

**A UNIVERSAL NANO-LEVEL CONSTITUTIVE
(MECHANO-VOLUME CHANGE) MODEL FOR
SWELLING CLAYEY SOILS**

BY
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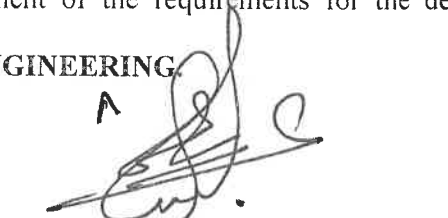
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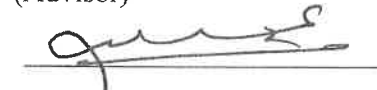
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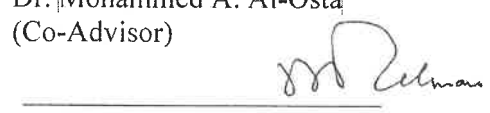

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Dedicated to my honorable teachers,
Sir Razaqat Ali Bajwa, to whom I owe all of my academic
achievements,
and
Dr. Habib ur Rehman, who has significant contribution to my career

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LIST OF ABBREVIATIONS

a:	parameter to account for the effect of density in the HMC Model
a:	back-fit parameters of the STJ Model (kPa)
a, b:	fitting parameters of the Hu et al. (2014) Model
b:	back-fit parameters of the STJ Model
c:	material parameter
C _b :	bond concentration
CEC:	cation exchange capacity (mEq/g)
e _{macro} :	macrostructure level void ratio
e _{micro} :	microstructure level void ratio
e _{NC} :	void ratio at the normally consolidated line (NCL)
E:	elastic modulus (kPa)
EXC:	exchange capacity (mEq/g)
f _i :	macro-micro coupling functions when SI is activated
f _d :	macro-micro coupling functions when SD is activated
f _c :	interaction function for microstructural compression path
f _s :	interaction function for microstructural swelling path
G:	shear modulus within the elastic domain (kPa)
G _{bo} :	bond undamaged shear modulus (kPa)
k ₁ , k _{II} :	parameter to account for the effect of unsaturated state
K:	parameter controlling the increase in cohesion with suction
K _{bo} :	bond undamaged bulk modulus (kPa)
K _{m.ref} :	reference bulk elastic modulus at the microstructure (kPa)

$K_{M.ref}$:	reference bulk elastic modulus at the macrostructure (kPa)
m :	parameter related to the effect on yield mean effective stress of the structure
m :	VG model parameter of the HMC Model
M :	slope of critical state lines
n :	VG model parameter of the HMC Model
n :	material parameter
N :	void ratio corresponding to 1 kPa
p^c :	reference stress (kPa)
p_o^M :	mean yield stress for saturated conditions (kPa)
p_a :	confining pressure (kPa)
p'_n :	isotropic stress at which no swelling or collapse takes place (kPa)
p'_{iyo} :	initial yield stress for expansive unsaturated soil (kPa)
$p'_c(0)$:	mean yield average skeleton stress under saturated conditions (kPa)
P'_{Myo} :	initial mean yield effective stress at the macrostructure (kPa)
$P'_{M.ref}$:	reference mean effective stress at the macrostructure (kPa)
r :	parameter defining the maximum soil stiffness
r_o :	initial damage state of the bond (kPa)
r_1 :	bond damage rate
S_I :	hardening parameter for suction increase (SI) yield surface (kPa)
S_D :	hardening parameter for suction decrease (SD) yield surface (kPa)
S^o_{rw} :	degree of saturation of wetting curve (%)
S :	specific surface area of crystal (m^2/g)
S^M_{Do} :	air entry value of capillary water retention curve (CWRC) (kPa)

S_{Do}^m :	air entry value of adsorptive water retention curve (AWRC) kPa
t :	thickness of the crystal (m)
v :	valence of exchangeable cation
W_{max} :	parameter for the hydration force (MJ/m ²)
W_{min} :	parameter for the hydration force (MJ/m ²)
α_m :	parameter controlling the microstructural soil stiffness (kPa ⁻¹)
α :	initial material parameter of the Sun and Sun (2011) Model
α_m :	hysteretic parameter of AWRC
α_M :	hysteretic parameter of CWRC
α :	Van Genuchten (VG) model parameter (kPa ⁻¹)
β^M :	plastic modulus of CWRC
β^m :	plastic modulus of AWRC
β_m :	parameter controlling the microstructural soil stiffness (kPa ⁻¹)
β :	parameter controlling the rate of increase of soil stiffness with suction (kPa ⁻¹)
$\beta_{m,min}$:	minimum plastic stiffness at the microstructure
β_M :	plastic stiffness at the macrostructure
γ :	initial material parameter of the Sun and Sun (2011) Model
γ^p :	plastic shear strain (%)
γ_s :	parameter related to the effect on yield mean effective stress of the suction
ϵ_1 :	axial strain (%)
ϵ_3 :	lateral strain (%)
κ :	compressibility coefficient along elastic stress paths
κ_s :	compressibility coefficient for changes in suction within the elastic region

κ_m :	parameter controlling the microstructural soil stiffness
κ_s :	gradient of scanning curve
κ^m :	elastic modulus of AWRC
κ^M :	elastic modulus of CWRC
λ_s :	stiffness parameter for changes in suction for the virgin state
$\lambda(0)$:	compressibility coefficient for saturated state along with virgin loading
λ_{sr} :	gradient of the drying-wetting curve
λ_{se} :	slope of the degree of saturation – void ratio curve
$\lambda(s)$:	slope of normal compression line at suction, s in kPa
λ :	slope of saturated normal compression line
μ, ν_e :	Poisson ratio
ζ :	parameter for rate of increase of macrostructure soil stiffness with suction (kPa^{-1})
σ_1 :	axial stress (kPa)
σ_3 :	lateral stress (kPa)
τ :	material parameter to identify the change in $\lambda(s)$ with suction (kPa^{-1})
ϕ_o :	initial porosity
ϕ_{Mo} :	reference porosity for the macrostructure for the permeability model
χ :	slope of the neutral line
χ_o :	bonding deformation parameter associated with undamaged state
χ_o :	parameter for the hydration force (m)

ABSTRACT

Full Name : [Muhammad Abdul Waheed]
Thesis Title : [A universal nano-level constitutive (mechano-volume change) model for swelling clayey soils]
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Clay minerals in soils and rocks exhibit large volume change upon exposure with water and this behavior becomes even more complex when the strata are being stressed by the engineering and environmental loads. Therefore, a realistic prediction of the hydro-mechanical behavior of the swelling soils is always a challenge due to their coupled swelling-mechanical response in the cases of geotechnical and geoenvironmental engineering problems, nuclear waste storage in clay-bearing rock repositories, shale gas extraction, and other uses of clay in the manufacturing industry. All the existing behavior models have restricted applications in engineering and other fields of practice mainly due to the partial consideration of the structure and fabric of swelling soils in the model formulation. In this study, a hydro-mechanical behavior model was formulated using the parameters acquired from the molecular-level simulations and modeling of the volume change and stress-strain behavior of the swelling soils. The molecular mechanics and molecular dynamic simulations were performed on the natural structure of the swelling soils formulated using the Monte Carlo technique. The mathematical model, developed from the simulation results, can predict the overall hydro-mechanical behavior of swelling soils for all possible combinations of clay minerals, non-clay minerals, salts causing cementation of the soil/rock structure, confining pressures, and the induced strain levels. The developed model has

successfully been validated through laboratory and field testing on the swelling soils in both the elastic and elastoplastic regions of the stress-strain behavior and also from the data of two (02) swelling clays (MX-80 and FEBEX Bentonite) from the existing literature, supporting the universal nature of the developed behavior model.

ملخص الرسالة

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عنوان الرسالة : نموذج محاكاة شامل في حجم النانو (تغيير الحجم الميكانيكي) للتربة الطينية المنتفخة

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تُظهر المعادن الطينية الموجودة في التربة والصخور تغييرًا كبيرًا في الحجم عند التعرض للماء، ويصبح هذا السلوك أكثر تعقيدًا عندما تتعرض الطبقات للضغط بسبب الأحمال الهندسية والبيئية. لذلك، فإن التنبؤ الواقعي بالسلوك الهيدروميكانيكي للتربة المتضخمة يمثل دائمًا تحديًا بسبب استجابتها الميكانيكية للانفخاض في حالات كثيرة مثل: المشاكل الهندسية الجيوتقنية والجيوب بيئية، تخزين النفايات النووية في المستودعات المصنوعة من الطين، استخراج الغاز الصخري. وغيرها من استخدامات الطين في الصناعة التحويلية. جميع نماذج السلوك الحالية لها تطبيقات مقيدة في الهندسة وغيرها من التطبيقات المختلفة وذلك يرجع أساسًا إلى الاعتبار الجزئي لبنية ونسيج التربة المعرض للانفخاض في صياغة النموذج. في هذه الدراسة، تمت صياغة نموذج للسلوك الهيدروميكانيكي باستخدام المعامل المأخوذة من عمليات المحاكاة على المستوى الجزيئي ونمذجة تغير الحجم وسلوك الإجهاد والانفعال للتربة المنتفخة. تم إجراء الميكانيكا الجزيئية والمحاكاة الديناميكية الجزيئية على التركيب الطبيعي للتربة المنتفخة المحضرة باستخدام تقنية ما تسمى (تقنية مونت كارلو Monte Carlo technique). يمكن للنموذج الحسابي الذي تم تطويره من نتائج المحاكاة، التنبؤ بالسلوك الهيدروميكانيكي العام للتربة المنتفخة لجميع التركيبات الممكنة من المعادن سواء كانت المعادن المكونة أو غير المكونة للطين أو الأملاح المسببة لتماسك بنية التربة / الصخور أو الضغوط المحصورة أو مستويات الإجهاد المستحثة. تم التحقق من صحة النموذج المطور بنجاح من خلال الاختبارات المعملية والميدانية على التربة المنتفخة في كل من المناطق المرنة وغير المرنة لسلوك الإجهاد والانفعال. بالإضافة إلى نوعين من التربة المنتفخة (MX-80 و FEBEX Bentonite). الموجودة في المقالات السابقة ، مما يدعم صحة ودقة نموذج المحاكاة الذي تم إنشاؤه.

CHAPTER 1

INTRODUCTION

1.1 Background

Clay minerals present in soils and rocks exhibit a high degree of volume change upon interaction with water and this behavior becomes even more complex when the strata are being stressed by the engineering and environmental loads. Swelling soils are known to be problematic because of their volume change characteristics resulting from a continuous variation in the moisture regime of the unsaturated and partially saturated zones. These volume changes are accompanied by variations in the mechanical behavior of swelling soils. The mechanical properties of natural and compacted clays are critical in the foundations' design and containment barriers for nuclear waste (Villar and Lloret, 2004; Sanchez et al., 2005; Komine and Watanabe, 2010; Cui, 2017; Tachibana et al., 2020). Foundations of the buildings are generally placed in partially saturated soil layers of the vadose zone. The increase in the moisture levels under the building foundations due to reduced evaporation, percolation of surface water(s), and potential for leakage from utilities lead to significant changes in the mechanical properties of these soils. The hydro-mechanical behavior of compacted clays is also critical in the design of clay barriers for nuclear waste. The clay barrier is initially placed in an unsaturated state and is exposed to moisture fluctuations during its lifetime caused by heat-emitting waste and hydration from the parent/host rock. Similarly, slopes and excavation work in mudrocks/clayey rocks also require special attention to study the hydro-mechanical behavior (Pinyol et al., 2007). Excavations in clayey rocks create unloading conditions (reduction in the confining stress) and expose the material to atmospheric interaction, causing

cyclic changes in the moisture levels. These changes in environmental and loading conditions lead to swelling of the exposed clayey rocks and the corresponding reduction in stiffness and strength. Also, the clays have applications in agricultural soils, landfill liners, and even in the field of medicine (Ahmed and Abduljawwad, 2017). Therefore, understanding the hydro-mechanical behavior of swelling soils is important for the application of this material in various disciplines and civil engineering options.

The structure of the natural and compacted clays is very complex since they constitute different minerals with multi-arrangement and complex interactions of the particles ranging from millimeters to nanometers (Gens and Alonso, 1992; Sharma, 1998). The overall material behavior of swelling clayey soils is controlled by the structure and fabric of swelling soils created by several factors such as clay-water-ion interactions, the interactions, relative distribution and proportion of clay and non-clay particles, density, and moisture conditions (Ahmed and Abduljawwad, 2018). Due to the above-described factors, the realistic modeling of clay-bearing soils/rocks has been very challenging for geotechnical experts. Clay minerals are nano-materials. Hence, the molecular-level simulations approach can be applied to determine the material performance of clay-bearing soils/rocks. Therefore, it can be inferred that molecular-level modelling concepts applied to nano-sized clay particles can predict the mechanical response of swelling clayey soils.

Several macro-level reports (Alonso et al., 1990; Gens & Alonso, 1992; Alonso et al., 1999; Gallipoli et al., 2003; Sanchez et al., 2005; Pinyol et al., 2007, Sun and Sun, 2011; Hu et al., 2014; Hu et al., 2015; Vilarrasa et al., 2015; Wang and Wei, 2015; Massin and Khalili, 2016; Chen et al., 2017; Massin, 2017; Qiao et al., 2019; Kyokawa, 2021), as well as molecular-level studies (Karaborni et al., 1996; Katti et al., 2005; Wang et al., 2007; Katti et al., 2009; Tao et al., 2010; Hantal et al., 2014; Katti et al., 2015; Ahmed and Abduljawwad, 2017; Rahromostaqim M. et al.,

2018; Thapa K. B., 2020; Du et al., 2021; Navarro et al., 2021), have been conducted to model the volume change and mechanical performance of swelling soils. All macro-level constitutive models are applicable to a specific behavior(s) and cannot be generalized in the form of a universal model (Ahmed and Abduljawad, 2017). The macro-level models also do not explicitly incorporate realistic nano-level clay interactions with water and ions in their formulations. Furthermore, the macro-level constitutive models use a complete matrix of volume change and strength tests on saturated and unsaturated soils (e.g., water retention tests, pressure-plate tests, isotropic compression tests, triaxial tests, etc.) to determine key model parameters that limit their application in the industry fields.

On the other hand, the existing molecular-level models for clay-bearing soils/rocks have mainly used single clay crystallite in their simulations without the incorporation of natural fabric and structure of clays. The existing molecular-level models, in addition, lack the formulation of a mathematical model to assess volume change and mechanical behavior. In light of the above-described limitations of macro and molecular level models, it is imperative to perform realistic modeling of swelling soils at the molecular level to predict the hydro-mechanical behavior with due consideration of clay interactions with water and ions at the nano-level and linking it to the macroscopic level by considering all possible variations in the structure and fabric of clay-bearing soils/rocks.

The advent of molecular-level modeling software, high-performance computers, and experimental advancement in unsaturated soils testing in the last two decades opened doors for modeling the real structure of clays at the molecular-level. Therefore, molecular-level models could be used for a wide range of materials, including clays.

1.2 Research Objectives

As explained in the previous section, the existing macro-level and molecular-level constitutive models have several limitations in the model formulations, such as mainly the non-consideration of clay interactions with water and ions at the nano-level and non-incorporation of natural clay fabric and structure. Therefore, there is a need for realistic modeling at the molecular level to describe the mechanical behavior and then couple it to the macro-level response. The modeling shall incorporate essential characteristics that influence the mechanical properties of swelling soils, including all possible variations in the fabric and structure of clays, chemical properties of clay, such as the type of clay minerals, physiochemical forces of attraction and repulsion arising from clay mineralogy, and interlayer cations (Alonso et al., 1987; Puppala et al., 2017; Zhou et al., 2022). Based on the above explained background, the main objectives of this research are summarized below:

- Molecular-level modeling of mechanical and volume change behavior of swelling clayey soils as a function of moisture content, density, CECs, exchangeable cations and cementation effects due to salts, thereby covering all possible variations of the fabric and structure of natural and compacted expansive clayey soils,
- Formulation of a mathematical hydro-mechanical behavior model (constitutive model) for swelling clayey soils,
- Coupling of mechanical behavior model with existing volume change model by Ahmed and Abduljawwad (2017), and

- Validation of the hydro-mechanical model through field and laboratory testing on samples collected from natural expansive clay deposits, reconstituted laboratory specimens (control specimens) and already published data in the literature.

1.3 Research Plan

The plan to accomplish the above-outlined objectives of this research consisted of the following phases: (i) molecular-level simulations of the hydro-mechanical behavior in materials studio software, (ii) formulation of a universal hydro-mechanical model, and (iii) laboratory and field validation of the model. Molecular-level simulations were carried out using material studio software, followed by the model formulation using simulation results. Validation of the model was performed through field and laboratory testing in the current study and available databases from the literature. All these phases of the study were discussed in the subsequent chapters. The model developed in this study would be based on the basic intrinsic parameters that are common in various types and kinds of clay-bearing soils/rocks available worldwide.

The flow process of the proposed research is illustrated in Figure 1-1 and brief details are presented as follows:

- As part of the research methodology, a program would be prepared to simulate the deposition of particles in a loose state and then a subsequent geological process of compaction and stress release in natural clayey soils at the molecular level. The interactions occurring during these processes, like the sorption of different ions and salts, would also be simulated. Molecular-level modeling for volume change and mechanical behavior of swelling clayey soils will be performed using various modules of the materials studio software.

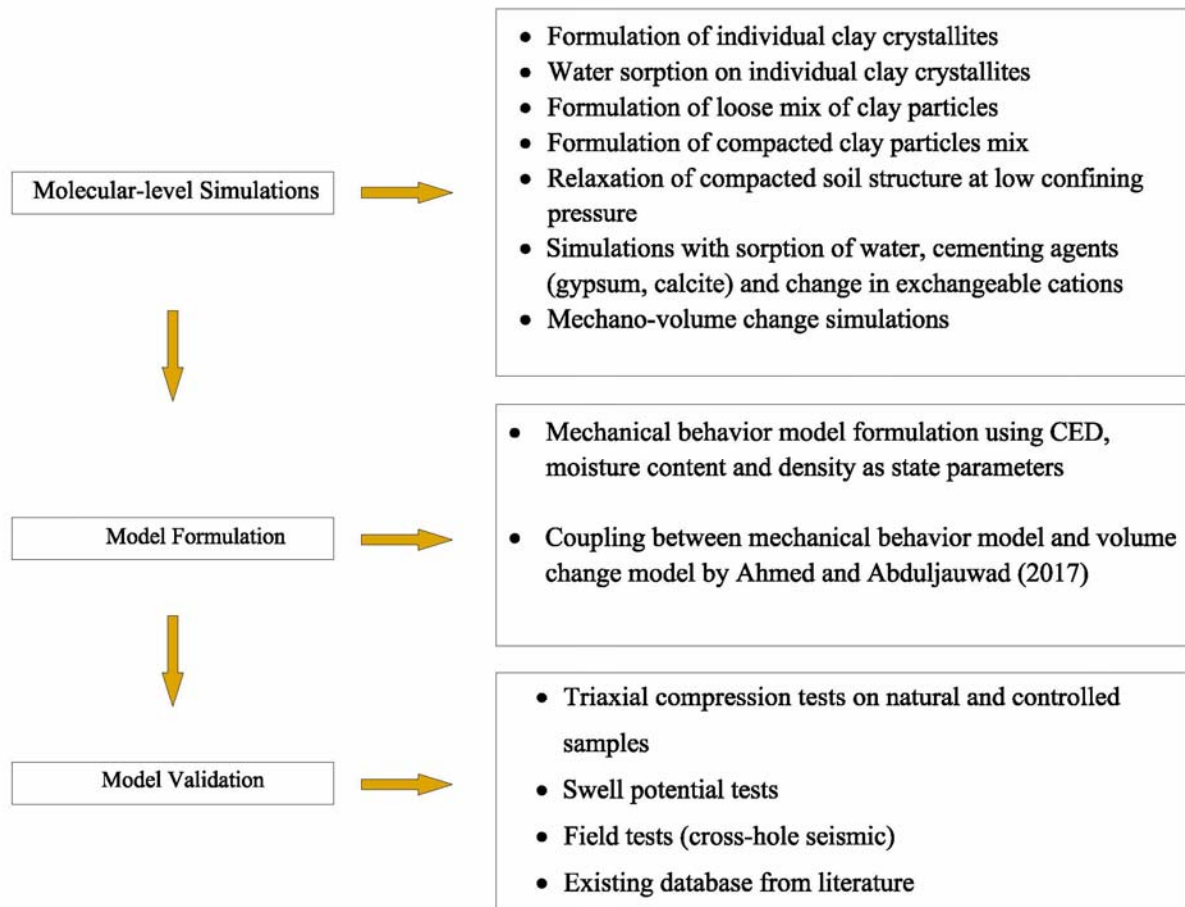


Figure 1-1 Framework of proposed hydro-mechanical model

- The trends of the hydro-mechanical response of swelling clayey soils obtained from the molecular-level simulations would be studied. The state variables, including modulus values at different strain levels and CED values of swelling clays with variations in density, moisture content, CECs, exchangeable cations and cementation effects, would be obtained from simulations. The plots would be generated between CED and modulus values against different strain levels and constitutive equations would be developed. These plots would serve as a nano-level mechanical model for swelling clayey soils.

- Both volume change and stress-strain phenomenon occur simultaneously and the complete response of swelling clayey soils to environmental and mechanical loading can only be obtained after coupling both behaviors in one model. Therefore, coupling of the mechanical behavior model with the existing nano-level volume change model by Ahmed and Abduljawad (2017) would be performed.
- The formulated model would be validated through field and laboratory testing on swelling clay samples. In addition, available databases in the literature would also be used for model validation.

CHAPTER 2

LITERATURE REVIEW

The mechanical behavior of compacted and natural swelling soils is critical in the design of foundations and seals for repositories of nuclear waste containment barriers (Villar and Lloret, 2004; Sanchez et al., 2005; Komine and Watanabe, 2010; Cui, 2017; Tachibana et al., 2020; Ye et al., 2020; Du et al., 2022). In addition, swelling soils also have other applications in shale gas hydraulic fracturing, municipal waste containment liners, agriculture soils, and medicine (Ahmed and Abduljawwad, 2017). Their wide presence in various fields of science has led to an increasing interest in understanding the mechanical behavior of these swelling soils.

Swelling soils exhibit volume changes when exposed to wetting, drying, loading, and unloading conditions and their stress-strain paths vary during these volume changes. The response of these soils becomes more complex in unsaturated/partially saturated zones where the foundations of structures are generally placed. Continuous fluctuations of moisture level in unsaturated zones result in volume change behavior, which consequently affects the mechanical properties of these soils. Volume change behavior of swelling soils is directly associated with changes in soil strength and stiffness (Gens and Alonso, 1992; Alonso et al., 1999; Sanchez et al., 2005).

The understanding of fabric and structure plays an essential role in describing the mechanical behavior of swelling soils (Alonso et al., 1987). The structure and fabric of swelling soils (generally clays) are very complex. Natural swelling soils consist of different minerals with a random arrangement of particle sizes ranging from millimeters to nanometer (Gens and Alonso, 1992; Sharma, 1998). The overall behavior of swelling soils mainly depends on the relative

proportion and distribution of these clay and non-clay particles, their interaction, cementation caused by non-clay salts (gypsum, calcite, etc.), degree of saturation, and overburden pressure (Ahmed and Abduljauwad, 2017a; Chen et al., 2019; Du et al., 2020). The final fabric and structure created by all the above factors have significant contributions to controlling the mechanical behavior of swelling soils. Owing to all these factors, it has become a challenge to realistically model the stress-strain behavior of swelling soils.

This chapter covers the general comprehension of the role of fabric and structure in the mechanical behavior of swelling clayey soils and presents a review of deficiencies in the existing constitutive models at both the macro/micro and molecular levels and their key features and significant limitations have been discussed.

2.1 Role of fabric in mechanical behavior

The structure of the natural and compacted swelling clayey soil is very complex since they constitute different minerals with random arrangements and complex interactions of the particles ranging from millimeters to nanometers. A typical swelling soil is composed of swelling and non-swelling clay minerals, active non-clay minerals such as gypsum, calcite, and inert non-clay minerals such as quartz. Active non-clay minerals interact with expansive clay minerals at deposition or change in the chemical environment and result in cementation between clay minerals by changing the cohesion/adhesion among these particles (Ahmed and Abduljauwad, 2017a). Furthermore, macro, micro and nano level pores exist in the swelling clayey soils with water and air phases.

The importance of the fabric and structure of unsaturated soils in understanding mechanical response was first investigated by Alonso et al. (1987). They reported that the matric suction or

water potential controls the mechanical behavior of unsaturated soils greatly depending on the fabric of the soil. They explained that the micro-fabric consists of three forms, namely elementary particle arrangements, particle assemblages, and pore spaces (Figure 2-1). If dominant in a fabric, elementary particle arrangements with intra-element pores combine to form assemblages or matrices with intra-matrix pore spaces. They also make aggregates or packets if a grain-like structure results from their integration and contain inter-aggregate and intra-aggregate voids. Sometimes, these elementary particle arrangements just act as connectors between sand and silt particles. All these three forms, matrices, aggregates, and connectors are presented in Figure 2-1 and are associated with the specific mechanical behavior of unsaturated soils. Matrix-type fabrics exhibit swelling, whereas aggregates and connectors are more prone to collapse. Generally, soils compacted dry of the optimum have "aggregates" type fabric, whereas soils compacted wet of the optimum exhibit a "matrix" type fabric. Depending upon the final form of fabric (matrices, aggregates, or connectors), they summarized some patterns of mechanical behavior of unsaturated soils, including the collapse of open-structure soils upon wetting under high applied stresses, expansion of soils on wetting under low confining stresses, the occurrence of irreversible volumetric deformations upon changes in suction and stiffening of soil against external stresses due to suction.

Gens and Alonso (1992) further elaborated that the soil structure consists of two levels: microstructure, and macrostructure. The microstructure level consists of elementary particle arrangement of clay platelets and intra-element pores. These elementary particle arrangements combine in a three-dimensional macrostructure to form matrices and aggregations with intra-matrix, inter-aggregate, and intra-aggregate pores (Figure 2-1). The microfabric of clay particles is embedded into a macrofabric of silt and sand particles. Sanchez et al. (2005) related the micro

and macrostructure model of expansive clays by Gens and Alonso (1992) with bimodal pore distributions at inter-aggregate and intra-aggregate pores (Figure 2-2). In the above reported studies, the microfabric and nanofabric are considered the same, which is not precisely true as clays are composed of nano-sized clay particles with intra and inter-particle voids and cannot be lumped with microfabric due to significant scale/size differences (Ahmed and Abduljawad, 2017a).

