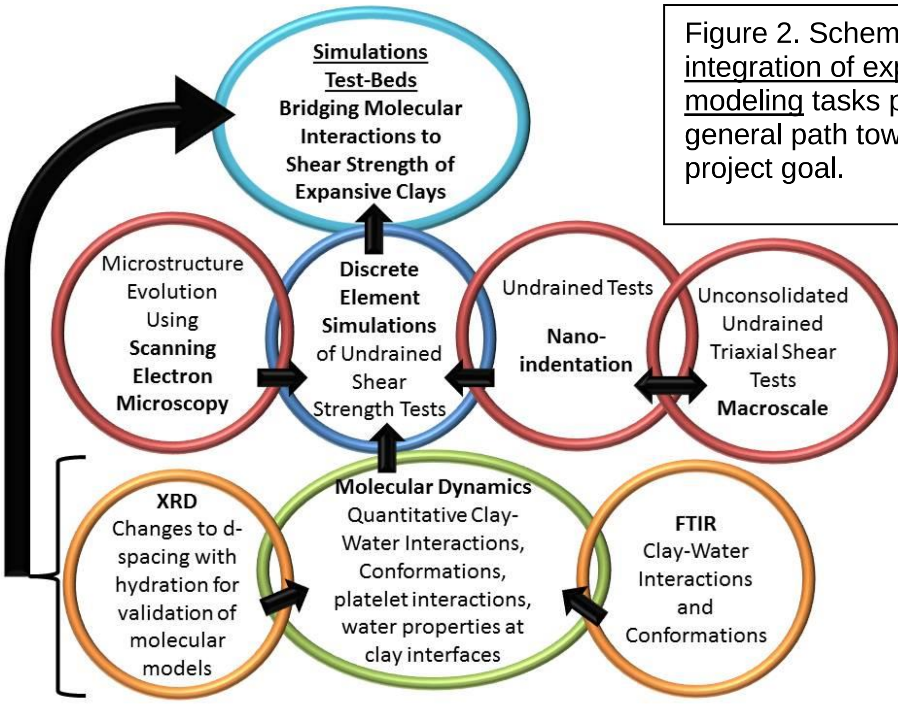

Figure 2. Schematic showing the integration of experimental and modeling tasks proposed and a general path towards achieving the project goal.

1.0 COMPUTATIONAL MULTISCALE MODELING

1.1 MOLECULAR MODELING AND SIMULATIONS

1.1.1 Construction of molecular models of clays and fluids Molecular models of clay minerals will be constructed and steered molecular dynamics (MD) simulations will be conducted. Experimental results will guide and validate the models and simulations. Steered molecular dynamics (SMD) software NAMD [5-7] and visualization and post-processing software VMD [8] will be used. SMD, which has been used previously by our group[9-27], is a type of MD where force or velocity is applied to an atom or atoms in a molecule, and the resulting displacements or forces are evaluated. Two models of standard clays and TIP3P[29] water will be constructed, (a) Na-Montmorillonite (SWy-2) using our prior work [17,19,28] and (b) Ca- Montmorillonite (STx-1b).

1.1.2 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, 36, 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. 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.

1.1.3 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°)[24]. Fig 3 shows examples of platelet interactions. The effect of model size will be evaluated and extrapolated to size range of real platelets obtained from atomic force microscopy[30] and SEM.

1.2 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[20] 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.

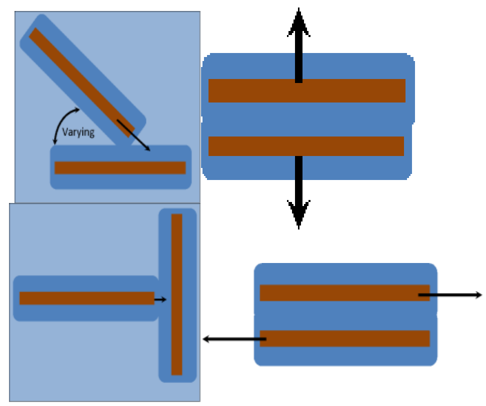

Figure 3. Various orientations considered for platelet-platelet interactions using SMD. Blue color is water and brown color depicts clay sheet.

2.0 EXPERIMENTS

Macroscale testing of Ca and 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 graduate students will work on this research project. Research results will be incorporated in the advanced soil mechanics course in the department of civil and environmental engineering.

Work Plan:

	Months					
Task **Months →**	1-6	7-12	13-18	19-24	25-31	32-36
Molecular Modeling						
Experimental tasks						
Discrete Element Modeling						
Reports		**12**		**24**		**36**
Seminar/Presentation		12		***24***		***36***
Journal/Conference Papers	***Major results: Submitted to peer reviewed papers***					

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

TRB Keywords: Expansive Clays, Swelling Soil, Soil Structure, Cohesive Soils, Clay Soils.

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