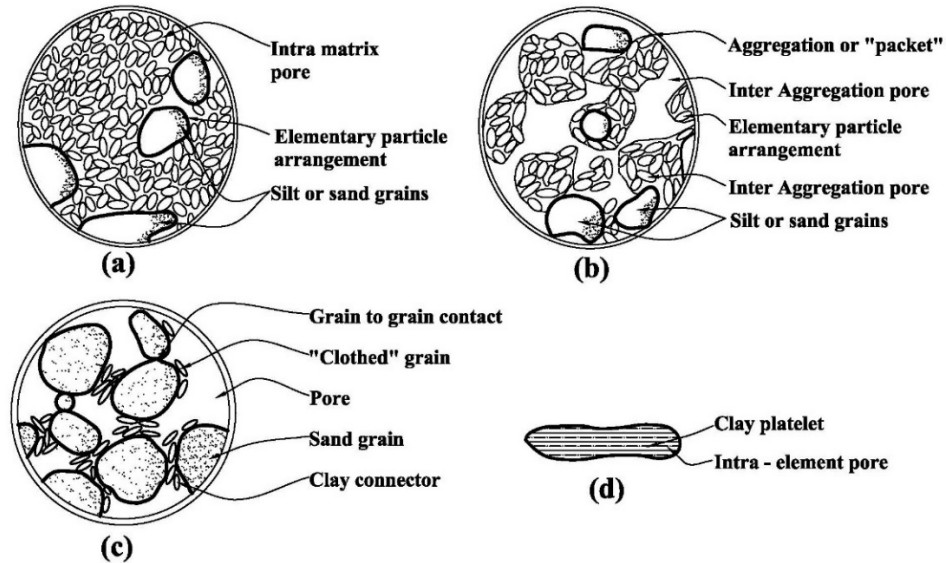


Figure 2-1 Types of microfabric; (a) Clay matrix, (b) Clay aggregations, (c) Clay connectors, (d) Basic clay platelet (Alonso et al., 1987).

Pinyol et al. (2007) further studied the cementation effect between clay aggregates and the role of cementation in the mechanical response of clayey rock (Figure 2-3). They described that the bond damage results in the closure of the macropores (collapse behavior) and rearrangement of clay aggregates into denser packing due to a sudden decrease in the void ratio.

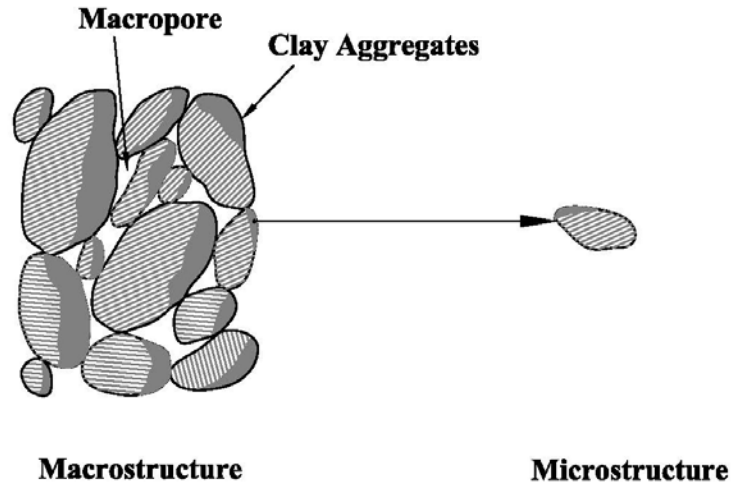


Figure 2-2 Schematic representation of macro and microstructure (Sanchez et al., 2005).

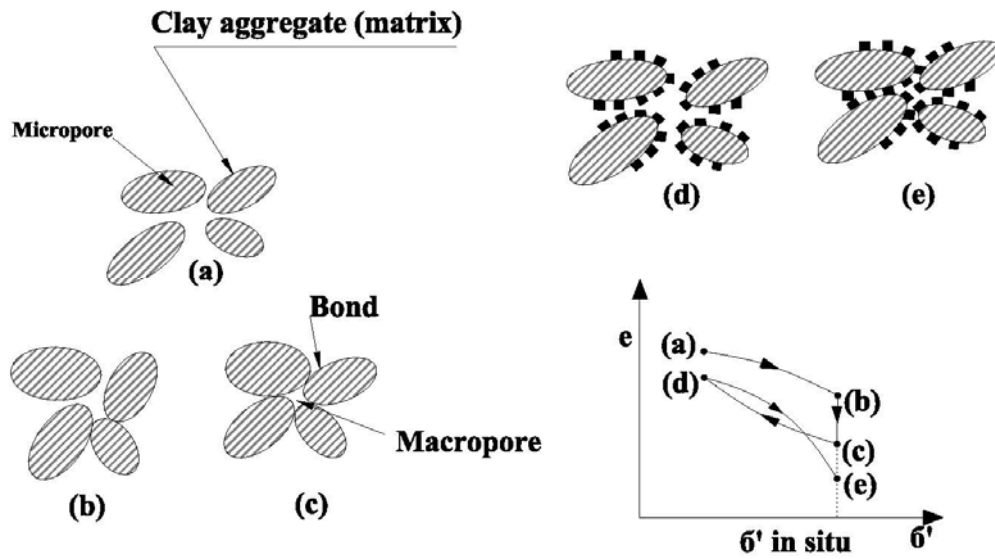


Figure 2-3 Stress-strain variation during unloading-reloading cycle on a clayey rock; (a), (b) and (c) Clay matrix compression and cementation under stress, (d) Unloading induced bond damage, (e) Re-loading induced bond damage (Pinyol et al., 2007).

Wang and Wei (2015) also divided the soil structure into micro and macrostructure. As illustrated in Figure 2-4, the configuration of elementary particle arrangements of expansive soils could be either dispersed or flocculated. These elementary particle arrangements join together to form aggregates that combine with other non-clay particles to create an overall fabric and structure of expansive clay. Further, they introduced a double porosity structure, demonstrating that mechanical loading under constant suction generally changes the macroporosity, whereas hydraulic loading (wetting or drying) mainly influences microporosity. Hydraulic loading (wetting or drying) also has an effect on macroporosity, depending on the stability of macrostructure, density, loading, and the intensity of the wetting-drying effect. The swelling of aggregates due to water flow generally increases microporosity, and the porosity becomes monomodal upon full saturation. On the other hand, the drying of aggregates (increase in suction) recovers a double porosity structure. Also, macroporosity decreases under the application of loading/compaction due to the closure of macropores. However, a slight increase in microporosity is also observed upon compaction due to the conversion of macropores to the micro-size range.

Vilarrasa et al. (2015) reported that expansive clays have a dual structure model (Figure 2-5) that defines the existence of two porosity levels, that is, microporosity and macroporosity. In the bimodal pore size distribution presented by them, 0.1 μm diameter is taken as the dividing size between intra-aggregate and inter-aggregate pores. Upon swelling, microporosity invades macroporosity, thereby causing a reduction in permeability. This decrease in permeability changes the suction characteristics and mechanical properties of expansive clays.

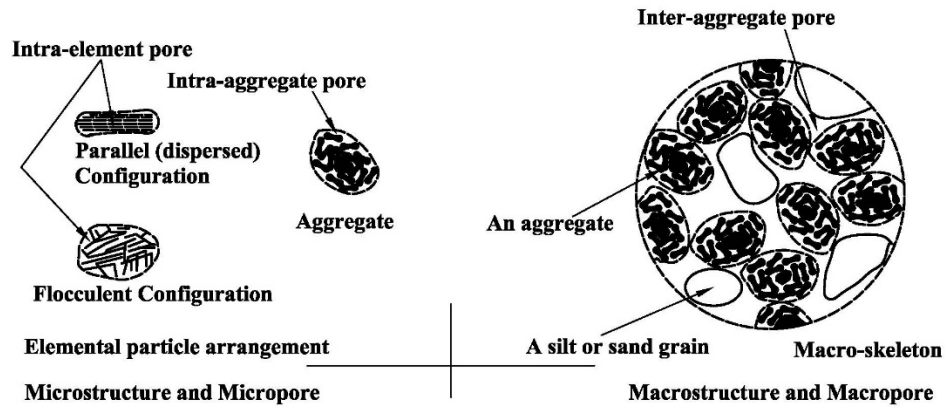


Figure 2-4 Double structure model (Wang and Wei, 2015).

Massin and Khalili (2016), Massin (2017), and Qiao et al. (2019) considered two structure levels, micro, and macro, as presented in Figure 2-6. Clay particle cluster is regarded as a primary component of the two structure levels. In their model, a clay layer consists of a tetrahedral–octahedral–tetrahedral (TOT) clay crystal that stacks to form a clay particle with about four layers of crystalline water, which is tightly bound within the structure of the clay particle in the interlayer space. The particle face is the side parallel to the clay layer, and diffuse double layers form around these particle faces. The equilibrium solution extends from the boundary of double-layer water, which is not very well defined. An assembly of clay particles is defined as clay aggregate. Clay aggregates combine to form a macrostructure, and voids between macrostructures are referred to as macrovoids. Several assumptions are usually made in predicting the mechanical response of such double-structure models. The aggregate response is considered elastic, and the aggregate is assumed to be fully saturated.

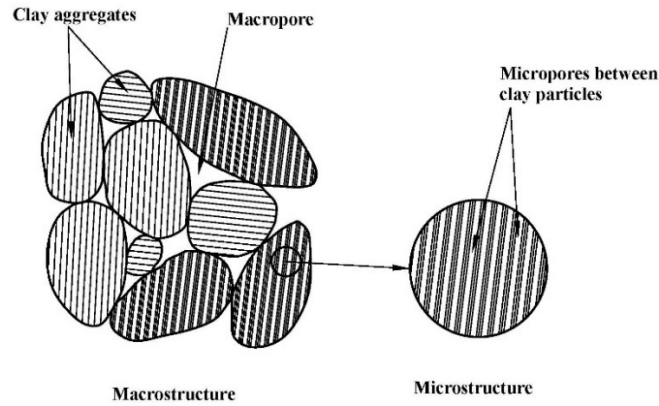


Figure 2-5 Dual-structure model; clay particles are represented by gray lines (Vilarrasa et al., 2015).

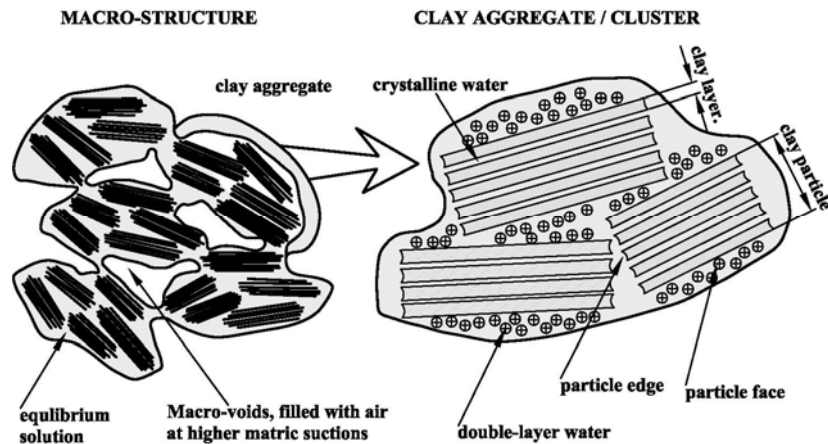


Figure 2-6 Two structure levels of compacted clay (Massin, 2017).

Kyokawa (2021) reported that the structure of an expansive unsaturated soil consists of clay minerals and non-expansive soil particles, as shown in Figure 2-7. They further highlighted that the expansive unsaturated soil is composed of soil skeleton at the macrostructure level having

water and air-filled pore voids, whereas the microstructure corresponds to nano-scale multilayered minerals with interlaminar space between the crystals.

Based on the above discussions, it can be inferred that all the existing studies for mechanical behavior account for partial consideration of the fabric and structure of clayey soils. All existing models assumed a dual structure of swelling clays at the micro and macro levels with corresponding pore spaces and ignored the clay fabric and interactions at the nano level. In fact, the microfabric is considered representative of both the micro and nano-level fabrics, which is not realistic. A recent study by Kyokawa (2021) extended the microfabric to interlaminar void at the nano level with several underlying assumptions, including full saturation of the interlaminar space and no consideration of the type of cation interaction between clay sheets.

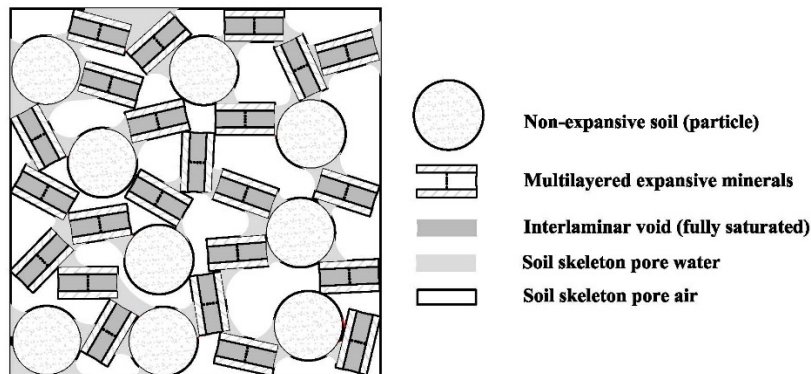


Figure 2-7 Schematic of an expansive unsaturated soil (Kyokawa, 2021).

2.2 Constitutive modeling of expansive soils

The existing constitutive models for swelling soils can be divided into two broad categories: macro-level models and molecular-level models. The macro-level constitutive models can be further divided into mechanical, hydromechanical, and hydro-mechano-chemical models. These models are generally based on the double structure of clays consisting of microstructure and macrostructure and do not consider the nano-level clay structure. In macro-level models, it remains a challenge to theoretically define the complex processes and interactions in swelling clays occurring at the atomistic level. Molecular-level modeling methods had been in the development phase in the late nineties and therefore, most of the early research on swelling clays at that period was performed at the macro-level.

It is also well established that the nano-level clay particles control the mechanical behavior of swelling soils (Katti et al., 2009; Tao et al., 2010; Hantal et al., 2014; Ahmed and Abduljawwad, 2017a; Thapa, 2020). The swelling mechanism presented by several authors, including Gouy (1910), Chapman (1913), Stern (1924), Ferrage et al. (2005), Laird (2006), Wayllace (2008), Rahromostaqim and Sahimi (2018) and Du et al. (2020) explained that the swelling of clays is mainly controlled at the nano-level. As the swelling-mechanical response of the swelling soils occurs simultaneously under given environmental and mechanical loading conditions, swelling mechanism in turn controls the mechanical behavior of swelling soils.

As the overall mechanical behavior of swelling soils is mainly governed by the processes and interactions at the molecular/nano level, the modelling of these soils should be performed at this level to ascertain their real behavior. However, if the clayey soil has an open structure fabric, the swelling may induce collapse under high confining stress, and macro-pore collapse will have a

significant contribution in controlling the overall mechanical behavior of swelling soils (Alonso et al., 1990). The key macro- and molecular-level models were discussed in subsequent sections of this chapter.

2.2.1 Macro-level constitutive models

Alonso et al. (1987) laid down a pathway for all recent models for expansive soils by presenting an integrated qualitative approach toward shear strength and a volumetric elastoplastic model. They qualitatively described the importance of the role of microfabrics in understanding the mechanical behavior of unsaturated soils. Three (03) state variables, that is, the net mean stress ($p = \sigma - u_a$), suction ($s = u_a - u_w$) and specific volume ($v = 1 + e$), were used to describe the isotropic state and the fourth stress variable [$q = (\sigma_1 - \sigma_3)/2$] was added to incorporate the effect of triaxial stress. Loading-Collapse (LC) and Suction-Increase (SI) yield curves were introduced to predict the irreversible volumetric strains for a given stress path in p - s space. A three-dimensional view of the yield surfaces is shown in Figure 2-8. In this model, the area bounded by both LC and SI yield surfaces represents the elastic zone. These yield surfaces were shifted based on a single hardening parameter controlled by plastic strains. The effect of shear stresses was introduced in the model by extension of the yield surface in three-dimensional p - q - s space using the concepts of the modified Cam-clay model for saturated soils. They argued that both the shear strength and stiffness of soil increase as the soil moves from a saturated to an unsaturated state.

The mathematical model for describing the stress-strain behavior of slightly expansive soils was developed by Alonso et al. (1990) and named the Barcelona Basic Model (BBM). Mathematical formulations were presented by defining elastic strains, yield surfaces, flow rule, and hardening law. Model predictions were made to predict the response of the model to shear stress at different

suctions using reference soil and stress-strain relationships computed for three different suction values of 0.10 MPa, 0.20 MPa, and 0.30 MPa shown in Figure 2-9. These curves demonstrate an increase in strength and stiffness with suction, presented in Figure 2-9a and Figure 2-9b, respectively. Responses of the partially saturated soils successfully explained by BBM were the increase in apparent pre-consolidation stress, stiffness, and shear strength with suction, reversible swelling strains at low confining stresses, and irreversible collapse strains at high confining stresses during wetting. No hydraulic hysteresis was the main assumption made in BBM.

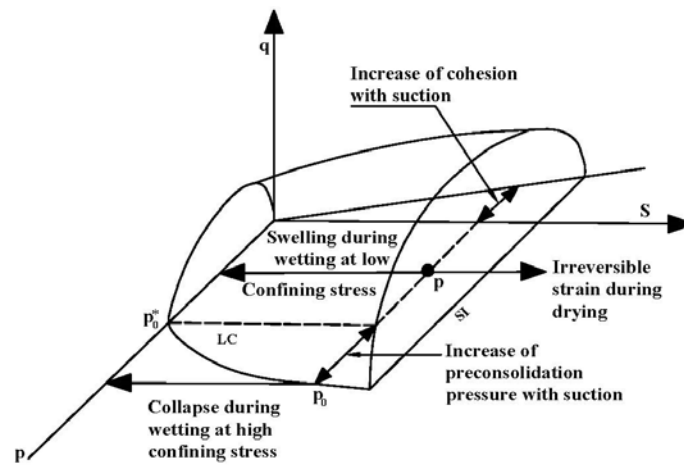


Figure 2-8 Three-dimensional view of BBM in (p , q , s) space (Alonso et al., 1999).

BBM was only applicable to non-expansive or slightly expansive and non-cemented partially saturated soils (sands, silts, and clays of low plasticity). BBM was extended to a more advanced model, Barcelona Expansive Model (BExM), by Gens and Alonso (1992), to understand the mechanical behavior of compacted expansive clays in sealing systems. It also covers the limitations of BBM to model plastic strain accumulation during suction cycles, a secondary swelling, and large irreversible swelling strains.

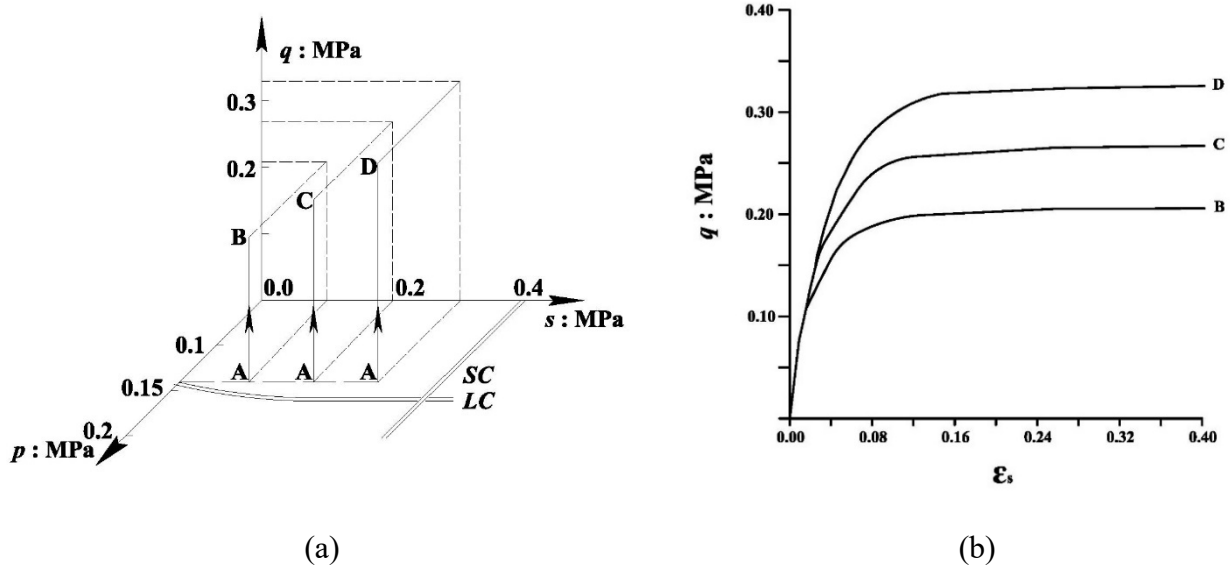


Figure 2-9 (a) Response of model to shear tests at different suctions, (b) Shear stress-shear strain plots showing an increase in stiffness with suction (Alonso et al., 1990).

The extended model, BExM, considered that the behavior of unsaturated soils is governed by the particle level interactions at two distinct levels of soil structure. Therefore, microstructure and macrostructure levels were introduced. They considered three levels of deformations: one at the microstructure level controlled by physio-chemical interactions, the second at the macrostructure level due to loading and collapse, and the third at the coupling between these two levels. BBM described the behavior at the macrostructure level. However, the extension of the model was carried out to explain strains at the other two levels. To explain strains at the microstructure level, they assumed that the deformations at this level are reversible and are not affected by the strains at the macrostructure level. This assumption leads to the development of the neutral line (NL) in p - s space over which the sum of suction and net stress ($p + s$) remains constant. Stress path movement towards the right of this line (suction and stress increase) results in compression, whereas the reverse causes swelling. Microstructure deformation results in macrostructure plastic strains depending upon the increase or decrease in void ratio under swelling or shrinkage stress

paths, respectively. These macrostructure plastic deformations, in turn, cause strain-hardening if LC expands or strain-softening if LC contracts. It was also concluded that the macrostructure plastic strains depend on the ratio of p over p_0 where p is the applied stress and p_0 is the apparent pre-consolidation stress. A decrease in p/p_0 represents a dense over-consolidated structure.

The mathematical form of the conceptual framework presented by Gens and Alonso (1992) was given by Alonso et al. (1999). They introduced two additional yield loci parallel to the neutral line (NL) in the p - s plane, one by a suction increase (SI) and the other by a suction decrease (SD). Both SI and SD represent the onset of macrostructure plastic deformations due to microstructural shrinkage and swelling and are linked to LC through coupling functions f_D and f_i (Figure 2-10). The coupling function, f_D , shows a decreasing trend with respect to p/p_0 , whereas the trend of f_i shows the opposite. With higher values of f_D , more is the microstructural swelling and, hence, it causes strain-softening in macrostructure.

BExM has several limitations, including the permanent saturation of the microfabric. However, inter-platelet voids may also remain unsaturated, particularly at high suction values. The assumption of only elastic strains at the microstructure level is not realistic due to the possible split of particles during swelling (Pinyol et al., 2007). Other limitations include no consideration of time-dependent effects and irreversible change in the degree of saturation during wetting-drying cycles. Another challenge with BExM is the determination of the micro parameters and coupling functions experimentally which requires the performance of complicated tests in saturated and unsaturated conditions, including swelling pressure tests, oedometer loading-unloading tests performed at constant suction and cyclic controlled-suction tests at different vertical stress values. Based on the results from these tests, κ_m is derived from the final suction cycle, followed by elastic and plastic deformations for each suction cycle. The interaction functions are then derived by

plotting the plastic strain ratio to microstructural strain against p/p_0 . The suction and stress cycles in these experiments should ideally be very small (Alonso et al., 2005). This, however, results in exceedingly large time for execution of these tests for high plastic swelling soils and limits the use of this model in engineering practice.

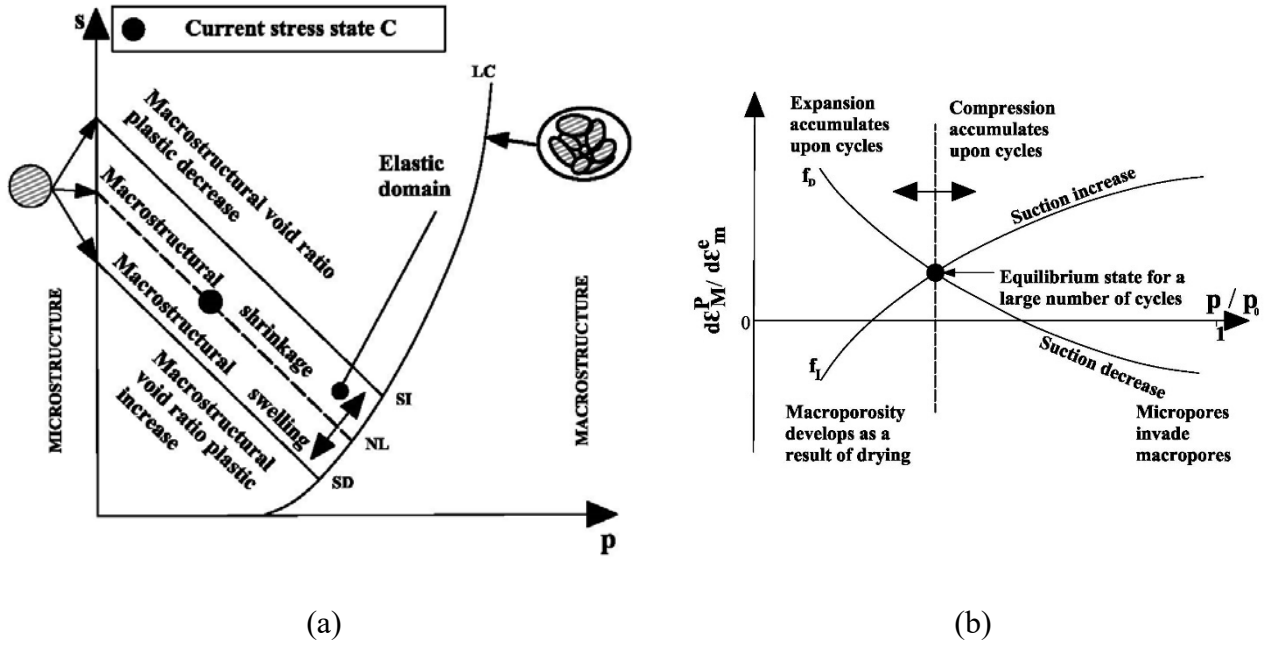


Figure 2-10 (a) BExM yield surface in the p - s plane, (b) Particle level interactions and coupling functions (Alonso et al., 1999).

A double structure model was later presented by Sanchez et al. (2005) and could be considered an extension of BExM. The model was based on generalized and classic plasticity theories. The mechanical law was formulated based on the elastoplastic model at the macrostructural level, the elastic model at the microstructure level, and the plastic model at the coupling between these two levels. Equations were derived for the above-described elastoplastic and elastic models at the macro and micro levels, respectively. As a result of the coupling interaction between the two levels, the macrostructure plastic strains were defined using two coupling functions: f_c for the

microstructural contraction (MC) path and f_s for the microstructure swelling (MS) path. The functions f_c and f_s have a similar trend as the functions f_i and f_D in BExM. Macrostructure softening results along the MS path, and macrostructure hardening along the MC path. Although the model well describes the volumetric deformations/strains due to changes in suction and stress, it does not predict changes in shear strength or stiffness of the swelling soils.

Another development in constitutive modeling was the work by Pinyol et al. (2007), who modeled the behavior of clayey rock composed of a clay matrix and a bonding network between the clay aggregates. They reported that the loading-unloading cycles on such rocks under stress and environmental changes result in swelling, material degradation, and progressive loss of material stiffness during cyclic loads. They further added that two constitutive laws, one for matrix material and the other for bonding between clay matrices, can be combined to describe the behavior of clayey rocks such as claystone. They used BBM (Gens and Alonso, 1992) and BExM (Alonso et al., 1999) to describe the matrix behavior at the macro and microlevels. Cementation/bond behavior was explained using an isotropic damage model for bond material. Bond-behavior was assumed elastic in an undamaged state. Bond deformation parameter (χ), bond concentration (C_b), damage rate (r_1), and damage variable (L) were defined to determine the degradation of bond stiffness due to a given strain energy. Smaller values of χ represent damaged material and transfer of stresses from the bond to matrix material. The bonding deformation parameter (χ) and bond concentration (C_b) also control the stress-strain response of such composite materials. Figure 2-11a shows that adequate bonding increases the deviatoric stress and the initial modulus. However, bond concentration significantly changes the peak strength without many variations in the initial modulus (Figure 2-11b). This model successfully explains the effect of wetting and drying on the material strength and stiffness of soft clayey rocks.

Both BBM (Gens and Alonso, 1992) and BExM (Alonso et al., 1999) do not consider water retention behavior, and this limitation led to the development of a macroscopic hydromechanical model for expansive unsaturated soils by Sun and Sun (2011). The degree of saturation and void ratio were considered state parameters to explain expansive soils' mechanical and water retention behavior, respectively. Data of compression curves presented by Cui et al. (2002) show that the compression index increases with the increase in suction if the soils are non-expansive. However, the compression index of expansive soils decreases, and the initial yield stress increases with the increase in suction. The elastoplastic model by Sun and Sun (2011) is based on the above-explained behavior of expansive soils and the existing hydromechanical model for non-expansive soils reported by Sun et al. (2007). Their constitutive model is composed of two surfaces, i.e., the initial yield curve (IYC) and equivalent void ratio curve (EVRC) on p' - s plane. Any stress state below IYC represents an elastic state, whereas the elastoplastic stress state lies above IYC. Predictions of shear tests by the proposed model under constant suction values are shown in Figure 2-12. It can be seen from this figure that both shear strength and stiffness increase with the increase in suction. One of the major assumptions of the model is the consideration that pore air pressure and pore water pressure are continuous throughout the soil mass, which is not a realistic assumption for expansive soils.

Wang and Wei (2015) developed a cyclic volume change model for compacted expansive soils under wetting-drying cycles. The basic model by Alonso et al. (1990) named BBM is combined with swelling-shrinkage strain components derived from experimental observations by the authors to develop this double structure model. This model divides the swelling-shrinkage strain components into two reversible and irreversible components. The reversible component mainly depends on the current suction value and follows the path of cyclic suction. It leads to compression

during drying and swelling during wetting. The irreversible component occurs at early wetting-drying cycles and could be swelling or compression depending on the difference in the soil macrostructure between the initial and equilibrium state. They used soaked and dried tests and cyclic suction-controlled tests to validate their model.

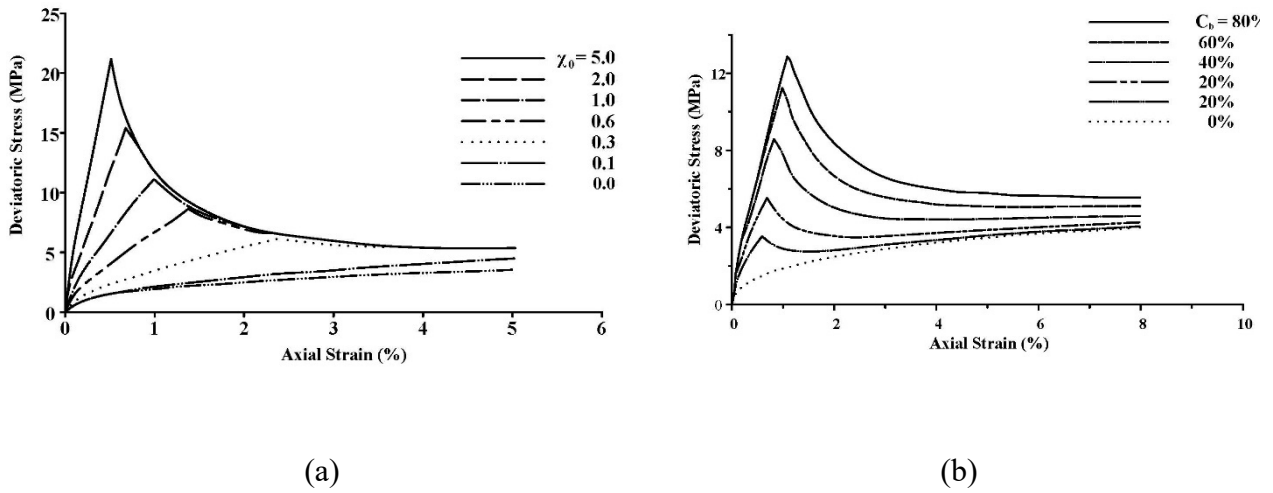


Figure 2-11 Triaxial behavior of bonded material (a) Effect of bonding deformation parameter (χ), (b) Effect of bond concentration (Pinyol et al., 2007).

Vilarrasa et al. (2015) developed a dual structure constitutive model for compacted expansive clays and implemented their model into the TOUGH2 (multiphase non-isothermal finite element code) and FLAC3D (Geomechanics finite difference code) simulator. They used the Barcelona Basic Model (BBM) for macrostructure behavior. They extended the double structure Barcelona Expansive Model (BExM) by Alonso et al. (1999) and Sanchez et al. (2005) for microstructure behavior along with the coupling functions. In addition to describing the well-explained patterns of the mechanical behavior of unsaturated soils by BBM and BExM, their model also predicts the accumulation of plastic strains due to wetting-drying cycles. It also shows that microstructural

swelling reduces the permeability of expansive soils due to the invasion of macrostructure by microstructure. The model is good at explaining the thermo-hydro-mechanical behavior of clays and their long-term performance as engineered barrier systems.

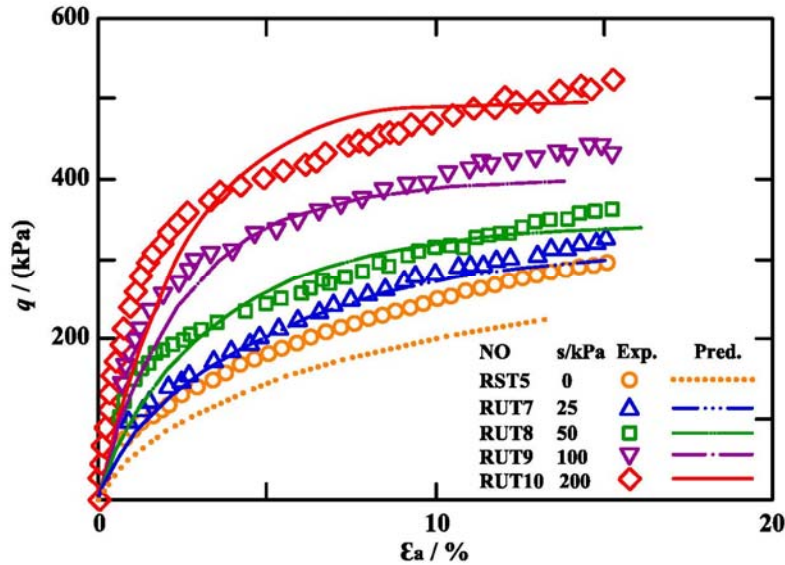


Figure 2-12 Comparison of triaxial shear tests and model predictions (Sun and Sun, 2011).

Chen et al. (2017) introduced a strain-hardening constitutive model to describe the stress-strain response of bentonite in the nuclear waste repository. The development of their model is based on three (03) stages of the failure mechanism of bentonite in uniaxial and triaxial tests, namely the compressive stage, the developing stage, and the crack-growing stage. They reasoned that the elastic-perfectly plastic Mohr-Coulomb model could not be used for bentonite as it does not incorporate the strain hardening of bentonite specimens tested under high confining pressure (Figure 2-13). Using experimental data, they established a relationship between plastic shear strain, confining pressure, and shear strength. The strain hardening model was then formulated using an

exponential increase of cohesion and angle of internal friction with plastic shear strains (Figure 2-14). Although the model is very simplistic in explaining the stress-strain response of bentonite under loading, it has several limitations, including the model's applicability to strain hardening phenomenon of one specific type of material (bentonite) and the assumption of the isotropic nature of bentonite in material properties and plastic hardening characteristics. Furthermore, the model does not incorporate the changes in strength due to suction cycles.

A recent development in the hydromechanical models for compacted bentonites was made by Qiao et al. (2019) through a double structure model named the STJ-DS model. It extends the double structure framework presented by Qiao et al. (2017). The model is the first of its kind where elastoplastic strains are considered at the microstructure level, and micropores are considered unsaturated. They explained that swelling of bentonites is controlled through five different processes, which are (i) crystalline swelling, (ii) DDL swelling, (iii) split of particles, (iv) capillary swelling, and (v) swelling due to unloading. The first three processes occur at the microstructure level, and the other two at the macrostructure level. However, all these processes are inter-linked and affect each other.

In this hydro-mechanical model, four levels were defined for the coupled framework of expansive soils (Figure 2-15), similar to the framework proposed by Massin (2013). They described that the deformations at the micro- and macro-structure levels are elastoplastic in nature. The overall stress-strain response of compacted expansive clays is basically the addition of stress-strain response at the micro and macro-structure scales. Similarly, the Adsorptive Water Retention Curve (AWRC) at the microstructure level and Capillary Water Retention Curve (CWRC) at the macrostructure level combine to create an overall water retention behavior of expansive clays. Therefore, mechanical and hydraulic models were formulated independently at the macrostructure

and microstructure levels. Hydromechanical coupling was achieved at each structure level through an independent water retention model and effective stress formulation. The overall material response was obtained using a coupling parameter (ζ) between the macrostructure and microstructure. To validate their formulations, the authors also compared the model simulations with swelling tests on FEBEX bentonite under constant vertical stress and constant volume.

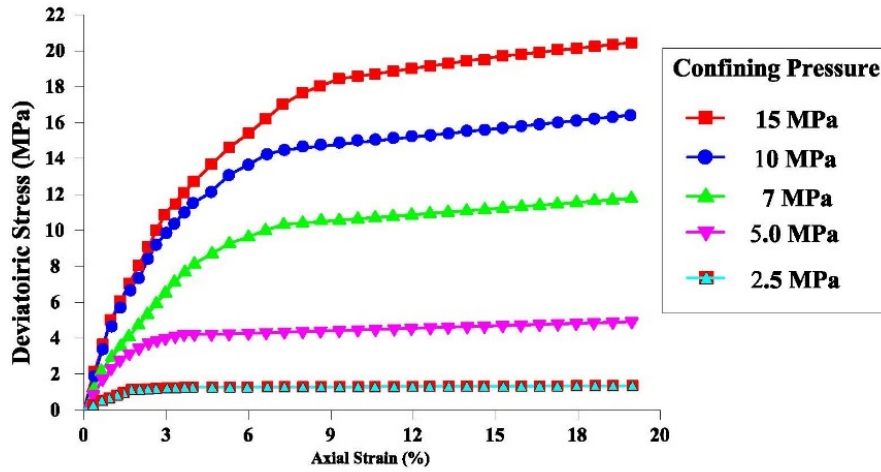
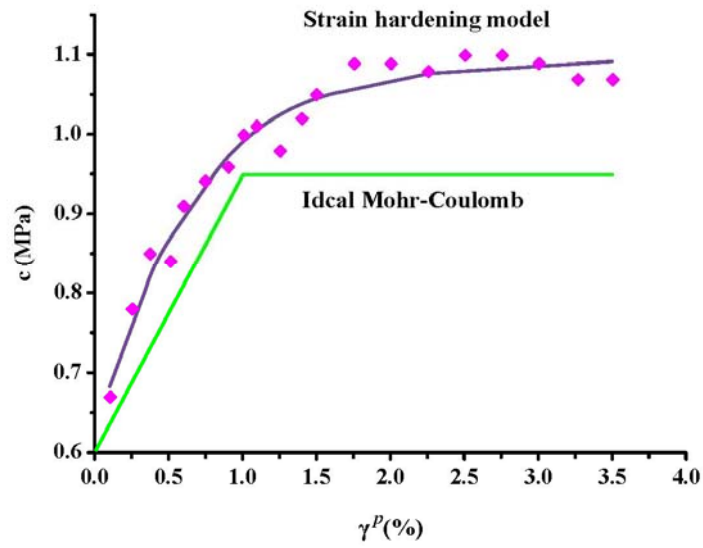
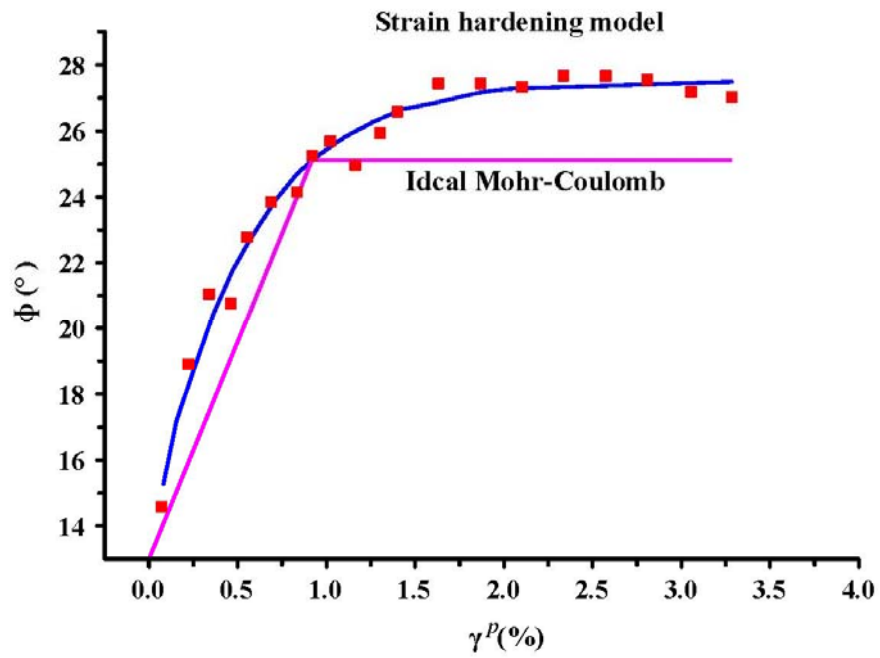


Figure 2-13 Stress-strain curves for bentonite specimens (Chen et al., 2017).

Among the most recent works on constitutive models of expansive clays is the hydro-mechano-chemical (HMC) model by Kyokawa (2021), which is based on the framework of the double structure model by Kyokawa et al. (2020). The double structure model by Kyokawa et al. (2020) constitutes the macrostructure soil skeleton and nano-scale interlaminar behavior of expansive clays in a fully saturated state. The HMC model, however, applies to expansive clays in an unsaturated state. The behavior at the macrostructure level is described by the Cam Clay model using the degree of saturation as an effective stress parameter through Bishop's effective stress. Two state parameters, Ψ and ρ , represent the effect of the degree of saturation on the soil skeleton void ratio. The interlaminar behavior is described through the interlaminar equilibrium of forces.



(a)



(b)

Figure 2-14 Strain hardening model (a) Cohesion with plastic strain, (b) Angle of internal friction with plastic strain (Chen et al., 2017).

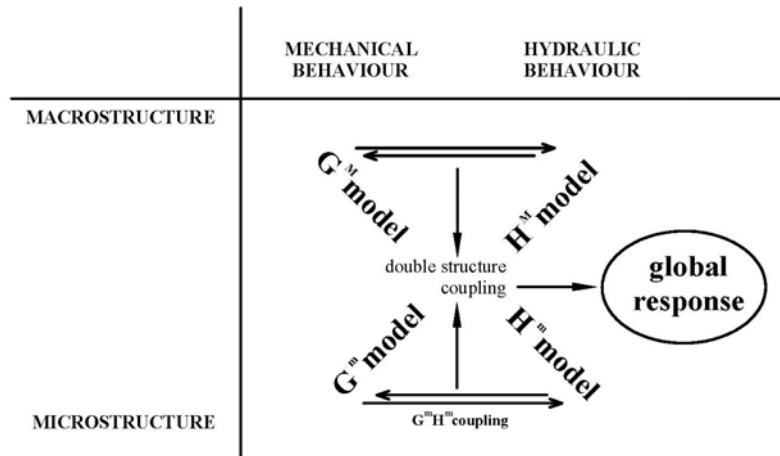


Figure 2-15 Schematic of Double-structure model (Qiao et al., 2019).

The mechanism of volume change due to wetting in the HMC model is described by the schematic diagram shown in Figure 2-16. As a result of the decrease in suction due to wetting, the soil skeleton (macrostructure) undergoes elastic swelling due to the reduction of effective stress and/or irreversible strains due to hydraulic collapse. At the interlaminar level, crystalline and osmotic swelling occur due to the hydration process. The net result of these hydro-mechano-chemical processes at both structure levels is the swelling of expansive clays. The model is also validated through a series of swelling pressure and oedometer tests at different suction levels. Despite being a nano-level constitutive model, the HMC model does not consider the effect of layer charge, type of cations in the interlayer, and type of liquid adsorbed at clay surfaces. Moreover, the interlaminar space is considered fully saturated, which is not true for high suction values. Also, the relationship between the degree of saturation and the effective stress parameter is linear, which is not valid for expansive unsaturated soils. Furthermore, the model is still required to be extended for hydraulic hysteresis. The HMC model does not provide the variation of strength and stiffness during

swelling. The mechanical model is only limited to estimating elastoplastic strains under mechanical and hydraulic loadings.

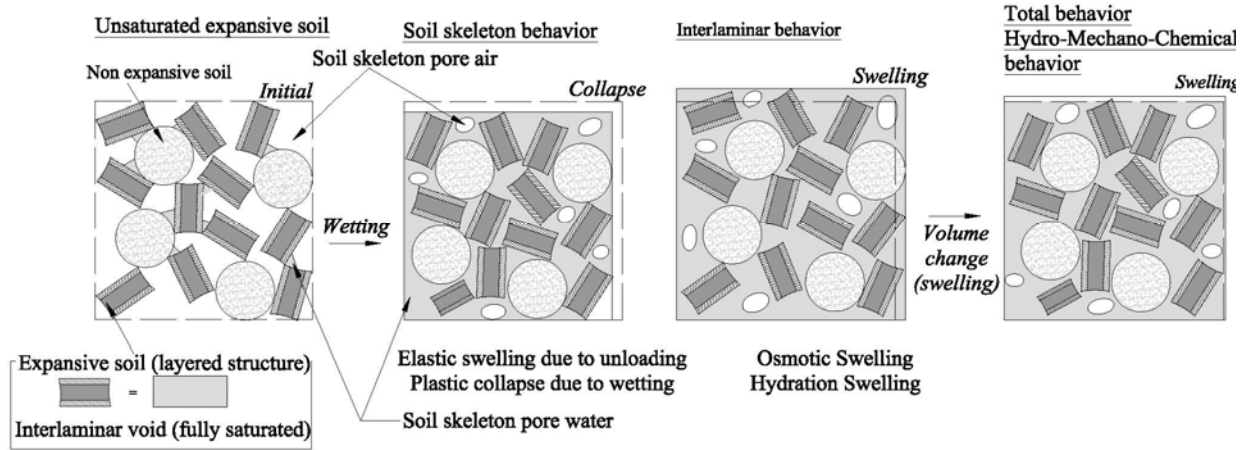


Figure 2-16 Mechanism of swelling behavior due to wetting (Kyokawa, 2021).

2.2.2 Molecular-level constitutive models

Skipper et al. (1995a, 1995b) performed Monte Carlo (MC) simulations on monolayer hydrates of clay minerals, dioctahedral montmorillonite and trioctahedral vermiculite. The types of interactions occurring in swelling clays consist of interaction between components of the clay-water system (i.e., water, cations and clay) and also between the molecules of individual components, i.e., water-water, clay-clay and cation-cation. In MC simulations, potential functions are used to describe interactions between molecules. They adopted MCY and TIP4P potential functions for water-water interactions. MCY considers Coulomb interactions, van der Waals attractions and electron overlap repulsions, whereas TIP4P describes these intermolecular interactions through parameters developed by fitting experimental data. This study focused on describing the effect of selected potential functions on such interactions. They also defined the intermolecular potential functions to illustrate interactions among water-sodium and water-

sodium-clay minerals and found good agreement with experimental observations. They used MONTE (Skipper, 1992) computer program for MC simulations of by selecting an isothermal-isobaric ensemble and a simulation cell of the size of about eight-unit cells (i.e., 21.12 Å x 18.28 Å). In the simulation process, macroscopic behavior was incorporated by adopting periodic boundary conditions and imposing a cut-off of 9 Å for short-range contributions of potential energy and the Ewald sum method for long-range Coulomb interaction energy. The comparison of their MC simulations with the experimental results revealed that the MCY model potential functions give closer results of average potential energy, layer spacing, and molecular structure for Wyoming-type montmorillonite and vermiculite. The study further concluded that the amount and distribution of layer charge in the clay sheets significantly affect the orientation of water molecules in the interlayer. Their study, however, is applicable to single clay crystallites and does not incorporate the complex fabric of natural and compacted expansive soils.

Karaborni et al. (1996) were among the first researchers who used the Monte Carlo technique and molecular dynamics (MD) to perform molecular-level simulations of sodium montmorillonite to understand the swelling mechanism of clays. Their model of clay-water-cations was similar to the one proposed by Skipper et al. (1995a, 1995b). Their simulations were based on surface force apparatus where the pressure is measured as a function of the fixed separation upon water intake. The distance between the two clay layers was fixed, and the system was allowed to take water molecules until equilibrium was reached. The process was repeated for an incremental increase in the interlayer distance until a relationship was obtained for the swelling of sodium montmorillonite. In this study, a rigid clay layer structure was employed, which was a limitation and was later covered by other studies (Katti et al., 2005) by adopting flexible clay layers. Molecular-level simulations were performed in a grand canonical ensemble. They defined two

states of sodium montmorillonite as stable and unstable states. In the stable state, water molecules were either locked in the hexagonal hole of clay, forming a strong bond between hydroxyl protons of clay and water oxygens, or a hydrogen bond existed between clay oxygens and water protons without any locked-in water molecules. Unstable states are the ones where the stable state configurations occur simultaneously and are the main reason for excessive non-uniform swelling of sodium montmorillonite. The simulation results showed that stable states are found at basal spacings of 9.7, 12.0, 15.5, and 18.3 Angstroms, demonstrating that the swelling occurs at a specific hydration sequence of sodium montmorillonite corresponding to unstable states.

As stated above that Karaborni et al. (1996) used rigid clay layer structure in the simulations. The use of constrained/rigid lattice saves substantial amounts of computer time by excluding degree of freedom due to the movement of atoms. In fact, almost all the studies on clay simulations adopted rigid clay lattice until a general force field was developed by Cygan et al. (2004) and they named it CLAYFF. A single point charge (SPC) water model was adopted in CLAYFF for water, oxygen and hydroxyl interactions. The total potential energy was taken as the addition of nonbonded (i.e., electrostatic and van der Waals) and bonded interactions (i.e., bond angle and bond stretch). Partial charges model was used for electrostatic interactions and van der Waals interactions were represented by Lennard-Jones parameters. To ensure full flexibility of the system, bonded interactions were introduced in the form of bond angle and bond stretch. Other salient features of CLAYFF include the assignment of modified charges to nearby oxygen atoms to avoid local charge imbalance during isomorphic substitution and inclusion of an angle bend term for describing hydroxyl groups. Molecular dynamics (MD) simulations with CLAYFF were performed using Open Force Field (OFF) module within the Cerius molecular modeling interface. The force field was applied to several classes of hydroxide (portlandite), oxyhydroxide (Boehmite)

and clay phases (Kaolinite, Pyrophyllite, Montmorillonite and Hydrotalcite) and successfully simulated the structures, surfaces and interfaces of clays and other inorganic materials.

Katti et al. (2005) performed steered molecular dynamics simulations on dry pyrophyllite to determine the stress-strain response of clay layers under applied forces. Pyrophyllite has a tetrahedral-octahedral-tetrahedral (TOT) structure and the bonding between clay layers is through van der Waals forces. Dry pyrophyllite was used to study the interactions of clay minerals only. They used NAMD software to run MD simulations at atmospheric pressure and room temperature by selecting $21.12\text{\AA} \times 18.28\text{\AA}$ clay layer size with an initial basal spacing of $10\text{\AA}$ and interlayer spacing of $3.44\text{\AA}$. The major part of their work is transforming the consistent force field (CFF) parameters by Teppen et al. (1997) to the CHARMM force field in NAMD software. After model construction and force field parameters selection, stress was applied on clay surfaces in the range of 0.0 to 1.65 GPa. The resulting strains in interlayer spacing and clay layers were recorded. The simulation results revealed that there is a linear relationship between stress and interlayer strain, and predominant deformation occurs in interlayer spacing. Based on the stress-strain relationship (Figure 2-17), the modulus values for two and three clay layers models were found to be 54.56 GPa and 45.26 GPa, respectively. The results also show a decreasing trend of modulus value with the increase in interlayer spacing. The proposed model by the authors uses dry pyrophyllite and, therefore, does not represent the interaction of clay with water and cations. However, the model provides a good way forward to apply the methodology used in determining the stress-strain response of other expansive clay minerals.

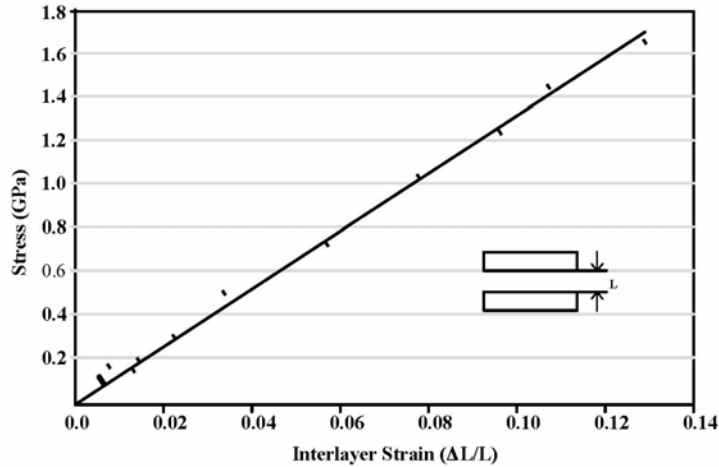


Figure 2-17 Stress-strain plot for clay interlayer (Katti et al., 2005).

Wang et al. (2007) studied the stress-strain response of different rock and clay minerals using MD simulations. In this study, a range of interatomic potentials was selected from past studies, which were appropriate for the chosen rock (quartz, albite, and calcite) and clay (montmorillonite, kaolinite, and palygorskite) minerals. For quartz and albite, interaction functions consisted of Coulomb (attractive or repulsive), short range repulsion, van Der Waals and Morse terms, whereas Coulomb attractions and short-range repulsions were considered for calcite. The potential functions used by Manevitch et al. (2004) were adopted for clays. The functions comprised of Coulomb attractions, van Der Waals, bond stretch potential and angle bending potential. Simulations were carried out on the program called TINKER, which was developed by Ponder. Molecular-level simulations were performed in the NPT (constant number of particles N , pressure P , and temperature T) ensemble. The model was subjected to uniaxial pressures, and the resulting strains were measured. Stress-strain curves were then generated from the model response to applied stresses (Figure 2-18), and all minerals showed non-linear behavior. Calcite showed the

lowest modulus, whereas kaolinite modulus value was even higher than quartz which is attributed to the relatively stable molecular structure of kaolinite. The modulus value of kaolinite was found to be 167 GPa against the published value of 192 GPa by Manevitch et al. (2004), showing a relatively good agreement. The model, however, has several limitations, including no consideration of clay-water interaction and the use of single clay crystallite in establishing the macroscopic stress-strain behavior of expansive clays.

Katti et al. (2009) adopted numerical and experimental approaches to understand sodium montmorillonite's swelling and mechanical behavior at a molecular level. This study examined the effect of swelling pressure on the microstructure of clay particles through the swelling pressure tests conducted in a specially designed swelling device. The experimental observations showed that the swelling of clay particles breaks down clay particles into smaller subdivisions and changes the orientation of clay particles as well. For the first time in literature, Discrete Element Method (DEM) simulations using ANSII C++ coding were used to investigate the effect of particle subdivision on the swelling properties of clays (Katti et al., 2009). The simulation results showed an increase in swelling with the increase in the number of subdivisions, the orientation of near-surface particles parallel to the surface, and the random orientation of particles in the inner zone.

In clays, two types of interactions occur: one between clay particles (double layer, van der Waal forces and Born's repulsion), and the second within the clay particles when they interact with each other (namely, van der Waals force, electrostatic force and hydrogen bond). The numerical method based on Molecular dynamics (MD) was adopted to simulate these clay interactions in this study.

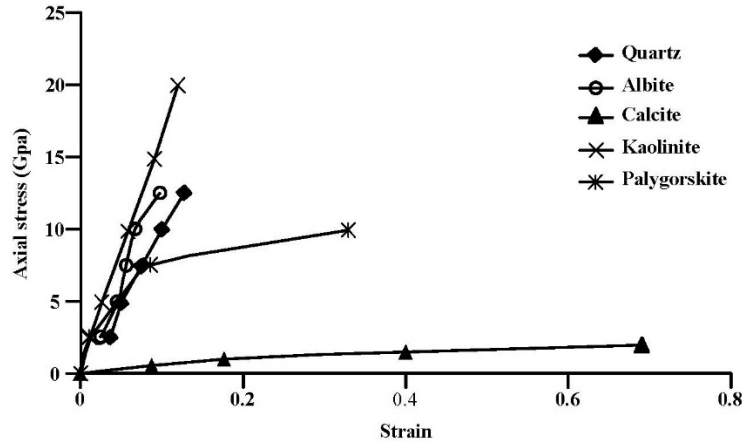


Figure 2-18 Stress-strain curves for rock and clay minerals (Wang et al., 2007).

Katti et al. (2009) performed molecular dynamics using the CHARMM force field in NAMD software to study changes in the stress-strain response of hydrated clays due to the breakdown of particles. A linear relationship between stress and interlayer strain was observed for dry sodium montmorillonite and for one layer of water. However, the relationship is non-linear for two and three layers of water in the interlayer (Figure 2-19). The main conclusion of their study was that the strain in the expansive clays is due to the deformation of interlayer water molecules and the distance between clay sheets and interlayer water.

Tao et al. (2010) investigated the effect of cations valence on the behavior of K^+ , Na^+ , and Ca^{+2} montmorillonites. Molecular dynamic simulations were performed using the LAMMPS package and CLAYFF force field, whereas SPC (single point charge) model is used for water behavior. CLAYFF force field has been found to yield good results at clay-water interfaces. Simulations were performed using three water contents corresponding to 64, 128, and 224 water molecules for all three selected clays. The study of the interaction between interlayer cations and water showed

that the cation-oxygens are densely packed in the hydration shell around the Na^+ and Ca^{+2} as compared to K^+ . It also suggests that Na^+ and Ca^{+2} have strong hydration energy as compared to K^+ . Clay oxygen atoms interact with interlayer cations predominantly through electrostatic and van der Waals potentials. A strong interaction exists between clay oxygen atoms and interlayer cations in the case of dehydrated clay and this interaction becomes relatively weaker due to the hydration of cations in hydrated clays. The simulation results also indicated that Ca-montmorillonite displays smaller basal spacing than K-montmorillonite, which exhibits smaller interlayer space than Na-montmorillonite. As a result, Na-montmorillonite has a more open structure and experiences more swelling for a given water content as compared to others. The authors also concluded that the swelling also depends on the hydration energy of the interlayer cations. The higher the hydration energy of the interlayer cation, the greater this difference is. Simulation results were also confirmed through previous experimental data and literature values.

Hantal et al. (2014) determined the elastic and failure properties of Illite using clay force field (CLAYFF) and reactive force field (ReaxFF). The pyrophyllite structure was used as the starting configuration for Illite. Isomorphic substitutions were then carried out in the top and bottom tetrahedral layers by replacing Si^{+4} with Al^{+3} and Al^{+3} with Mg^{+2} . Potassium ions were used as cations in the clay interlayer to balance negative charges produced by isomorphic substitution. The complex processes of chemical reactions were simulated through ReaxFF using parameter-set developed by Pitman and Van Duin (2012). This parameter-set covers a series of chemical reactions involving compounds of silicon and aluminium. MD simulations were performed at constant temperature and volume with the LAMMPS program. Deformations were applied, and the resulting stress was calculated for each deformation step. The elastic properties of Illite were determined using a numerical method in ReaxFF and analytical derivatives of intermolecular

interactions in CLAYFF. The macroscopic elastic modulus of Illite was obtained using the Voigt-Reuss-Hill (VRH) approximation. It was observed that ReaxFF generally yields smaller values of moduli than CLAYFF. The shear modulus value of Illite in ReaxFF and CLAYFF was 18 GPa and 35.17 GPa, respectively. Clays are usually considered transversely isotropic (TI) materials, and both force fields were checked to provide a reliable description of Illite as transversely isotropic (TI) material. The criteria used were similarity of elasticity tensors, deviation of elasticity tensors from ideal TI material, and fracture toughness. Based on these criteria, CLAYFF reasonably provides a good approximation of the elastic properties of Illite. A typical stress-strain curve obtained using CLAYFF is shown in Figure 2-20.

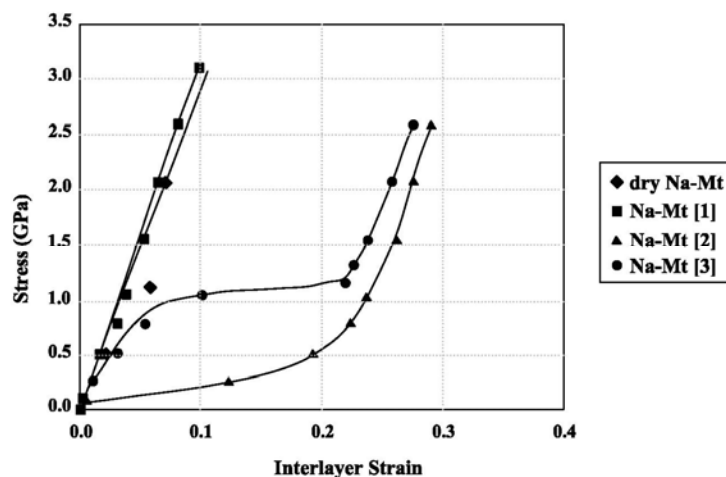


Figure 2-19 Stress-strain plot for clay interlayer for various levels of hydration (Katti et al. 2009).

Katti et al. (2015) presented the molecular dynamics approach to study the effect of hydration and the associated swelling mechanism of initially dry and partially hydrated sodium montmorillonite (Na-MMT) by constructing a solvation/water box around the clay particles. The authors used the CHARMM force field in NAMD software using the transformed parameters of the consistent force

field (CFF) by Teppen et al. (1997). Molecular-level simulations were performed in the NPT (constant number of particles N , pressure P , and temperature T) ensemble. The structure of pyrophyllite was used as the starting configuration of montmorillonite. Isomorphic substitutions were then performed by replacing Al^{+3} with Mg^{+2} and Fe^{+3} . Interaction energies were monitored during the simulations to evaluate interactions between different components of the clay-water-cation system. The Na-MMT sheets have a net negative charge, and sodium cations were introduced in the clay interlayer to balance negative charges. The van der Waals attraction between cations and clay sheets holds the clay sheets together (Cornelis and Dutrow, 2007). The solvation model was constructed by making a water box around dry Na-montmorillonite and slightly hydrated Na-montmorillonite with varying interlayer water contents ranging from 0% to 14.38%. Results of MD simulations for initially dry clay inside the solvation box showed the collapse of the clay interlayer. There was no change in basal spacing, which indicates that no swelling occurs. However, water molecules were observed to form a cluster around the clay sheets. The reason for the absence of swelling in initially dry Na-montmorillonite was observed to be the strong attraction between Na-ions and clay sheets which reduces the effective space between clay sheets and prevents water molecules' interaction with clay and Na-ions. In contrast, initially, hydrated models show the flow of water molecules into the interlayer of clay sheets, increasing the basal spacing and swelling of clay minerals. Their study reveals that the initial hydration of clays is essential to cause swelling, which is generally the case of natural clays.

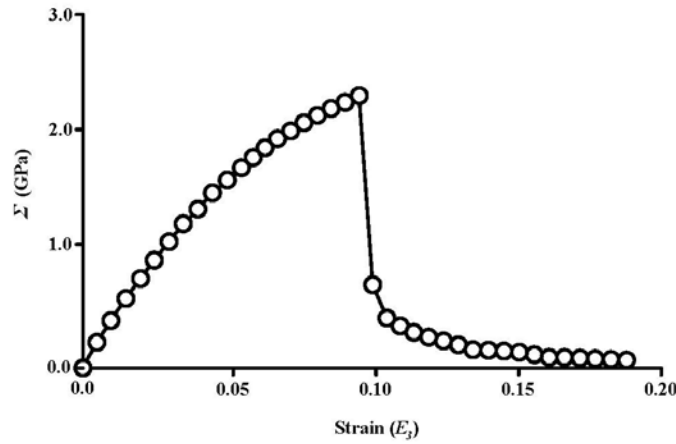


Figure 2-20 Stress-strain curve using ClayFF (Hantal et al., 2014).

Sun et al. (2015) used molecular dynamics as a tool for swelling pressure simulations. The modelling was performed with the CLAYFF force field in the Gromacs simulation package. The clay structure comprising of two layers of sodium montmorillonite was adopted for simulations using a spring model. The restraining force of the spring was assumed to be equal to the swelling pressure. The simulations were performed for different spring constants representing the range of density conditions of clay, and swelling pressure was found to increase exponentially with the increase in dry density. The predictions of swelling pressure from the simulations were exceedingly higher than the experimental observations. The authors relate this discrepancy to the simplification of the adopted clay-water system with no consideration of the complex structure and composition of natural swelling clays. Also, the proper spring constant of the molecular structure is hard to determine (Du et al., 2021).

Ahmed and Abduljawwad (2017a) were the first to present a comprehensive nano-level constitutive model to predict the swelling behavior of natural and compacted clayey soils. They named it the

universal nanoscopic constitutive model. Their model covers all possible clay fabric and structure variations due to possible variations in clay and non-clay particles, their interaction, cementations, degree of saturation, and overburden pressure.

Molecular-level modelling of the swelling behavior in the universal model was performed using molecular mechanics (MM), molecular dynamics (MD), and Monte Carlo (MC) techniques in Material Studio. The simulations modeled all possible variations in soil constituents, interlayer cations and anions, cementation salts, cation exchange capacity (CEC), density, and moisture conditions of expansive clayey soils. Molecular-level simulation results for the loose and compacted state of fabrics are shown in Figure 2-21.

Their volume change model considered the following three state parameters: (i) cohesive energy density, (ii) moisture content, and (iii) density. The cohesive energy density (CED) concept, which is the amount of energy needed to transition of 1 mol of material from the liquid to the gaseous phase, was adopted for the first time as a nano-level parameter to explain the swelling phenomenon at the molecular level. CED plots were generated against moisture content for all simulation cases, and a typical plot is shown in Figure 2-22a. The study reveals that the total CED increases with the increase in CEC and decrease in water content. Density, cementation, and bivalent cations also show a similar trend. However, the van der Waals CED reduces and becomes repulsive in nature with the same variation of the above parameters. They defined three zones with different volume change behaviors (Figure 2-22b) based on changes in CEC and other possible interactions with non-clay minerals and salts. They also formulated a complete mathematical model for swell and swell pressure predictions and validated it through corresponding tests on natural undisturbed and laboratory-controlled specimens. However, their model is limited to the swelling behavior of

swelling clayey soils only and cannot be adopted to predict the stress-strain response of swelling clayey soils.

Thapa (2020) studied the mechanical properties of swelling clays at a molecular level using the molecular dynamics (MD) approach. They evaluated the shear strength and stress-strain response of dry and hydrated sodium montmorillonite using various fluids of different polarities in the interlayer. A 4x2 Na-MMT model was developed to study the clay-water-cation interactions. In this study, the clay model has 6-unit cells in the x-direction and 3-unit cells in the y-direction. The individual clay sheets have a negative charge due to isomorphic substitution where nine (09) Al^{+3} cations are replaced with Mg^{+2} and another nine (09) with Fe^{+3} . Sodium cations were introduced in the clay interlayer to balance negative charges as a result of isomorphic substitution. Sodium montmorillonite and fluid models were developed using Material Studio and PSFGen of Visual Molecular Dynamics (VMD) software. The CHARMM force field in NAMD software was used to study the clay-fluid interaction. Constant-force steered molecular dynamics (SMD) simulations were carried out using an isothermal-isobaric ensemble (NPT) with 6 unit cells in the x-direction and 3 unit cells in the y-direction. Normal stresses were applied in the range of 0 to 8.88 GPa to measure strain in the direction of the normal force. After constant-force SMD simulations, constant-velocity SMD simulations were performed by applying shear force in the horizontal direction. Upon exposure to different fluids, it was observed that the interlayer spacing increases with the increase in the polarity of the fluid. Shear stress was also applied on Na-montmorillonite models with different interlayer fluids at 0%, 10%, and 20% fluid contents, and the response of the molecular model was observed in terms of shear displacement. The response of models at various normal stress and fluid content conditions shows that the shear stress increases with the increase in normal stress and polarity of fluids.

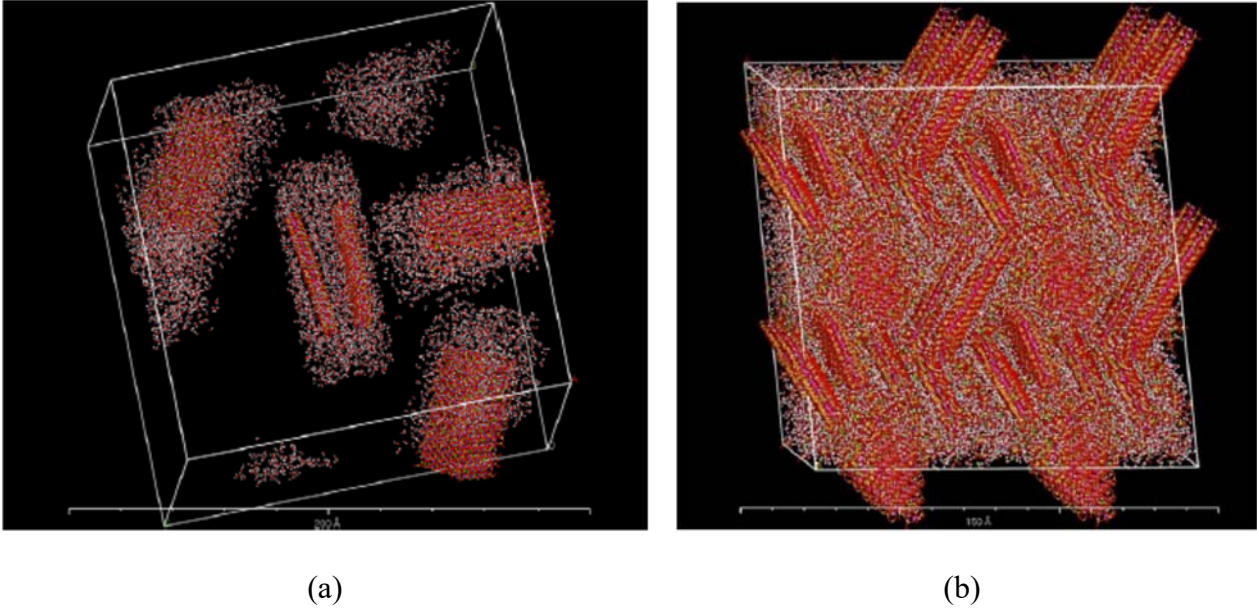
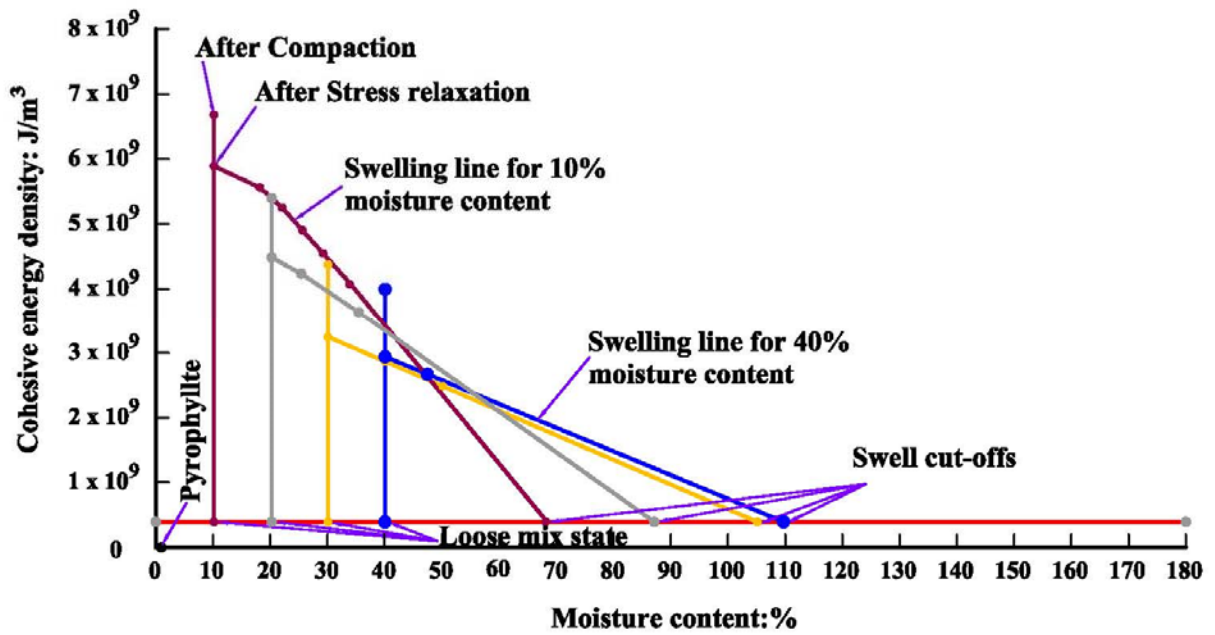
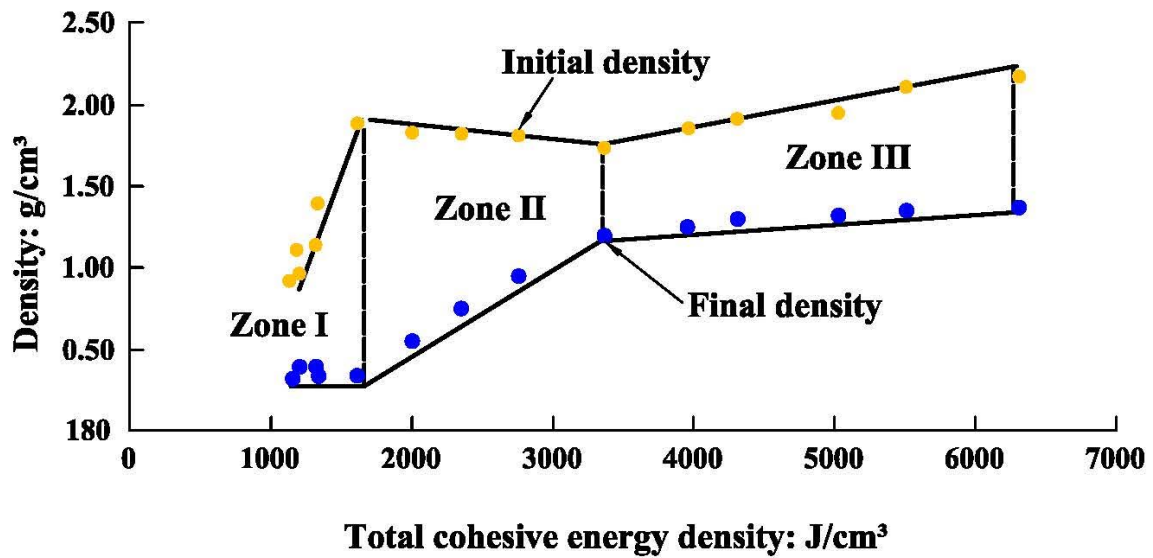


Figure 2-21 Molecular-level simulations (a) loose soil fabric before compaction, (b) fabric compacted to maximum density (Ahmed and Abduljawwad, 2017a).

Thapa (2020) further used the nanoindentation technique to measure the nanomechanical properties of sodium montmorillonite. The nano-scale experiments were performed on dry and water-hydrated clays to study the influence of swelling on the nano-mechanical properties of clay. A controlled uniaxial swelling (CUS) device was used to prepare the samples at different swelling levels (0%, 10%, and 20%). These samples were then used to perform unconfined compression and nano-indentation tests at various levels of swelling. Stress-strain behavior from the unconfined compressive strength (UCS) test for different values of swelling is shown in Figure 2-23a. It appears that the stress-strain curve for 0% swelling is steeper than for 10% and 20% swelling, and the UCS of sodium montmorillonite decreases with the increase in swelling level. A 6mm x 12mm specimen was used for the nanoindentation experiment, and tests were performed at a controlled displacement of 500 nm to determine the elastic modulus values. Load-displacement curves from nanoindentation tests for dry, 0%, 10%, and 20% swelling are shown in Figure 2-23b.



(a)



(b)

Figure 2-22 (a) CED and moisture content plot, (b) CED and density plot (Ahmed and Abduljawwad, 2017a).

The curve for 0% swelling is steeper than the curves for 10% and 20% swelling. It is also observed that the elastic modulus decreases with the increase in swelling, which indicates that clays become softer upon swelling.

Molecular dynamics (MD) simulations have also been utilized by Underwood and Bourg (2020) for various properties of clay-water assemblages, including porosity, pore-size distribution, anisotropy, enthalpy, the free energy of hydration, total suction and diffusion of water ions as a function of dehydration. The modelling was performed with the CLAYFF force field in the Gromacs simulation package. The study concluded that the molecular level simulations can provide realistic predictions of microstructure, mechanics, energetics, and transport properties of clay-water systems and, therefore, can be applied for swelling and mechanical behavior of swelling soils.

Navarro et al. (2021) used molecular dynamics models (MDM) to study the microstructural behavior of compacted bentonites. The study used MDM results to verify the changes in microstructure void ratio (e_m) with the changes in suction by linking the molecular dynamics models of Sun et al. (2015) and Akinwunmi et al. (2020) with the experimental results from Cases et al. (1992), Berend et al. (1995), Salles et al. (2009), and Montes et al. (2003). The MDM results compare well with the experimental values of e_m , suggesting the use of molecular dynamics in numerical simulations for studying the hydro-mechanical behavior of compacted bentonites.

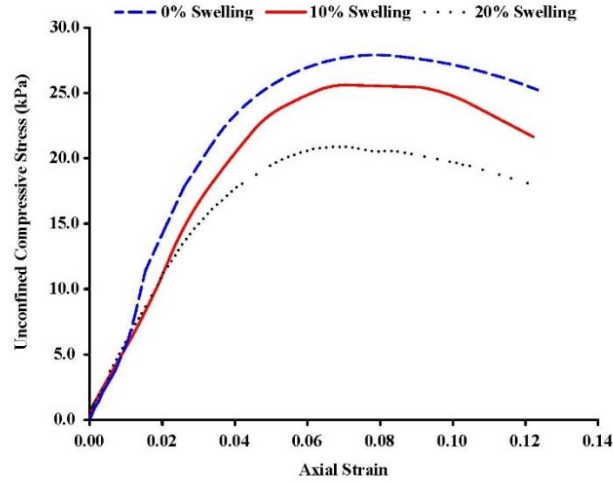
Du et al. (2021) combined molecular dynamics simulations with traditional DDL theory for the prediction of swelling pressure and named their model a potential energy method. The potential energy method comprised of: (i) determination of macro-parameters such as CEC, dry density, and mineralogy, (ii) calculation of micro-parameters (lattice distance, numbers of water molecules and

cations), (iii) establishment of a molecular model in Material Studio 8.0 software using CLAYFF force field, (iv) determination of electrostatic (repulsive) and van der Waals (attractive) forces, and (v) prediction of swelling pressure based on a model equation. The model was also validated with the traditional DDL method using the results reported in the literature (Schanz et al., 2013; Schanz and Tripathy, 2009) and the molecular oedometer method. The developed model is very helpful in engineering practice as it provides charts for swelling pressure prediction of montmorillonite with monovalent/divalent interlayer cations for a range of dry densities and CEC conditions. However, the model has limited application due to the use of only a two-layer montmorillonite structure without the incorporation of complex fabric and structure of swelling soils originating from the interaction of clay minerals with non-clay minerals and salts.

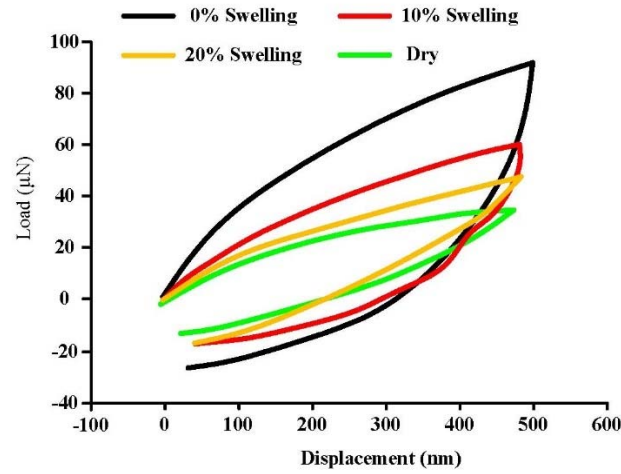
2.3 Conclusive remarks

A detailed comparison of the key features and limitations of the landmark constitutive models at both macro and molecular levels is presented in Tables 2-1 and 2-2, respectively.

The major limitations of the macro-level constitutive models are: firstly, all the presented models do not take any consideration of the nano-level clay interactions, including the effect of layer charge and type of cations in the interlayer, which significantly affects the mechanical behavior of swelling soils. Secondly, the natural fabric of swelling soils consists of random arrangements of clay particles, and their interaction with the non-clay particles and salts is not accounted for in the model formulations. In addition, all macro-level models are applicable to a specific behavior(s) with several underlying assumptions.



(a)



(b)

Figure 2-23 (a) Stress-strain response from UCS tests for 0%, 10% and 20% swelling, (b) Load-displacement curve from nanoindentation experiment for dry, 0%, 10% and 20% swelling (Thapa, 2020).

Furthermore, all the macro-level models use a set of parameters (Table 2-1) that require a completely independent laboratory testing campaign. For example, the Barcelona Basic Model (BBM) is characterized by a minimum of ten (10) parameters in addition to the initial state parameters. The model parameters in the Barcelona Expansive Model (BExM) further increase the

parameters due to the incorporation of coupling functions. The Hydro-mechanical Constitutive Model by Sun and Sun (2011) requires thirteen (13) parameters which four different laboratory tests can obtain, including isotropic compression tests with loading-unloading cycles on saturated soil, consolidated undrained triaxial tests on saturated soil, isotropic compression tests at different suction values and a test for measuring water retention behavior. The Dual Structure Constitutive Model by Vilarrasa et al. (2015) needs eight (08) to eleven (11) parameters in addition to the parameters defined by BBM. In summary, to use existing macro-level constitutive models, the user is required to perform a number of laboratory tests (e.g., isotropic compression tests, triaxial tests, pressure-plate tests, water retention tests, permeability tests, etc.). Due to the above-described facts, the application of macro-level models in engineering practice is very limited (Sun et al., 2000).

Molecular-level simulations for the stress-strain behavior of swelling soils have been performed by several authors, as summarized in Table 2-2. However, these studies have concentrated on one mineral only (mostly bentonite) without incorporating the complex fabric and structure of compacted/natural clays. Moreover, the interaction of clay minerals with other non-clay minerals and salts has also not been considered. One of the major limitations of all molecular-level studies is the lack of mathematical formulation to predict the stress-strain behavior of swelling soils.

The nano-level constitutive model presented in this study provides a state-of-the-art technique at the molecular level for modeling the swelling soils to predict the stiffness moduli and stress-strain response. The model encompasses any combination of clay minerals with other interacting non-clay minerals and the cementing agents.

Table 2-1 Summary of macro-level constitutive models

Model	Key Features	Major Limitations/Assumptions	Key Model Parameters
Barcelona Basic Model (BBM) by Alonso et al. (1990)	- A mathematical model for describing the stress-strain behavior - Modified Cam Clay adopted as limiting condition of unsaturated formulation - Applicable for slightly expansive or non-expansive soils	- Based on macrostructure only - Linear increase of apparent cohesion with suction - Linear $e-\ln(p)$ relationship - No consideration of water retention behavior	- Compressibility under mean stress changes: $\lambda(0)$, κ, β, r, p^c. - Compressibility under suction changes: λ_s, κ_s. G, M, k.
Barcelona Expansive Model (BExM) by Gens & Alonso (1992) and Alonso et al. (1999)	- Conceptual framework only by Gens & Alonso (1992) - Complete mathematical model by Alonso et al. (1999) - Two distinct levels of soil structure, i.e., microstructure level and macrostructure level	- Permanent saturation of the microfabric - Elastic strains at the microstructure level - No consideration of water retention behavior - No consideration of nano-level clay interactions	κ, κ_s, κ_m, β, r, p^c, $\lambda(0)$, M, p_o^M - Hardening Parameters: S_I and S_D - Micro-Macro Coupling Functions: f_I (SI active) and f_D (SD active)
Double Structure Barcelona Expansive Model (BExM) by Sanchez et al. (2005)	- Use of BExM for macrostructural behavior - A mathematical model for describing the stress-strain behavior using generalized equations - Non-linear elastic model for microstructural behavior - Generalized plasticity model for coupling between micro and macro levels	- No consideration of water retention behavior - Elastic strains at the microstructure level - No consideration of nano-level clay interactions - Natural clay fabric at the micro-level is not incorporated	- Macrostructural behavior: $\lambda(0)$, κ, κ_s, ζ, r, p_c - Microstructural behavior: χ, κ_m, α_m, β_m - Interaction functions: f_c, f_s, e_{macro}, e_{micro}
Constitutive Model for Claystone by Pinyol et al. (2007)	- Two behavior levels i.e., clay matrix and cementation - Use of BExM for matrix behavior - Bond/cementation behavior by damage model for bond material	- No consideration of nano-level clay interactions - Natural clay fabric at the micro-level is not incorporated	- Expansive Matrix: same as BExM - Cementation: C_b, K_{bo}, G_{bo}, Γ_o, Γ_I - Coupling: χ_o
Hydromechanical Constitutive Model by Sun and Sun (2011)	- Incorporation of water retention behavior along with mechanical behavior - Macroscopic elastoplastic model for expansive soils	- No consideration of nano-level clay interactions - Natural clay fabric at the micro-level is not incorporated - Pore air pressure and pore water pressure are continuous throughout the soil mass	- Stress-strain behavior: $\lambda(0)$, κ, ζ, τ, p'_n, M, γ, α, p'_{iyo} - Water retention behavior: λ_{sf}, κ_s, S^o_{rw} - Hydraulic-mechanical coupling: γ

Table 2-1 Summary of macro-level constitutive models (continued)

Model	Key Features	Major Limitations/Assumptions	Key Model Parameters
Dual Structure Constitutive Model by Vilarrasa et al. (2015)	- An elastoplastic thermo-hydro-mechanical model for expansive soils - Use of BBM for matrix behavior and modification of BExM for microstructure and coupling functions - Incorporates the effect of microstructural swelling on the permeability of expansive soils	- Strain evolution patterns with suction cycles show nonlinearity, which is not supported by experimental evidence - Permanent saturation of the microfabric - Elastic strains at the microstructure level - No consideration of water retention characteristics - No consideration of nano-level clay interactions	- Macrostructure level: same as BBM - Microstructural behavior: $\alpha_m, \beta_m, \phi_o, \phi_{Mo}$ - Interaction functions: $f_c, f_s, e_{macro}, e_{micro}$
Strain Hardening Constitutive Model by Chen et al. (2017)	- A stress-strain model based on the strain hardening phenomenon - Extension of Mohr-Coulomb criterion using dilatancy effect theory	- Applicable to one specific type of material (bentonite) - Bentonite is regarded as isotropic in nature - Macroscopic in nature based on experimental observations only - No consideration of changes in strength due to suction cycles.	$\sigma_1, \sigma_3, E, \mu, \varepsilon_1, \varepsilon_3, \gamma^p$
STJ-Double Structure Model by Qiao et al. (2019)	- Mechanical and hydraulic models were formulated independently at the macrostructure and microstructure levels - Elastoplastic strains are considered at the microstructure level - Micropores are considered unsaturated	- Applicable to one specific type of material (bentonite) - No consideration of nano-level clay interactions	- Microstructure level: $S_{Do}^m, \kappa^m, \alpha^m, \beta^m, K_{m.ref}, \beta_{m.min}, a, b$ - Macrostructure level: $S_{Do}^M, \kappa^M, \alpha^M, \beta^M, c, K_{M.ref}, \beta_M, n, P'_{M.ref}, M, m, \gamma_s, P'_{Myo}$
HMC Double Structure Model by Kyokawa (2021)	- A hydro-mechano-chemical model for unsaturated expansive clays - A nano-level constitutive model - Cam Clay-based model at macrostructure level - Interlaminar behavior through interlaminar force equilibrium	- Interlaminar space is assumed to be fully saturated - Hydraulic hysteresis is not considered - A linear relationship between the degree of saturation and effective stress parameter - No consideration of the effect of layer charge and type of cations	- Microstructure level: $\lambda, \kappa, M, v_e, e_{NC}, p_a, a, k_1, k_{11}$ - Water retention curve: α, m, n - Clay mineral specifications: $t, S, CEC, EXC, v, W_{max}, W_{min}, \chi_o$

Table 2-2 Summary of molecular-level constitutive models

Model	Key Features	Major Limitations/Assumptions	Key Model Parameters
Stress-strain Simulations by Katti et al. (2005)	• Steered molecular dynamics (SMD) simulations on pyrophyllite • Transformation of parameters of the consistent force field (CFF) by Teppen et al. (1997) to CHARMM force field in NAMD software • Stress-strain relationship for the interlayer of clay mineral	• Use of dry pyrophyllite and no interaction of clay with water and cations • Application of forces normal to the simulation cell • Use of single clay crystallites; no incorporation of complex fabric and structure of compacted/natural clays • No swelling simulations	• No mathematical formulation
Stress-strain Simulations by Wang et al. (2007)	• Applicable to different rock and clay minerals using MD simulations • Non-linear stress-strain behavior • Simulations of three clay minerals using potential functions by Manevitch et al. (2004)	• No interaction of clay with water and cations • Application of uniaxial pressures for strain calculations • Use of single clay crystallites; no incorporation of complex fabric and structure of compacted/natural clays • No swelling simulations	• No mathematical formulation
Mechanical and Swelling Simulations by Katti et al. (2009)	• A numerical and experimental approach • Discrete Element Method (DEM) simulations using ANSYS C++ coding for swelling • Molecular dynamics using CHARMM force field in NAMD software for stress-strain response	• Applicable to one specific type of material (Na-montmorillonite) • Application of forces normal to the simulation cell • Use of single clay crystallites; no incorporation of complex fabric and structure of compacted/natural clays	• No mathematical formulation
Stress-strain Simulations by Hantal et al. (2014)	• Mechanical properties of Illite using clay force field (ClayFF) and reactive force field (ReaxFF) • Voigt-Reuss-Hill (VRH) approximation for modulus determination	• Applicable to one specific type of material (Illite) • Use of single clay crystallites; no incorporation of complex fabric and structure of compacted/natural clays	• No mathematical formulation
Universal nano-level constitutive model by Ahmed and Abduljawad (2017a)	• Nano-level constitutive model for swelling behavior of natural and compacted clay soils • Covers all possible variations in clay fabric and structure • Molecular mechanics (MM), molecular dynamics (MD) and Monte Carlo (MC) simulations in Material Studio • Three state parameters; (i) cohesive energy density, (ii) moisture content, and (iii) density	• Model shows some deviations in soils with macro features (cracks, fissures etc.)	• A complete mathematical model with following input parameters: CEC, moisture content, dry density and mineralogical composition

Table 2-2 Summary of molecular-level constitutive models (continued)

Model	Key Features	Major Limitations/Assumptions	Key Model Parameters
Mechanical Simulations by Thapa (2020)	• Development of clay and fluid models using Material Studio and PSFGen of Visual Molecular Dynamics (VMD) software • Constant-force and constant-velocity SMD simulations for normal forces and shear forces, respectively • Use of nanoindentation experimental technique to measure nanomechanical properties	• Applicable to one specific type of material (Na-montmorillonite) • No incorporation of complex fabric and structure of compacted/natural clays	• No mathematical formulation

CHAPTER 3

MOLECULAR-LEVEL SIMULATIONS

This research comprised of three major levels: Molecular-level simulations, model formulation; and model validation. Molecular-level simulations were carried out in material studio software followed by the model formulation using simulation results. Validation of the model was then performed through field and laboratory testing in the current study and available databases from the literature. Molecular-level simulations are discussed in this chapter, whereas other phases of the study would be discussed in the subsequent chapters.

3.1 Model construction

The natural composition of swelling soils is very complex owing to the presence of swelling clay minerals such as Na-montmorillonite (Na-Mt), non-swelling clay minerals such as kaolinite and the interaction of these clay minerals with other non-clay minerals like quartz, gypsum, calcite and other salts. Cations and anions from these salts interact with the swelling clay minerals and cause cementation. Quartz acts as filler in the pore spaces and does not contribute to the volume change process. Furthermore, macro, micro and nano level pores exist in a swelling soil with water and air phases. The overall volume change and mechanical behavior of the swelling soils are thus controlled by the swelling clay minerals, density, degree of saturation and cementation between clay minerals. All such possible clay-water-ion compositions and interactions in swelling soils are simulated in this study through Materials

Studio software (Accelrys Software, 2019) using molecular dynamics (MD), molecular mechanics (MM), and Monte Carlo (MC) techniques.

It is well established that the swelling mechanism of clays is governed by the interactions and processes among the nano-level clay particles, called as crystallites (Ferrage et al., 2005; Laird, 2006; Wayllace, 2008; Rahromostaqim and Sahimi, 2018; Du et al., 2020). The swelling response, in turn, defines the mechanical performance of these soils/rocks (Katti et al., 2009; Tao et al., 2010; Hantal et al., 2014; Ahmed and Abduljauwad, 2017; Thapa, 2020). In this study, the swelling-mechanical response of clays is modeled through molecular-level simulations of Na-montmorillonite with different cation exchange capacities (54, 90, and 144 meq/100 g). Na-montmorillonite has a tetrahedral-octahedral-tetrahedral (TOT) structure in which silica tetrahedral sheets are composed of one silicon atom surrounded by four oxygen atoms and the octahedral sheets contain aluminum or magnesium that are octahedrally connected by hydroxyls and oxygen. The clay particles form by stacking of these sheets with dimensions of an order of nanometre and a length or width to thickness ratio of about 2000:1 (Sharma 1998).

Based on the already published values in literature (Arnott, 1965; Jonas and Oliver, 1967; Sucha et al., 1999; Uhlik et al., 2000; Marinkovic et al., 2001; Simic and Uhlik, 2006) and XRD findings by Ahmed and Abduljauwad (2017), a basic crystallite size of 2.6 x 5.4 x 2.0 nm was selected for the simulation of Na-montmorillonite (Figure 3-1a). These individual crystallites were then grouped in a periodic unit cell, utilizing the MC to form bigger clay particles. The clay particles combine to form aggregates that join with other non-clay particles to generate overall fabric and structure of clay-bearing soils/rocks having micropores between clay particles, inter-aggregate and intra-aggregate pore spaces. Most of the unit molecules used

in this study were obtained from the Nanoscale Simulation Laboratory at the University of Akron, USA (NSL, 2013). These unit molecules consist of Na-montmorillonite with different cation exchange capacities (54, 90, and 144 meq/100 g), water, Calcite, Gypsum, and pyrophyllite. Some other molecules were also drafted using Materials Studio software. All these molecules' charges were validated using the method of charge equilibration QEq (Accelrys Software, 2019).

3.2 Simulation parameters

One of the basic steps in molecular-level simulations is the sorption of water molecules in the clay crystallites to simulate the swelling process. The sorption module of the software was used for the sorption of water on the selected clay crystallites using MC method (Figure 3-1b). The MC method checks the fixing of the defined number of water molecules at best-fit places. The MC uses the random placement principle to fit water molecules in the best possible configuration through 'exchange', 'conformer', 'rotate', 'translate', and 'regrow' ratios. Various values of these parameters were tried and the resulting clay-water configurations were verified against the known behaviors like hydration radii of Na^+ cations and the expansion of clay lattice with change in water content in the interlayer. The finally selected values of these parameters, verifying these known behaviors, were 0.39, 0.20, 0.20, 0.20, and 0.20, respectively, against probabilities of 0.39, 0.20, 0.20, 0.20, and 0.20. The modified universal force field was used in the simulations through the Forcite module of the software. Berendsen thermostat, Berendsen barostat, and NPT (constant number of particles, pressure, and temperature) ensemble were selected to perform the simulations. A decay constant of 0.1 ps was used in both the Berendsen thermostat and barostat, with a temperature of 298 K in the

thermostat and a pressure of 100 kPa in the barostat. After the water molecules' sorption, the system's energy was minimized using geometry optimization and the MD technique in the Forcite module (Accelrys Software, 2019).

3.3 Simulation parameters verification

As explained earlier, the verification and calibration of above-described parameters in the simulation study was carried out using the relationship between the moisture content and d-spacing in Na-montmorillonite. It has been found through previous studies (Rahromostaqim et al., 2018; Ferrage. et al., 2005; Du et al., 2021) that d-spacing increases with an increase in water molecules in the clay layers. The increase in d-spacing of the study model with water molecules is shown in Figure 3-1c and is found to be in good agreement with previous experimental, numerical, and simulation studies.

3.4 Simulation methodology

A six (06) step simulation methodology comprising: (i) water molecules sorption on the individual clay crystallites, (ii) salts sorption, such as calcite and gypsum, on clay crystallites, (iii) creation of soil fabric in the loose state by random sorption of four crystallites in the unit periodic cell, (iv) compaction of the soil to the required density, (v) stress relief of the compacted unit cell, and (vi) sorption of water to produce different swelling stages, was adopted using selected variations of cation exchange capacity (CEC), exchangeable cations, density, moisture content, and salts (Ahmed and Abduljawad, 2017).

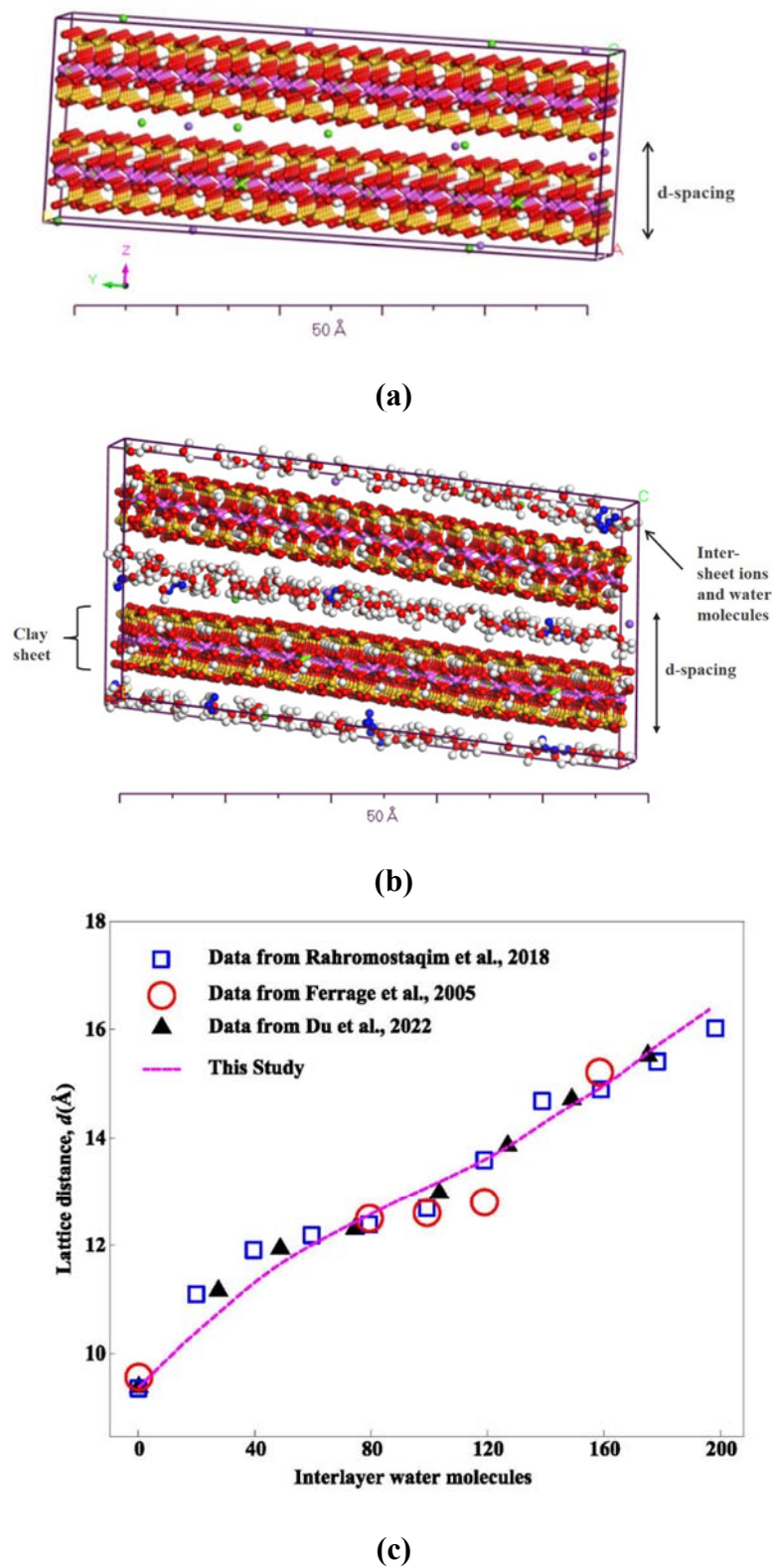


Figure 3-1 (a) Single crystallite of Na-Montmorillonite, (b) Sorption of water on single crystallite of Na-Mt, (c) Increase in lattice distance of Na-Mt after water sorption

These steps of the simulation program were repeated for three CEC changes in Na-montmorillonite (144 meq/100g, 54 meq/100g, and 90 meq/100g) and subsequent variations in density, moisture conditions, exchangeable cations, and salts. In the simulation for Na-montmorillonite at three different CECs (Na as 100% exchangeable cation), the clay particles were compacted at 0.01, 0.1, and 1.0 GPa at moisture contents of 10, 20, 30, and 40%. Cementation agents, such as Calcite (CaCO_3) and Gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), were added to Na-montmorillonite at 10 to 20%. Simulation permutations with these salts were performed at 10% for Calcite and 10 and 30% for Gypsum. Exchangeable cations (i.e., Na^+ , K^+ , Mg^{+2} , and Ca^{+2}) were also varied at 20, 40, and 60% with different combinations to investigate their effect on swelling and subsequent mechanical behavior.

3.4.1 Sorption of water molecules and salts on clay crystallites

The sorption of water molecules on the selected clay crystallites was achieved using the sorption module. After sorption of a maximum number of possible water molecules in every 25000 steps, the system's energy was minimized using the software's molecular dynamics technique in the Forcite module. After the sorption of water molecules on single clay crystallites, the individual ions, e.g., Ca^{+2} , SO_4^{-2} , etc., were sorbed on the water-bearing clay crystallites to simulate the process of cementation due to salts. A typical post-sorption particle of Na-montmorillonite is shown in Figure 3-2a, and an enlarged view showing various inter-layer and intra-layer cations is provided in Figure 3-2b.

3.4.2 Creation of soil fabric in loose state

During the deposition process, the clay particles first pack in a loose state and then get compacted under the consolidation process. Therefore, it was essential to simulate clays' fabric at both stages. Using the Sorption module, simulation of the loose state is performed through random sorption of four crystallites with periodic boundary conditions in a $12.5 \times 12.5 \times 12.5$ nm cubic unit cell (Figure 3-3a).

3.4.3 Simulation of compacted clay particles

These loose particles were then compacted to the maximum achievable density using the NPT ensemble in the Forcite molecular dynamics module (Figure 3-3b). Confining pressures of 0.01, 0.10, and 1.0 GPa were employed to model the different types and levels of laboratory compaction and geological pressures. Each simulation was run for a varying period (ranging from 10 to 30 ns). The simulation time period was extended to a maximum limit where it was made sure that no more increase in density, under that confining pressure is achievable and it has become constant. This is the stage where the particles have achieved the maximum possible packing by occupying all the possible empty spaces. This packing is governed by the size, shape and gradation of the clay particles.

3.4.4 Simulation of stress relief and swelling stages

Swelling soils are subjected to the release of geological pressures (stress relief), making them overconsolidated in nature and prone to swelling. In the previous step, the Forcite MD module was run at a confining pressure of 0.001 GPa to simulate the stress relief of the compacted unit

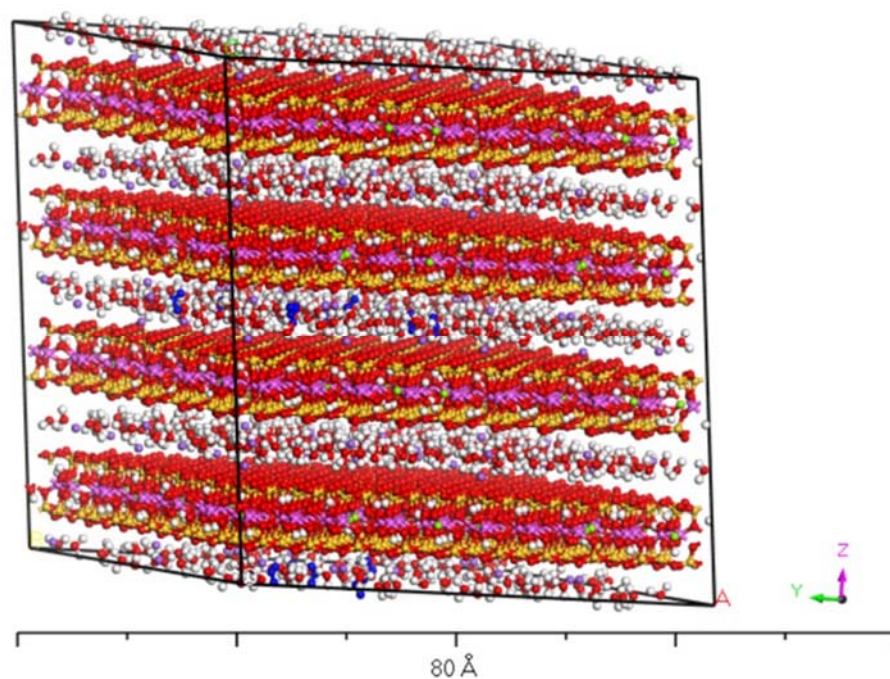
cell. The selected pressure of 0.001 GPa could be considered representative of the over-consolidation pressure in most of the clay-bearing soils/rocks. The mixture of clay particles after stress relief was subjected to the sorption of water molecules to create different swelling stages. The process was repeated for different percentages of moisture content. In this study, each absorption/adsorption run was carried out using the Monte Carlo technique. In this simulation, the water molecules start absorbing/adsorbing to the highest energy point in the clay structure and continue till all the energy (water deficiency) points are covered by water molecules. Hence, in this manner, the simulation is continued till the adsorption/absorption process of the water molecules is completed.

3.4.5 Cohesive energy density and mechanical properties

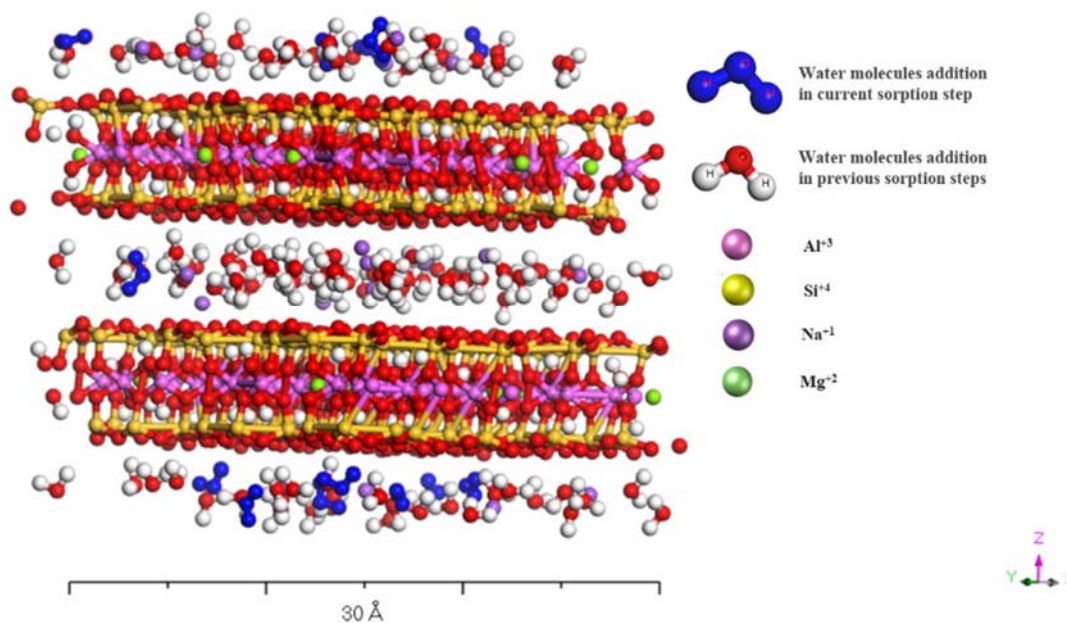
The mechanical behavior model formulated in this study considered cohesive energy density (CED), dry density, and moisture content as three (03) state parameters. CED is the energy required to separate molecules from each other and is given as:

$$E_{coh} = -E_{inter} = E_{intra} - E_{total} \quad (1)$$

where E_{coh} is the cohesive energy of all molecules in Joule, E_{total} is the total energy of the system, and E_{inter} and E_{intra} are the intermolecular and intramolecular energies, respectively. The cohesive energy per unit volume defines the CED and is generally represented in units of J/cm³. It is the measure of mutual attraction between the molecules.



(a)



(b)

Figure 3-2 (a) Water sorbed particles of Na-montmorillonite, (b) A close up view of Na-Montmorillonite particle after water and cations sorption

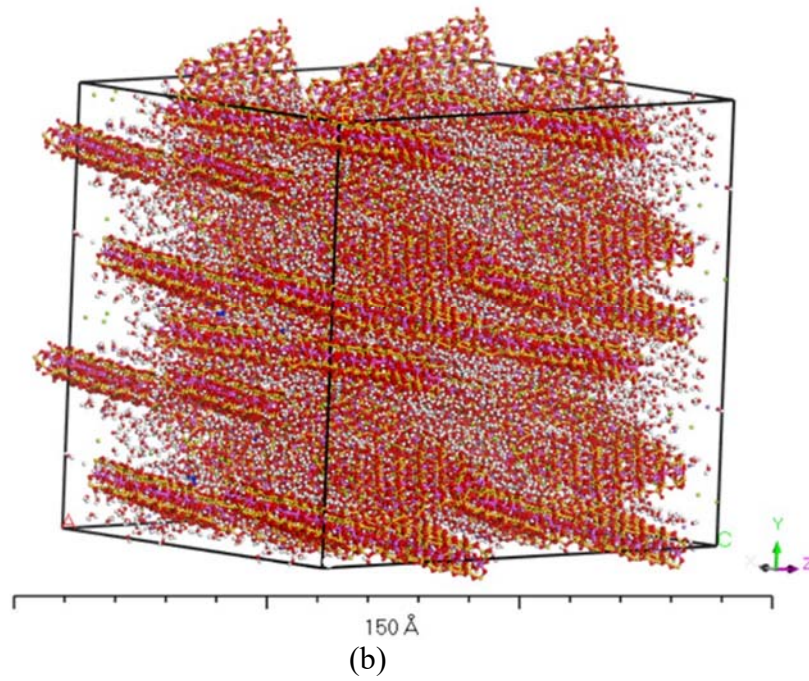
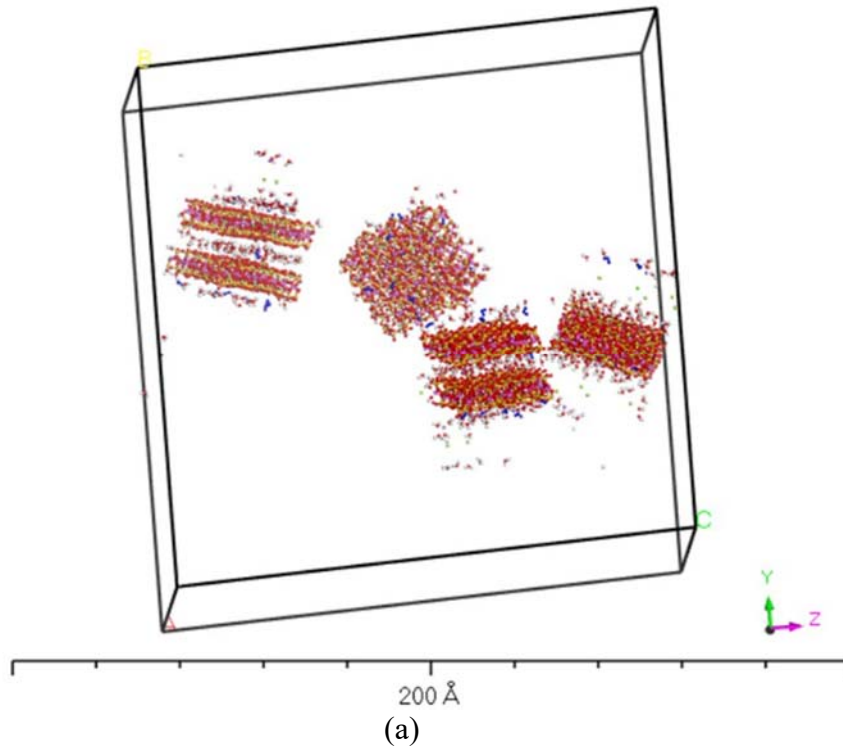


Figure 3-3 (a) Cubic unit periodic cell representation of four water sorbed crystallites, (b) Dispersed fabric at 0.001 GPa pressure and 10% moisture content

Both the CED concept and volume change processes of swelling soils are quite analogous to each other. Therefore, the CED parameter is found to correlate well with all possible variations in the structure of clay-bearing soils/rocks resulting from changes in density, moisture content, CEC, and exchangeable cations (Ahmed and Abduljawad, 2017). The Forcite module of material studio software was used to determine CED for all likely variations in the soil/rock structure.

The CED value depends on the net result of all interactions taking place in a clay-water-ion system, including ionic hydration, adsorption, double layer repulsion, electrostatic attractions and van der Waals interactions. The CED parameter varies with the changes in density, moisture content, cementation, exchangeable cations, and CEC and is directly/indirectly associated with all of these variables. In this study, the clay crystallites with high CEC have been observed to yield high CED values as compared to low CEC crystallites for the same density and moisture. This is because of the higher number of hydrogen bonds in high CEC clays due to the higher charge deficiency centers, which results in more electrostatic attractions in clay particles. The CED also shows an increasing trend with the increased bivalent cations and cementation. This is due to the extra bonding created by the cations and anions of cementing agents such as Calcite, Gypsum, etc., and/or exchangeable cations other than sodium. The clay crystallites with high densities have been found to achieve higher CED values due to the close proximity of the crystallites or the lesser moisture contents. The increase in CED owes to the additional attractions due to the close range of attractive forces on the crystallites. However, as the clay particles come closer due to the high electrostatic attraction, the van der Waals forces become repulsive, resulting in additional expansion. For the same CEC, the higher water content results in a decrease in the CED value due to the

balancing of charge deficiency centers by water molecules thereby lowering the electrostatic attractions. In conclusion, the CED parameter depends on density, moisture content, cementation, exchangeable cations, and CEC and it controls the swelling and mechanical response of clay-bearing strata.

The mechanical properties were determined using the Forcite module in the material studio at each swelling stage. The constant strain method was used for the modulus determination at strain levels varying from 0.001% to 10% in four steps against each strain level. The software uses the Voigt-Reuss-Hill (VRH) approximation to determine the moduli values. The adopted simulation methodology in this study considered all possible variations in the strain levels (0.001% to 10%) that are generally observed in geotechnical engineering and therefore, it is applicable to assess moduli values in elastic and elastoplastic regions of stress-strain behavior of swelling soils. A three-dimensional view showing the swelling soil structure with inter-aggregate and intra-aggregate pore spaces after CED and modulus simulations is shown in Figure 3-4.

There could be a directional arrangement of the clay particles during the compaction process. 3D views of the repeated cells shown in Figures 3-3 and 3-4 reveal the nature of the fabrics, which consist of various directional arrangements of clay particles. The mechanical properties determined for these 3D fabrics are representative of the three-dimensional stress case and, hence, cover the effects of the anisotropy if there are any.

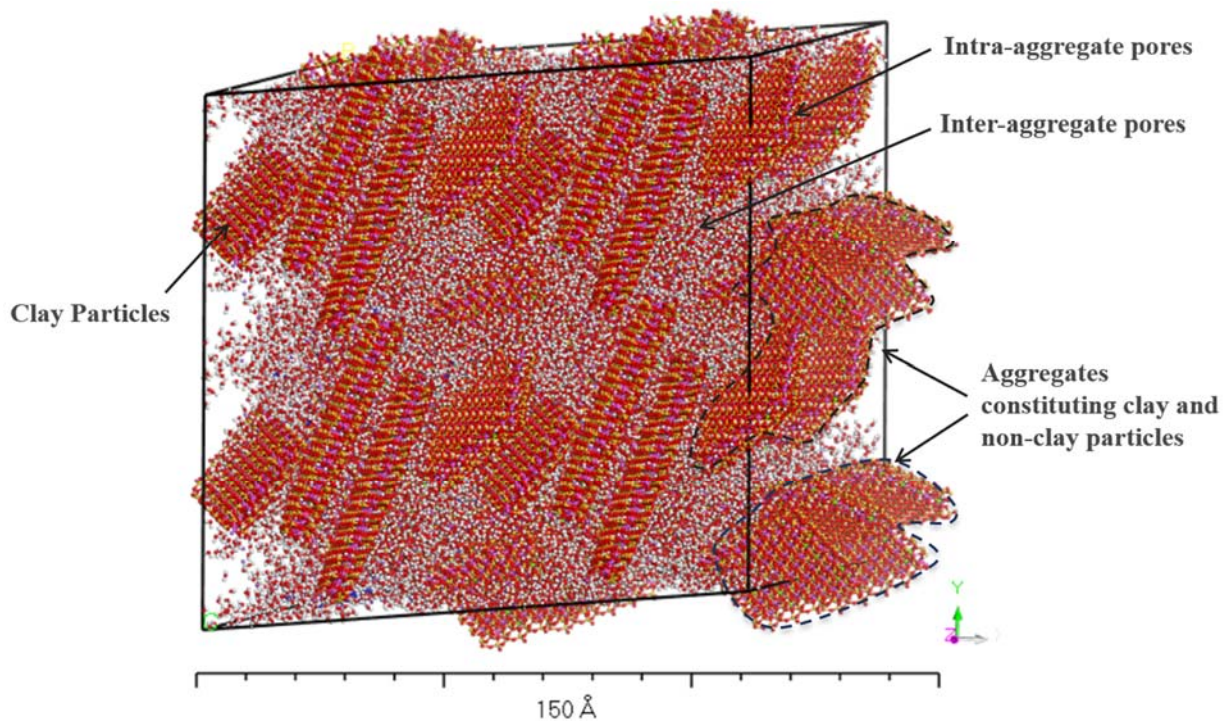


Figure 3-4 Three-dimensional view of multiple unit cells after CED and modulus simulations of Na-montmorillonite with non-clay particles (water content = 10%, strain level = 1.0%)

CHAPTER 4

MODEL FORMULATION AND VALIDATION

As explained in Chapter 3, CED can be effectively used in predicting the volume change and mechanical behavior of swelling soils due to its sensitivity to changes in CEC, exchangeable cations, cementation, density conditions, and water. Therefore, this study has applied it as a state parameter to predict the swelling behavior and mechanical properties of swelling soils at different stages of swelling.

4.1 Nano-level hydro-mechanical model

The Forcite module of materials studio software is used to determine the CED and the corresponding modulus values. The simulation permutations were repeated for the adopted cases with varying density, cementation, moisture conditions, and exchangeable cations at strain levels of 0.001% to 10%. The outcomes of the simulations are plotted as a mechanical behavior model in Figure 4-1.

The mechanical behavior model is developed using a molecular level simulation approach, but the resulting structure and fabric of soil modeled in the software consists of both nano and micro-level pores, which are typically present in any overconsolidated hard clay/clayey rock structure. This is evident from the three-dimensional (3D) structure created using periodic boundary conditions (Figure 3-4). Periodic boundary conditions create multiple unit cells of resulting structure by replicating model in all the three dimensions infinitely. Percentages of large-sized pores are almost

minimal in the case of heavily overconsolidated clay-bearing soils/rocks because of high densities, while there could be relatively high percentages of macropores in low density strata.

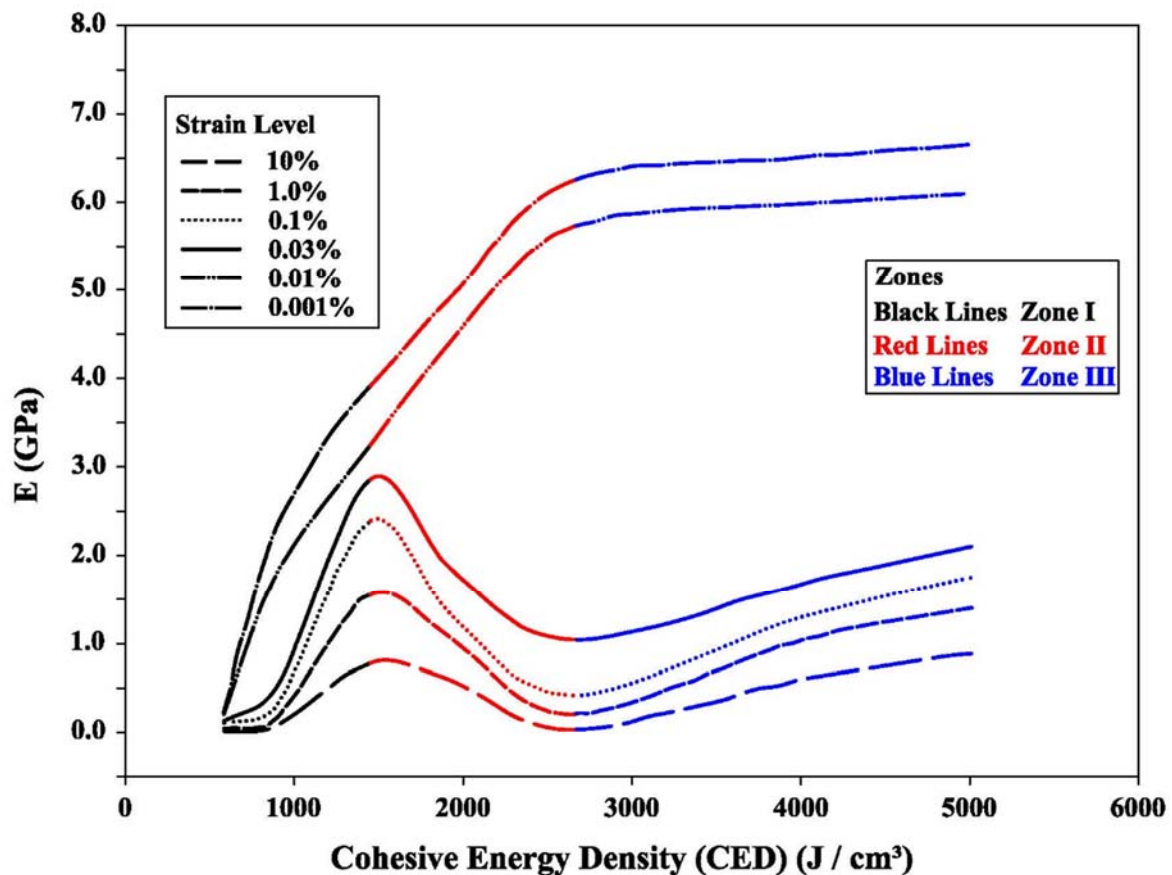


Figure 4-1 Mechanical behavior model plot for swelling soils

Two (02) types of trends can be observed from the mechanical behavior model plot, one at small strain levels (0.01% and 0.001%) and the other at large strain levels (0.03% to 10%). Small strains range is applicable to foundations subjected to dynamic loads and corresponding field geophysical tests i.e., in-situ cross-hole and downhole tests. The large strain range is

related to foundations, retaining walls, and conventional soil testing approaches (Atkinson and Sallfors, 1991; Mair, 1993).

Three zones are obvious at a large strain level (Figure 4-1). Zone I is bordered by CED values of 584 J/cm^3 and 1450 J/cm^3 . In this zone, the modulus values demonstrate an increasing trend with the raise in CED. This is mainly attributed to the increase in CEC with no contribution from cementation between the particles. There is a tendency of reduction in the modulus values with an increase in CED in Zone II, bounded by CED values of 1450 J/cm^3 and about 2640 J/cm^3 . Theoretically, the increase in CED in Zone II is only possible due to either reduction in moisture content or an increase in cementation due to salts such as Calcite, Gypsum, etc. It has been observed in molecular simulations that the presence of cementation in swelling soils yields higher CED values than the limiting value of 2640 J/cm^3 for Zone II. Therefore, it can be interpreted that the increase in CED in Zone II is primarily due to a reduction in moisture content (dry nature of soil). The reduction in moisture content will cause the crumbling of dry clays and, ultimately, loss of strength and stiffness. In Zone III ($\text{CED} > 2640 \text{ J/cm}^3$), there is again a trend in the minor rise in the modulus values with the increase in CED. The increase in CED in this zone is caused by an increase in cementation due to the binding salts, which have resulted in an increase in modulus values. It can also be observed that keeping constant CED (i.e., moisture content, density, cementation, and CEC), the modulus values decay with an increase in strain level from 0.03% to 10% (Figure 4-1).

The above discussion explained the material behavior at large strain levels, which is absent at small strain levels (0.01% and lesser). The modulus values at the small strain levels tend to increase at different rates in all zones. The behavior at small strain levels is essentially linearly elastic in nature, while it is elasto-plastic at higher strain levels. The modulus value at small

strain level increases with the increase in CED value. The increase in CED value is associated with the increase in density and cementation and/or decrease in the degree of saturation. A similar trend is also observed by Pintado X. et al. (2019), where the modulus values at low strain levels increase with the dry density and at lower degrees of saturation. The small strain levels apply to foundations subjected to dynamic loads and low-strain geophysical tests. The small strain levels apply to foundations subjected to dynamic loads and low-strain geophysical tests.

Using the mechanical behavior model plots, fundamental equations are developed comprising the relationship between CED and modulus values, E, at various strain levels where E is the secant modulus. The relationships for all three zones of the plots for large and small strain levels are represented below:

$$E_{LI} = \{1.2363(1.7137\varepsilon^{-0.184}) (CED)^2 - 1629(1.6774\varepsilon^{-0.163}) (CED) + 542692(1.6838\varepsilon^{-0.157})\} / \Delta IDD / \Delta p_c \quad (2)$$

$$E_{LII} = \{0.2954(-0.762\ln(\varepsilon) + 0.4073) (CED)^2 + 575(1.8977\ln(\varepsilon) - 2.7568) (CED) + 567877(-2.582\ln(\varepsilon) + 6.3925)\} / \Delta IDD / \Delta p_c \quad (3)$$

$$E_{LIII} = \{-0.0502(-0.149\ln(\varepsilon) + 1.6255) (CED)^2 + 754(-0.132\ln(\varepsilon) + 1.4661) (CED) - 1614985(-0.078\ln(\varepsilon) + 1.3227)\} / \Delta IDD / \Delta p_c \quad (4)$$

Equations (2) to (4) represent relationships for large strain levels. For small strain levels, Equations (5) to (7) can be used and are shown below:

$$E_{SI} = \{-2.9073(-116.67\varepsilon+2.1667) (CED)^2 + 9432(-81.835\varepsilon+1.8184) (CED) - 4314026(-76.667\varepsilon+1.7667)\} / \Delta IDD / \Delta p_c \quad (5)$$

$$E_{SII} = \{0.5496(-63.662\varepsilon-0.3634) (CED)^2 + 4324(35.906\varepsilon+0.6409) (CED) + 1863674(-120.07\varepsilon+0.2007)\} / \Delta IDD / \Delta p_c \quad (6)$$

$$E_{SIII} = \{0.0302(-47.093\varepsilon-0.5291) (CED)^2 + 391(23.987\varepsilon+0.7613) (CED) + 4896810(-14.845\varepsilon+1.1484)\} / \Delta IDD / \Delta p_c \quad (7)$$

The numbers in the subscripts in Equations (2) to (7) represent the respective zone of the plot whereas large and small strain levels are shown by L and S, respectively. CED represents the cohesive energy density in J/cm³, and ε is the strain level. As the simulated model has been constructed considering the natural composition of swelling soils using a combination of clay and non-clay minerals with pore spaces, the strain, ε , in Equations (2) to (7) represents total strain of the swelling soil. A linear interpolation could be performed for strain levels between 0.03% and 0.01%.

The CED can be calculated by Equations (8) to (12) obtained by Ahmed and Abduljawwad (2017) in their swelling behavior model as follows:

$$CED = 0.0625 (IWC)^3 - 3.575 (IWC)^2 + 10.5 (IWC) + 2830 + \Delta CED_{CEC} + \Delta CED_{cat} \quad (8)$$

where IWC is the initial water content. The correction due to CEC (ΔCED_{CEC}) is then applied using the following expressions:

For CEC > 90meq/100g:

$$\Delta CED_{CEC} = [0.0717 (IWC)^3 - 3.775 (IWC)^2 - 22.917 (IWC) + 3785](CEC-90)/(54) \quad (9)$$

For $CEC < 90 \text{ meq/100g}$:

$$\Delta CED_{CEC} = -[0.0002 (IWC)^3 + 0.74 (IWC)^2 - 57.4171 (IWC) + 1528](90-CEC)/(36) \quad (10)$$

Equation (8) should also be corrected for binding/cementing salts and exchangeable cations (ΔCED_{cat}) as follows:

$$\begin{aligned} \Delta CED_{cat} = & [7100(C/0.1) + 7250(L/0.1) + 5050(G/0.2) + 3010(KCl/0.1) \\ & + 3250(KP/0.1) + 3510(D/0.1) + 10200(P/0.1)] (10/IWC)0.85 + Ca(500) \\ & + Mg(300) + K(100) \end{aligned} \quad (11)$$

where C is Calcite; L is hydrated lime, G is Gypsum; KCl is potassium chloride fraction of Na-montmorillonite (smectite) content, and Ca is exchangeable calcium cation; Mg is exchangeable magnesium cation; P is Palygorskite; K is potassium exchangeable cation fraction of the total cations.

For CECs other than 54 meq/100g, Equation (8) is normalized as:

$$CED_m = e^{(0.01263 \times 54 + \ln(CED) - 0.01263 CEC)} \quad (12)$$

Furthermore, a correction for the confinement effect, p_c , is also suggested in this study for the modulus values to account for the field stress conditions. This correction is given as:

$$\Delta p_c = (p_c/102)^{0.333} \quad (13)$$

The CEC of clay-bearing soils/rocks is controlled by the relative amount of swelling-clay minerals in the sample. Therefore, in addition to correction for confinement effect to get final modified modulus value (E_m), CED_m is also modified by the ratio of swelling-clay minerals to get the final CED value of the specimen for the mechanical behavior model.

4.2 Up-scaling of the model

Based on the level of compaction or consolidation, natural or engineered swelling clays contain varying proportions of micro to macropores. The percentages of macropores are almost minimal in the case of heavily overconsolidated/compacted clay-bearing soils/rocks owing to their high densities, while there could be relatively high percentages of macropores in low density strata. Therefore, the models formulated using molecular-level simulations may require upscaling for the cases where macropores are predominantly present. In this study, therefore, a correction, ΔIDD , in the form of upscaling is applied to account for the macropores in the swelling soils. The factor ΔIDD represents the difference in densities of clay-bearing soils/rocks at molecular and macroscopic levels due to the presence of macropores and generally ranges from about 1.0 to 3.0 depending upon the proportion of macropores in the strata. The upscaling mechanism is described below in the form of equations.

The initial dry density (IDD) of the swelling soils resulting from molecular-level simulations is related to the normalized CED value, CED_m , through the following correlations (Ahmed and Abduljauwad, 2017):

$$IDD_{CED_m} = (0.002CED_m - 1.3476) \text{ for } CED_m < 1610 \quad (14)$$

$$IDD_{CED_m} = (-0.00008CED_m + 2.0203) \text{ for } CED_m > 1610 \text{ and } < 3360 \quad (15)$$

$$IDD_{CEDm} = (-3 \times 10^{-9} (CED_m)^2 + 0.0002CED_m + 1.1971) \text{ for } CED_m > 3360 \quad (16)$$

The factor, ΔIDD is defined as follows:

$$\Delta IDD = IDD_{CEDm} / IDD_{specimen} \quad (17)$$

where IDD_{CEDm} is the initial dry density from molecular-level simulations, and $IDD_{specimen}$ is the initial dry density of strata. The modulus values obtained from the mechanical behavior model are reduced by the factor ΔIDD to account for macropores in the strata and to get the final modulus values.

4.3 Model validation

The model validation is mainly comprised of a testing program consisting of basic characterization tests, mineralogical study, and deformation properties, followed by the determination of CED and modulus values from the test results. Model validation has been carried out in two steps: (i) E-moduli validation at various strain levels from field and laboratory tests performed in this study and from an existing database, and (ii) validation through complete stress-strain plots.

4.3.1 E-moduli validation from current study

The mechanical behavior model is validated through laboratory testing on natural swelling soil samples and reconstituted laboratory specimens (control specimens) utilizing several proportions of soil constituents. Many soil constituents were selected to denote the utmost feasible composition of the natural swelling soils. Thus, individual soil constituents were attained from various known sources to prepare control samples. Natural soil samples were

acquired from the Qatif and Hofuf areas of Saudi Arabia, known for their swelling soils (Hameed, 1991; Abduljawwad & Al-Sulaimani, 1993; Abduljawwad et al., 1998; Ahmed et al., 2007). The large intact lumps and block samples of swelling soils were obtained from the dug test pits and were wrapped with plastic sheets to maintain the natural moisture content of these samples. Laboratory compacted bentonite samples were prepared from the Bentonite collected from a known source in Saudi Arabia (Kano Est., KSA). Bentonite was taken out of bags, oven-dried for 24 hours, and then put into air-tight containers for further sampling and testing. The control specimens were then prepared by static compaction in a compression machine.

Calcium carbonate was collected from Techno Pharmchem, India, and Gypsum samples were taken from Phosphate Plant, RIC, KSA. Sand samples were collected from the dunes in Jubail, KSA (Table 4-1) and mixed with Bentonite to formulate control specimens with different CED.

Basic characterization tests consisting of the grain size distribution (ASTM D6913), moisture content determination (ASTM D2216), and Atterberg limits (ASTM D4318) were performed on field-collected swelling clays and control specimens. Cation Exchange Capacity (CEC) tests were also carried out on swelling soils using Rayment & Higginson (1992) Method 15A2. The results of basic characterization tests are summarized in Table 4-2.

Table 4-1 Gradation analysis of sand used in this study

ASTM Sieve no.	10	20	40	60	100	200
Size (mm)	2.0	0.85	0.425	0.25	0.15	0.075
Passing (%)	100	92	58	35	19	2

X-ray diffraction (XRD) tests were performed using an Ultima IV X-Ray Diffractometer with copper radiation generated at 40 kV and 40 mA at the Research Institute (RI) in KFUPM. In this study, both quantitative and qualitative evaluations were performed to determine the type and amount of clay and non-clay minerals present in the samples. Randomly orientated samples (powdered specimens) were prepared by drying the sample in the oven and pressing it against the metal surface. Relative percentages of different clay and non-clay minerals in natural expansive clay samples of Hofuf and Qatif area and Bentonite are presented in Table 4-3.

Table 4-2 Summary of basic characterization tests

Material	Designation	Source	Classification	Atterberg Limits			CEC
				LL	PL	PI	
Bentonite	B	Kanoo Est., KSA	CH	442	85	357	71.3
Qatif Clay	Q	Qatif, KSA	CH	157	54	103	51.0
Hofuf Clay	H	Hofuf, KSA	CH	73	31	42	12.7
Calcium carbonate	C	Techno Pharmchem, India	-	-	-	-	-
Gypsum	G	Phosphate Plant, RIC, KSA	-	-	-	-	-
Sand	S	Jubail, KSA	SP	NP	NP	NP	-

Note: CH, high-plasticity clay; SP, poorly graded sand; NP, non-plastic; LL, liquid limit; PL, plastic limit; PI, plasticity index.

Table 4-3 Relative amount of minerals in clay-bearing soil samples

Clay Type	Relative Percentage (%)						
	Smectite	Palygorskite	Illite	Kaolinite	Calcite	Quartz	Gypsum
Bentonite	60	-	10	25	-	5	-
Qatif Clay	32	7	21	-	22	9	9
Hofuf Clay	3	5	35	-	40	17	-

To study the stress-strain response for the possible changes in fabric and structure, moisture-density relationships were established for the control specimens using the modified Proctor test procedures as per ASTM D1557. The results of the modified proctor test are provided in Figure 4-2. The control samples with recognized amounts of clay and non-clay minerals were arranged by static compaction in a compression machine at the moisture content and density on the "dry side of optimum," "optimum," and "wet side of optimum" using the results of the modified Proctor test to create different forms of fabric and structure. The undisturbed natural swelling soil samples were tested at the natural moisture contents and densities. The testing matrix for the experimental laboratory program carried out in this study is summarized in Table 4-4. These control and natural undisturbed specimens were then subjected to Unconsolidated Undrained (UU) Triaxial Compression tests as per ASTM D2850 to determine the stress-deformation properties. The stress-strain plots of UU Triaxial Compression tests for the controlled specimens and natural samples at a cell pressure of 300 kPa (the stress conditions the material will face in the field under most project conditions) are shown in Figure 4-3.

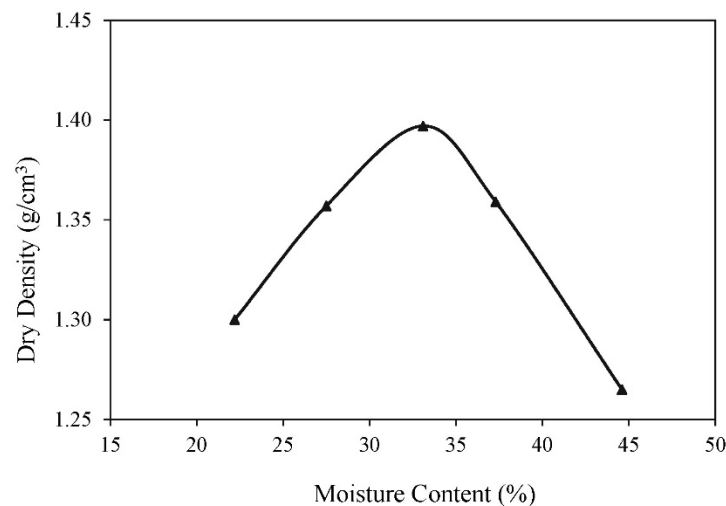


Figure 4-2 Moisture–density relationship (modified Proctor test)

Crosshole seismic tests were performed as per ASTM D4428 using Olson CS Equipment on swelling soils of the Hofuf area to validate the mechanical behavior model at low strain levels of 0.01% and lesser. In this test, three boreholes (spaced 3.0 m from center to center) were drilled in a straight line. The seismic waves were generated in one of the boreholes (called a "shot hole"), and its horizontal travel time was recorded in the other two boreholes (referred to as "receiver holes"). The holes were drilled and prepared for the tests before the testing by placing PVC pipes and grouting the annular space. The field procedure consisted of the generation of seismic waves in the shot hole and recording the time of arrival of waves in the receiver holes. The readings were recorded at 1.50m, 2.0m, 6.50m, 7.0m, and 7.50m in swelling clay layers at two different locations. Based on the velocity of propagation of the waves (shear and compression) in the medium, the modulus values of the sub-surface layers were determined. A summary of the results of cross-hole tests is tabulated in Table 4-5.

4.3.2 E-moduli validation from existing literature

The molecular-level simulation results were validated from the existing literature using data from two (02) swelling clays (MX-80 and FEBEX Bentonite). The FEBEX and MX-80 are the bentonites used as Engineered Barrier Systems in Finland, Sweden, and Spain. The mineralogical composition and materials properties of both FEBEX (calcium bentonite) and MX-80 (sodium bentonite) samples have been presented in Tables 4-6 and 4-7. The information about MX-80 is taken from Kiviranta and Kumpulainen (2011) and Kiviranta et al. (2016), whereas the information about FEBEX properties is collected from Enresa (2000).

Table 4-4 Testing matrix for laboratory program carried out in this study

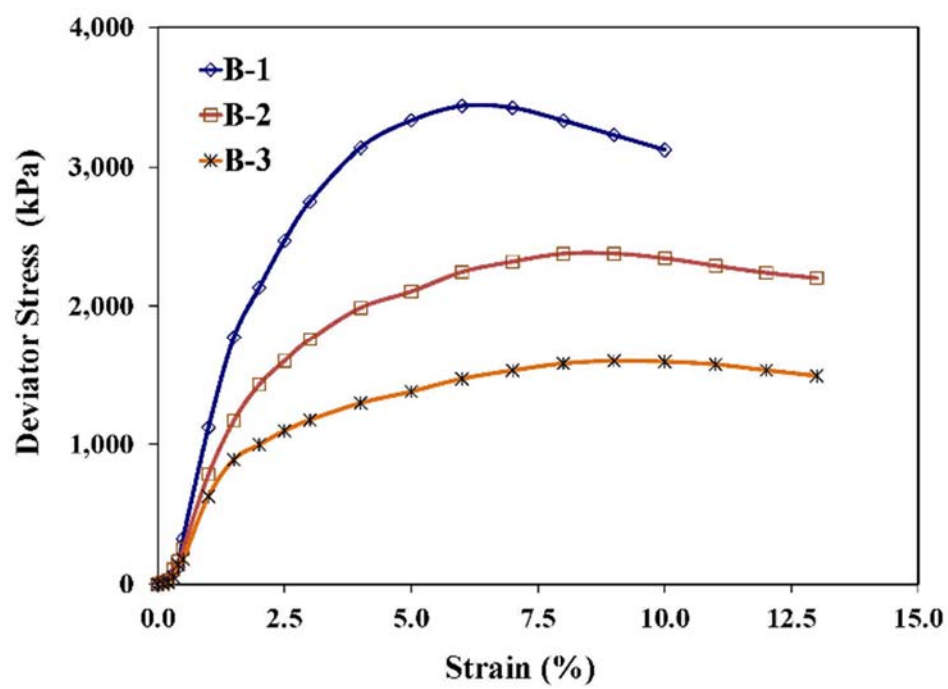
Sample ID	Constituent type and percent	Moisture content state	Moisture content (%)	Initial dry density (g/cm ³)
B-1	B100	Dry of OMC	25.00	1.327
B-2	B100	OMC	33.10	1.397
B-3	B100	Wet of OMC	39.90	1.327
BS-1	B90S10	Dry of OMC	25.00	1.327
BS-2	B70S30	Dry of OMC	25.00	1.327
BS-3	B90S10	OMC	33.10	1.397
BS-4	B80S20	OMC	33.10	1.397
BS-5	B70S30	OMC	33.10	1.397
BS-6	B90S10	Wet of OMC	39.90	1.327
BG-1	B90G10	OMC	33.10	1.397
BG-2	B85G15	OMC	33.10	1.397
BG-3	B80G20	OMC	33.10	1.397
BC-1	B85C15	Wet of OMC	39.90	1.327
Q-1	Natural Clay Samples	NMC	50.60	1.200
H-1	Natural Clay Samples	NMC	45.00	1.240

Note: B, Bentonite; G, Gypsum; C, Calcite; S, sand; OMC, optimum moisture content; NMC, natural moisture content.

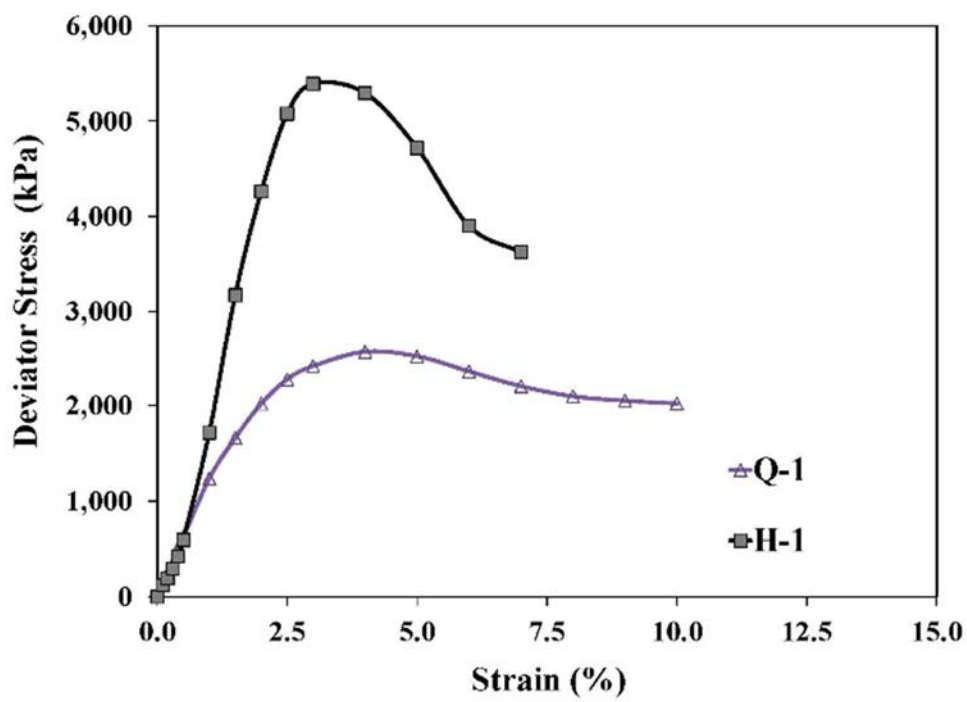
Table 4-5 Crosshole seismic test results in swelling clays of Hofuf

Sample ID	Depth of Source & Receiver (m)	Distance from S to R1 (m)	Travel Time of Wave from S to R1 (msec)		Distance from S to R2 (m)	Travel Time of Wave from S to R2 (msec)		Average Wave Velocity (m/sec)		Density ρ (g/cm ³)	Poisson's ratio ν	Modulus E (M Pa)
			P	S		P	S	P	S			
H-2	1.50	3.00	1.61	5.07	6.00	3.62	11.78	1760	551	1.820	0.44	1595
H-3	2.00	3.00	1.62	5.09	6.00	3.59	11.91	1762	547	1.840	0.44	1591
H-4	6.50	3.00	1.58	5.38	6.00	3.47	11.62	1814	537	1.920	0.45	1608
H-5	7.00	3.00	1.49	5.22	6.00	3.61	11.44	1838	550	1.930	0.45	1692
H-6	7.50	3.00	1.49	5.17	6.00	3.56	11.39	1849	554	1.930	0.45	1716

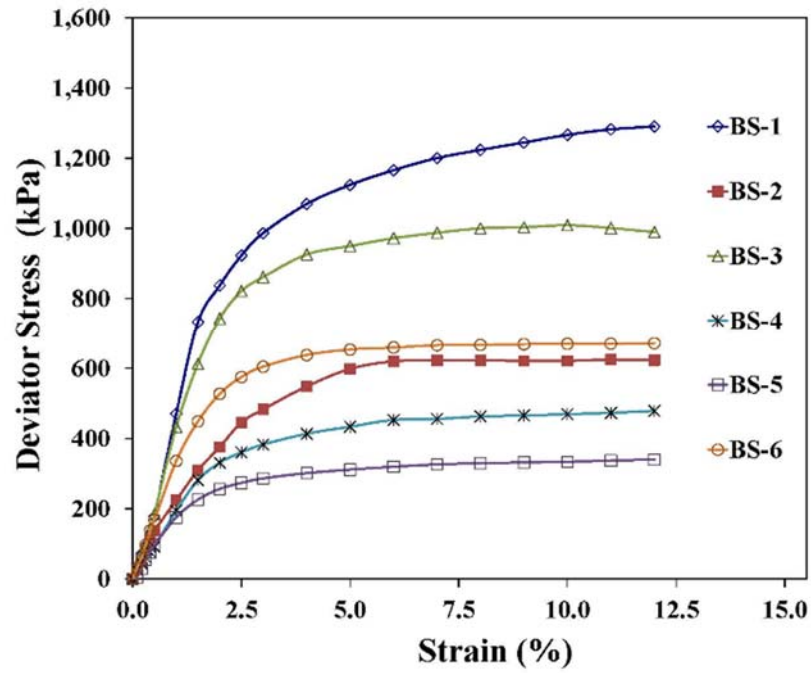
Notes: S=Shot hole; R1=First receiver hole; R2=Second receiver hole; P=Primary wave; S=Secondary wave



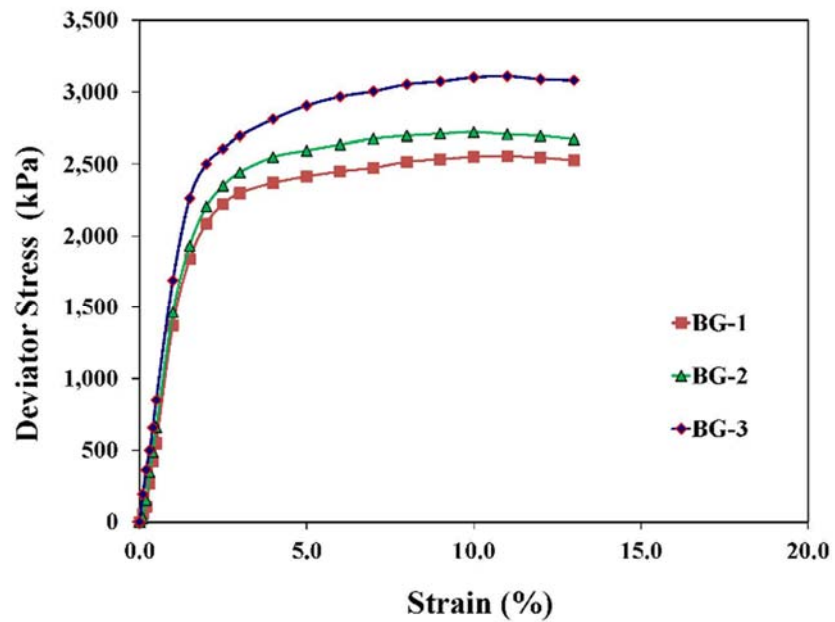
(a)



(b)



(c)



(d)

Figure 4-3 Stress-strain plots; (a) Bentonite samples on dry of optimum (B-1), optimum (B-2) and wet of optimum (B-3), (b) Swelling clay samples of Qatif and Hofuf at natural moisture content, (c) Bentonite mixed with sand, (d) Bentonite mixed with Gypsum

Table 4-6 Relative amount of minerals in FEBEX and MX-80

Clay Type	Relative Percentage (%)					
	Smectite	Quartz	Plagioclase	Cristobalite	Calcite	K- feldspar
FEBEX	92 ± 3	2 ± 1	2 ± 1	2 ± 1	0.50	Traces
MX-80	88.2 ± 5.2	3.5 ± 0.1	2.9 ± 0.7	Traces	-	2.4 ± 1.50

Table 4-7 Material properties of FEBEX and MX-80

Clay Type	Cation exchange capacity (eq/kg)	Liquid Limit (%)	Plasticity Index (%)	Specific Surface (m ² /g)	Density of solid particles (g/cm ³)
FEBEX	1.02	102	49	725	2.70
MX-80	0.86	500	450	624	2.78

Data on the mechanical properties of MX-80 and FEBEX bentonites were collected from Pintado X. et al. (2019). The resonant column tests on these bentonites were performed on different dry densities and degrees of saturation, and shear modulus ($G_{\max}$ or G_0) values were determined (Tables 4-8 and 4-9).

Table 4-8 Shear modulus values in FEBEX bentonite at $p = 0.80$ MPa

Specimen ID	Initial moisture content (%)	Initial Dry Density (mg/m ³)	Initial degree of saturation (%)	G_0 (GPa)
F-1	14.70	1.58	54	370
F-2	21.30	1.66	87	502
F-3	4.70	1.65	19	310
F-4	3.70	1.66	15	265
F-5	10.40	1.72	47	429
F-6	10.60	1.74	49	409
F-7	3.70	1.68	16	290
F-8	12.70	1.62	50	387

Note: p , confinement pressure.

Table 4-9 Shear modulus values in MX-80 Bentonite at $p = 0.80$ MPa

Specimen ID	Initial moisture content (%)	Initial Dry Density (mg/m³)	Initial degree of saturation (%)	Go (GPa)
MX-1	10.70	1.75	51	521
MX-2	19.00	1.56	69	409
MX-3	17.30	1.62	68	463
MX-4	24.70	1.58	92	253
MX-5	18.40	1.64	74	454
MX-6	21.10	1.68	89	303
MX-7	26.50	1.58	96	242
MX-8	17.00	1.61	67	394
MX-9	21.70	1.63	86	342
MX-10	15.40	1.66	63	449

Note: p , confinement pressure.

4.3.3 Stress-strain model validation

The model can be applied to predict stress-strain curves for clay-bearing soils/rocks. It can be used to predict the complete stress-strain behavior, including elastic, elastoplastic, peak strength, and post peak behavior. Since the model is developed from the realistic simulations of the interaction between clay and non-clay minerals, pore water, and dissolved salts, it results in the stress-strain plots, which constitute by default the elastic and elastoplastic behaviors.

The following step-wise procedure is adopted to generate stress-strain curves from the mechanical behavior model:

Step 1: The nano-level model parameter, cohesive energy density (CED), at initial conditions of moisture content and dry density, is determined using Equation (8).

Step 2: Equations (5) to (7) are used to find modulus value for the initial sample conditions at low strain level of 0.001%.

Step 3: The modulus values for successive strain increments of 0.01% to 10% are calculated using Equations (2) to (4).

Step 4: During the sample shearing stage, the CED and density of the sample change in response to various strain levels. This change in CED and density for each strain increment can be determined by a factor equal to $10^{-4} \times (E_2 - E_1)$. The E-value for next step is then determined against new CED and density values after each strain increment.

Step 5: The deviator stress can then be obtained from E-values after each strain increment using Equation (18), and results can be plotted as stress-strain curves.

$$E = \frac{\sigma_1 - 2\nu\sigma_3}{\epsilon} \quad 18$$

where σ_1 and σ_3 are the major and minor principal stresses, ν is Poisson's ratio, and ϵ is the strain.

CHAPTER 5

RESULTS AND DISCUSSIONS

This chapter contains the major findings and discussions of the three major levels of this research, i.e., molecular-level simulations, model formulation, and model validation.

5.1 Hydro-mechanical behavior

Based on the mineralogical composition, CEC, initial moisture content, and density values, CED values were determined for the samples used in this study and also for MX-80 and FEBEX bentonites using the relationships presented in Equations (8) to (12) and the results are provided in Table 5-1. The modulus (E_i) values for the natural undisturbed and control specimens of swelling soils at any given strain level were estimated using stress-strain plots of UU triaxial compression tests (Figure 4-3) using the hyperbolic function (Kondner, 1963).

For MX-80 and FEBEX bentonites, the hardening soil model (Equation 19) introduced in Plaxis was used to estimate the variation of G and the corresponding E with strain level.

$$G(\gamma) = \frac{G_o}{1 + 0.385 \frac{\gamma}{\gamma_{0.7}}} \quad (19)$$

In Equation (19), $\gamma_{0.7}$ corresponds to the strain at which the modulus G is $0.722G_o$. The following relationship given by Pintado et al. (2019) was used for $\gamma_{0.7}$ and shear modulus at a small strain.

$$\gamma_{0.7} = 2.60 \times 10^{-7} \times G_o^2 \quad (20)$$

The modulus values were determined for all the tested specimens of natural and compacted clays, and the results are summarized in Table 5-2. Table 5-2 also includes the modulus values obtained from the crosshole seismic tests, represented by sample IDs H-2 to H-6 to validate the mechanical behavior model at low strain levels. The estimated modulus values for two (02) swelling clays (MX-80 and FEBEX bentonite) against varying CED values are also presented in Table 5-3. The calculated modulus values were then plotted on the mechanical behavior model plots developed in this study (Figure 5-1).

Based on these results, the CED values range from 1130 J/cm³ to 9543 J/cm³, with moisture contents varying from 25.0% to 50.6% for both natural and control samples. The test results presented in Table 5-1 dictate that the final CED values of the tested samples vary from 633 J/cm³ to 4103 J/cm³, and the modulus values range from 0.021 to 1.0 GPa at strain levels varying from 0.10% to 10.0%. The modulus values from low-strain crosshole tests were found to be 5.77 to 6.09 GPa against the final CED values of 3995 to 4137 J/cm³.

As discussed earlier, three zones can be identified from the mechanical behavior model plot: (i) Zone I between a CED value of 584 J/cm³ and 1450 J/cm³ in which the modulus values increase with an increase in CED, (ii) Zone II from a CED value of 1450 J/cm³ to 2640 J/cm³ where there is a tendency of reduction in the modulus values with the increase in CED, and (iii) Zone III having CED of more than 2640 J/cm³ showing an increasing trend in the modulus values with the increase in CED due to cementation.

It can be observed from Figure 5-1 that all tested bentonite samples fall in Zone I. The final CED values of the tested bentonite samples range from 791 J/cm³ to 931 J/cm³. The modulus value at a 1.0% strain level and a CED of 791 J/cm³ are estimated as 0.106 GPa, whereas it is

0.236 GPa at a CED of 931 J/cm³. This confirms an increasing trend in the modulus values in Zone I with an increase in CED. The FEBEX bentonite samples are lying in Zone II of the mechanical model. The decrease in modulus values is observed in FEBEX bentonite samples with an increase in CED, which can be very well correlated with the lower moisture content of 4.70%, 3.70%, and 3.70% in samples F-3, F-4, and F-7, respectively. The undisturbed natural samples of swelling clays of Hofuf and Qatif areas fall in Zone III. The mineralogical composition of Hofuf and Qatif clays shows the presence of Gypsum and Calcite (Table 4-3) in the samples. The CED values of Hofuf and Qatif clays are calculated as 4103 J/cm³ and 3167 J/cm³, respectively. The higher CED values in Zone III are caused by an increase in cementation due to binding salts, which increases the stiffness values with CED. The modulus values of Hofuf and Qatif clays are estimated to be 0.891 GPa and 0.387 GPa, respectively, at a 1.0% strain level, validating an increasing trend of modulus values with CED in Zone III.

A comparison is also provided in Tables 5-2 and 5-3 between the laboratory and field-determined modulus values from crosshole tests and the ones predicted by the mechanical behavior model through Equations (2) to (7). It can be seen from the results that the modulus values of the tested samples at strain levels of 0.001 to 10% are in very close agreement with the model predictions. However, a major discrepancy was seen for the bentonite samples with Calcite as a cementing agent, which can be due to the relatively low solubility of Calcite in distilled water.

Table 5-1 Cohesive energy density (CED) values

Specimen Details			Mineralogy							Exchangeable Cations					CED	
Sample ID	Initial water content (%)	Initial dry density (g/cm ³)	Swelling clay minerals (%)	Palygorskite (%)	Non-clay / Non-swell (%)	Gypsum (%)	Fraction of Swelling clay minerals	Calcite (%)	Fraction of Swelling clay minerals	CEC	Na	Ca	Mg	K	CED (J/cm ³)	CEDm (J/cm ³)
B-1	25.00	1.327	70	0	30	0	0	0	0	71.3	0.76	0.14	0.10	0.10	1545	1330
B-2	33.10	1.397	70	0	30	0	0	0	0	71.3	0.76	0.14	0.10	0.10	1296	1130
B-3	39.90	1.327	70	0	30	0	0	0	0	71.3	0.76	0.14	0.10	0.10	1305	1138
BS-1	25.00	1.327	63	0	37	0	0	0	0	71.3	0.76	0.14	0.10	0.10	1545	1330
BS-3	33.10	1.397	63	0	37	0	0	0	0	71.3	0.76	0.14	0.10	0.10	1296	1130
BS-6	39.90	1.327	63	0	37	0	0	0	0	71.3	0.76	0.14	0.10	0.10	1305	1138
BG-1	33.10	1.397	63	0	37	10	0.06	0	0	71.3	0.76	0.14	0.10	0.10	1296	1783
BC-1	39.90	1.327	59.5	0	40.5	0	0	15	0.09	71.3	0.76	0.14	0.10	0.10	1305	3356
Q-1	50.60	1.200	53	7	40	9	0.048	22	0.132	51.0	0.50	0.50	0.00	0.00	1066	5278
H-1	45.00	1.240	38	5	57	0	0	40	0.17	12.7	0.50	0.50	0.00	0.00	611	9543
F-1	14.70	1.580	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3046	2004
F-2	21.30	1.660	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	2542	1681
F-3	4.70	1.650	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3607	2597
F-4	3.70	1.660	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3635	2716
F-5	10.40	1.720	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3338	2223
F-6	10.60	1.740	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3326	2212
F-7	3.70	1.680	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3635	2716
F-8	12.70	1.620	89	0	11	0	0	0.5	0.004	102	0.24	0.42	0.31	0.03	3189	2105
MX-1	10.70	1.750	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	2499	1779
MX-2	19.00	1.560	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	2089	1506
MX-3	17.30	1.620	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	2181	1567
MX-4	24.70	1.580	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	1787	1305
MX-5	18.40	1.640	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	2122	1528
MX-6	21.10	1.680	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	1975	1430
MX-7	26.50	1.580	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	1702	1248
MX-8	17.00	1.610	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	2197	1578
MX-9	21.70	1.630	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	1943	1408
MX-10	15.40	1.660	83	0	17	0	0	0	0	86	0.61	0.27	0.10	0.02	2281	1634

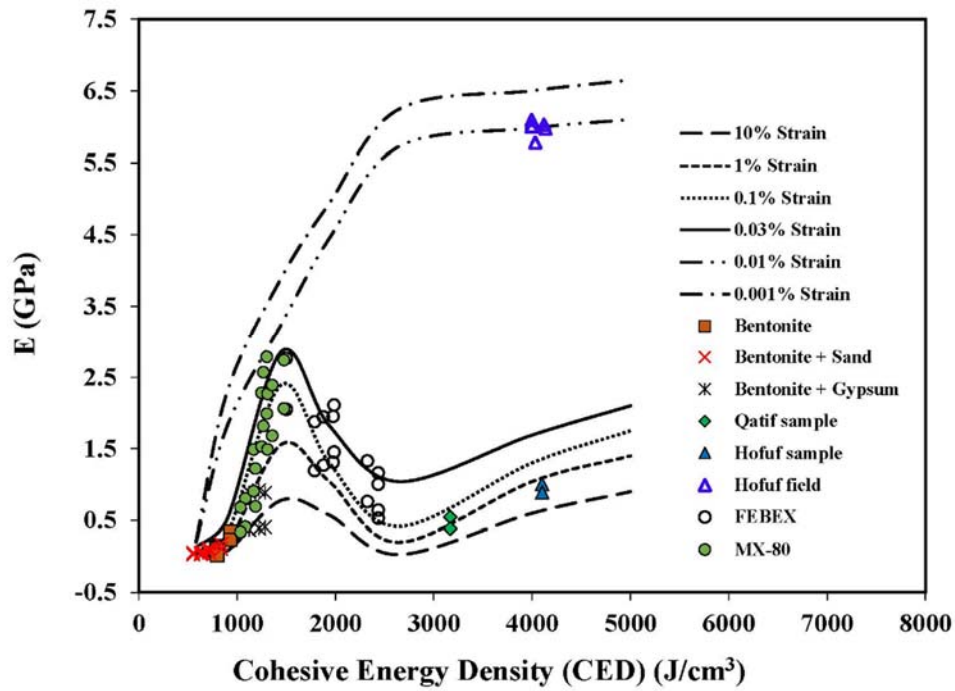
Table 5-2 Modulus determination from test results and comparison with mechanical model predictions

Sample ID	Initial moisture content (%)	Initial dry density (g/cm ³)	CED _m	Strain Level, γ (%)	E _i (kPa)	IDD _{CED_m} (g/cm ³)	Δ IDD	Δp_c	CEC Ratio	Final CED	E _m (GPa)	Model prediction, E _{model} (GPa)
B-1	25.00	1.327	1330	0.10	183900	1.71	1.29	1.43	0.70	931	0.339	0.414
B-2	33.10	1.397	1130	0.10	117300	1.23	0.88	1.43	0.70	791	0.148	0.191
B-3	39.90	1.327	1138	0.10	96700	1.25	0.94	1.43	0.70	797	0.130	0.197
B-1	25.00	1.327	1330	1.00	127800	1.71	1.29	1.43	0.70	931	0.236	0.206
B-2	33.10	1.397	1130	1.00	84200	1.23	0.88	1.43	0.70	791	0.106	0.078
B-3	39.90	1.327	1138	1.00	59300	1.25	0.94	1.43	0.70	797	0.080	0.082
B-3	39.90	1.327	1138	10.0	15500	1.25	0.94	1.43	0.70	797	0.021	0.021
BS-1	25.00	1.327	1330	0.10	94500	1.71	1.29	1.43	0.63	838	0.174	0.252
BS-2	25.00	1.327	1330	0.10	33500	1.71	1.29	1.43	0.49	652	0.062	0.094
BS-3	33.10	1.397	1130	0.10	84000	1.23	0.88	1.43	0.63	712	0.106	0.121
BS-6	39.90	1.327	1138	0.10	80400	1.25	0.94	1.43	0.63	717	0.108	0.124
BS-1	25.00	1.327	1330	1.00	59500	1.71	1.29	1.43	0.63	838	0.110	0.112
BS-4	33.10	1.397	1130	1.00	24300	1.23	0.88	1.43	0.56	633	0.031	0.033
BS-6	39.90	1.327	1138	1.00	40500	1.25	0.94	1.43	0.63	717	0.054	0.044
BG-1	33.10	1.397	1783	0.10	417885	2.07	1.48	1.43	0.63	1123	0.888	0.928
BG-2	33.10	1.397	2055	0.10	437250	2.05	1.47	1.43	0.60	1223	0.919	1.287
BG-1	33.10	1.397	1783	1.00	173900	2.07	1.48	1.43	0.63	1123	0.370	0.517
BC-1	39.90	1.327	3356	0.10	151400	1.93	1.46	1.43	0.60	1997	0.316	1.370
BC-1	39.90	1.327	3356	1.00	69100	1.93	1.46	1.43	0.60	1997	0.144	0.945
Q-1	50.60	1.20	5278	0.10	182800	2.50	2.08	1.43	0.60	3167	0.544	0.809
Q-1	50.60	1.20	5278	1.00	129800	2.50	2.08	1.43	0.60	3167	0.387	0.546
H-1	45.00	1.24	9543	0.10	262800	3.32	2.67	1.43	0.43	4103	1.007	1.386
H-1	45.00	1.24	9543	1.00	232500	3.32	2.67	1.43	0.43	4103	0.891	1.026
H-2	44.70	1.26	9589	0.001	1595022	3.32	2.64	1.43	0.43	4123	6.028	7.113
H-3	44.50	1.27	9620	0.001	1590565	3.33	2.62	1.43	0.43	4137	5.974	7.119
H-4	46.10	1.31	9378	0.001	1607738	3.29	2.51	1.43	0.43	4033	5.778	7.072
H-5	46.70	1.32	9292	0.001	1691631	3.27	2.48	1.43	0.43	3995	6.005	7.055
H-6	46.70	1.32	9292	0.001	1715810	3.27	2.48	1.43	0.43	3995	6.091	7.055

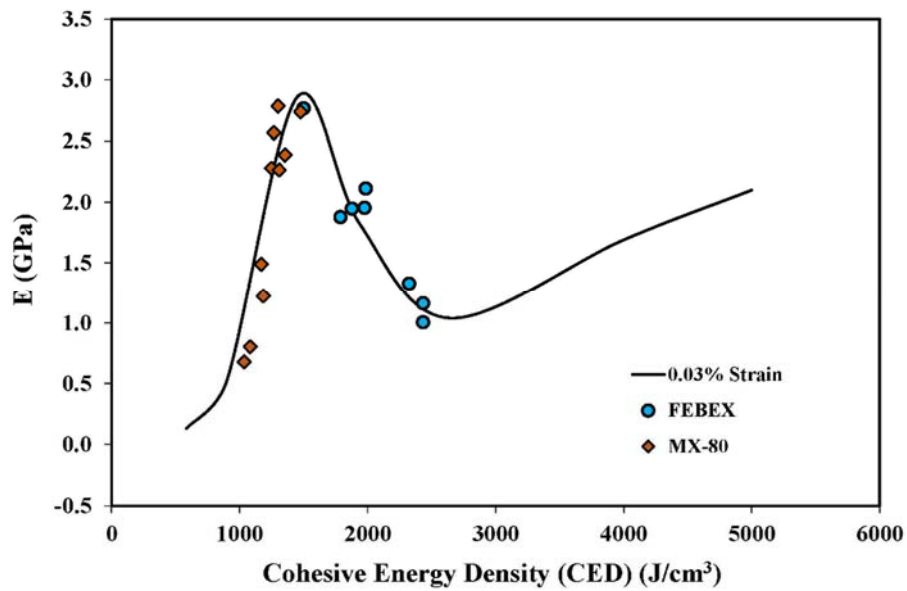
Note: E_i, modulus value from field and laboratory tests; E_m, final modified modulus value after corrections and upscaling.

Table 5-3 Modulus determination for FEBEX and MX-80 and comparison with mechanical model predictions

Sample ID	Initial moisture content (%)	Initial dry density (g/cm ³)	Degree of saturation (%)	CED _m	G _o (MPa)	Strain Level, γ (%)	Strain Level, $\gamma_{0.7}$ (%)	G _{γ} (MPa)	E _i (MPa)	IDD _{CED_m} (g/cm ³)	Δ IDD	$\Delta\rho_c$	CEC Ratio	Final CED	E _m (GPa)	Model prediction, E _{model} (GPa)
F-1	14.70	1.58	54	2009	370	0.03	0.036	279	726	2.05	1.30	1.99	0.89	1788	1.875	2.003
F-2	21.30	1.66	87	1685	502	0.03	0.066	427	1110	2.08	1.25	1.99	0.89	1500	2.765	2.701
F-3	4.70	1.65	19	2612	310	0.03	0.025	212	551	2.00	1.21	1.99	0.89	2325	1.327	1.107
F-4	3.70	1.66	15	2735	265	0.03	0.018	162	422	1.99	1.20	1.99	0.89	2434	1.005	0.989
F-5	10.40	1.72	47	2231	429	0.03	0.048	346	899	2.03	1.18	1.99	0.89	1985	2.111	1.613
F-6	10.60	1.74	49	2220	409	0.03	0.043	323	840	2.03	1.17	1.99	0.89	1976	1.952	1.630
F-7	3.70	1.68	16	2735	290	0.03	0.022	190	493	1.99	1.18	1.99	0.89	2434	1.160	0.989
F-8	12.70	1.62	50	2111	387	0.03	0.039	298	776	2.04	1.26	1.99	0.89	1879	1.946	1.815
F-1	14.70	1.58	54	2009	370	0.10	0.036	178	462	2.05	1.30	1.99	0.89	1788	1.193	1.720
F-2	21.30	1.66	87	1685	502	0.10	0.066	316	822	2.08	1.25	1.99	0.89	1500	2.049	2.297
F-3	4.70	1.65	19	2612	310	0.10	0.025	122	317	2.00	1.21	1.99	0.89	2325	0.764	0.931
F-4	3.70	1.66	15	2735	265	0.10	0.018	85	222	1.99	1.20	1.99	0.89	2434	0.528	0.816
F-5	10.40	1.72	47	2231	429	0.10	0.048	238	618	2.03	1.18	1.99	0.89	1985	1.452	1.388
F-6	10.60	1.74	49	2220	409	0.10	0.043	217	564	2.03	1.17	1.99	0.89	1976	1.310	1.403
F-7	3.70	1.68	16	2735	290	0.10	0.022	105	273	1.99	1.18	1.99	0.89	2434	0.642	0.816
F-8	12.70	1.62	50	2111	387	0.10	0.039	195	506	2.04	1.26	1.99	0.89	1879	1.269	1.561
MX-1	10.70	1.75	51	1779	521	0.03	0.071	448	1164	2.07	1.19	1.99	0.83	1477	2.739	2.764
MX-2	19.00	1.56	69	1506	409	0.03	0.043	323	840	2.13	1.37	1.99	0.83	1250	2.279	1.847
MX-3	17.30	1.62	68	1567	463	0.03	0.056	384	997	2.28	1.41	1.99	0.83	1301	2.785	2.125
MX-4	24.70	1.58	92	1305	253	0.03	0.017	149	388	1.65	1.04	1.99	0.83	1083	0.804	1.080
MX-5	18.40	1.64	74	1528	454	0.03	0.054	374	971	2.18	1.33	1.99	0.83	1268	2.567	1.943
MX-6	21.10	1.68	89	1430	303	0.03	0.024	204	531	1.95	1.16	1.99	0.83	1187	1.223	1.530
MX-7	26.50	1.58	96	1248	242	0.03	0.015	138	358	1.51	0.96	1.99	0.83	1035	0.679	0.904
MX-8	17.00	1.61	67	1578	394	0.03	0.040	306	796	2.30	1.43	1.99	0.83	1310	2.263	2.176
MX-9	21.70	1.63	86	1408	342	0.03	0.030	248	644	1.90	1.16	1.99	0.83	1169	1.489	1.447
MX-10	15.40	1.66	63	1634	449	0.03	0.052	368	957	2.09	1.26	1.99	0.83	1356	2.388	2.451
MX-1	10.70	1.75	51	1779	521	0.10	0.071	337	876	2.07	1.19	1.99	0.83	1477	2.062	2.347
MX-2	19.00	1.56	69	1506	409	0.10	0.043	217	564	2.13	1.37	1.99	0.83	1250	1.530	1.398
MX-3	17.30	1.62	68	1567	463	0.10	0.056	274	712	2.28	1.41	1.99	0.83	1301	1.988	1.616
MX-5	18.40	1.64	74	1528	454	0.10	0.054	264	687	2.18	1.33	1.99	0.83	1268	1.816	1.473
MX-8	17.00	1.61	67	1578	394	0.10	0.040	202	524	2.30	1.43	1.99	0.83	1310	1.490	1.655
MX-9	21.70	1.63	86	1408	342	0.10	0.030	151	392	1.90	1.16	1.99	0.83	1169	0.907	1.085
MX-10	15.40	1.66	63	1634	449	0.10	0.052	259	673	2.09	1.26	1.99	0.83	1356	1.680	1.871

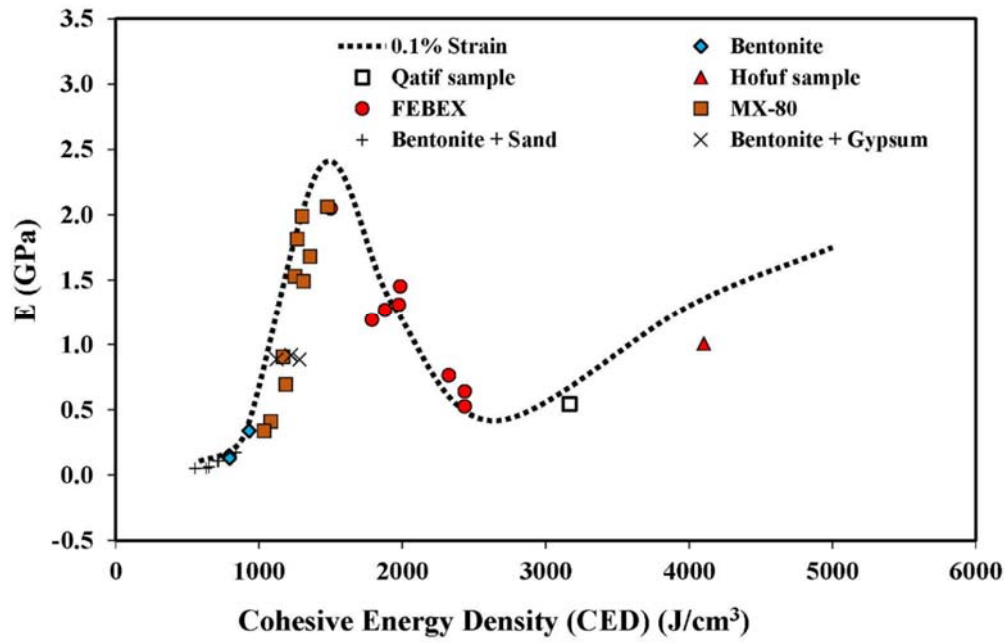


(a)

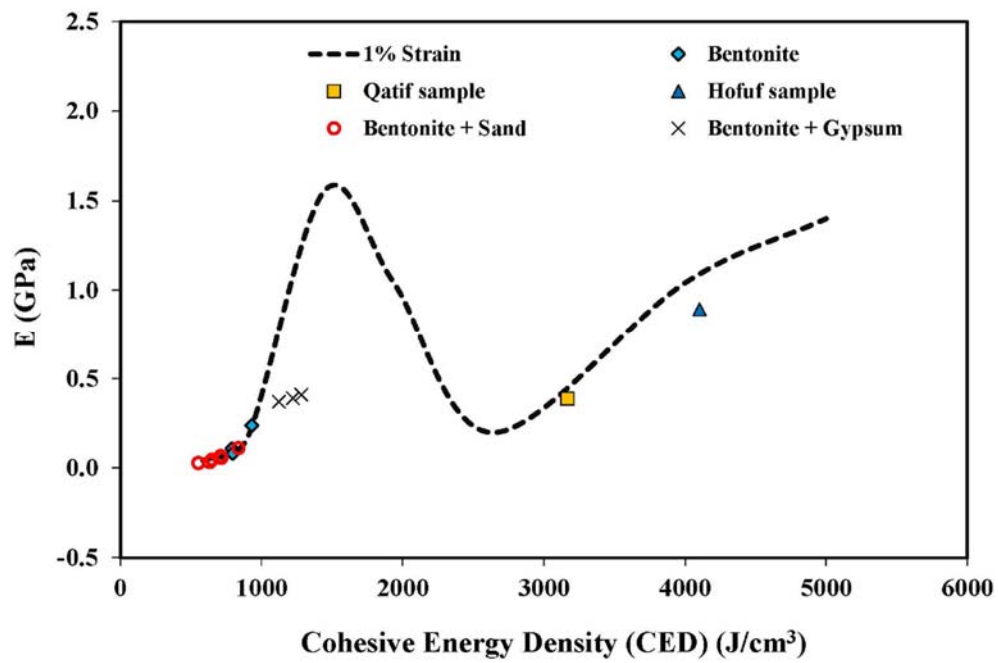


(b)

Figure 5-1 Mechanical behavior model validation; (a) Plot of all laboratory and field tests, (b) FEBEX and MX-80 samples on 0.03% strain level



(c)



(d)

Figure 5-1 Mechanical behavior model validation; (c) 0.10% strain level, (d) 1.0% strain level

Typically, foundations of civil engineering structures are placed in partially saturated soil layers. The moisture levels of the subsurface strata often increase after construction due to reduced evaporation, percolation of surface water(s), and the potential of leakage from utilities. An increase in the moisture level in the swelling soils below the foundations results in the swelling strains and associated reduction in the CED value depending upon the exchangeable cations, CECs, and binding/cementing agents present in the strata. In response to the swelling strains, the modulus value also decreases as a function of the difference between initial and final densities with respect to changes in CED value. This reduction in modulus value causes additional compressive strains under the constant superimposed loads from the structure. The net result of these coupled swelling and compressive strains defines the overall hydro-mechanical response of swelling soils under the foundations. The overall hydro-mechanical response is formulated through the coupling of the mechanical behavior model developed in this study with the existing nano-level swell behavior model by Ahmed and Abduljauwad (2017). The swell potential can be determined using the swell behavior model (Ahmed and Abduljauwad, 2017) from the following Equation:

$$\text{Swell (\%)} = (\text{FDD} - \text{IDD}) / \text{FDD} \times 100 \quad (21)$$

The initial dry densities (IDD) are calculated using Equation (13) to Equation (15). The final dry densities (FDD) are related to CED_m through the following correlations (Ahmed and Abduljauwad, 2017):

$$\text{FDD}_{\text{CED}_m} = \{ \text{IDD} + [(0.000007 \text{CED}_m + 0.3443) - \text{IDD}] \} \times (102/P)^{0.5} \text{CED}_m \text{ for } \text{CED}_m < 1610 \quad (22)$$

$$FDD_{CED_m} = \{IDD + [(0.0005CED_m - 0.4517) - IDD]\} \times (102/P)^{0.5} CED_m \text{ for } CED_m > 1610$$

and < 3360 (23)

$$FDD_{CED_m} = \{IDD + [(0.00006CED_m + 1.0082) - IDD]\} \times (102/P)^{0.5} CED_m \text{ for } CED_m > 3360$$

(24)

where FDD is in units of g/cm³, CED is in J/cm³, and P, seating/confining pressure, is in kPa.

Incremental swelling can be estimated on each incremental intake of water content using slope = (IDD-FDD)/(FWC-IWC). Final water content can also be assessed from the swelling behavior model as:

$$FWC = 0.0789CED_{vw} + 56.648 \text{ for } CED_{vw} < -87$$

(25)

$$FWC = 0.0039(CED_{vw})^2 + 1.0587 CED_{vw} + 106.44 \text{ for } CED_{vw} > -87$$

(26)

where FWC, final water content, is in units of percent and CED_{vw} is in J/cm³ and can be calculated from Equation (27) (Ahmed and Abduljawwad, 2017).

$$CED_{vw} = -0.081IWC^2 + 7.5421IWC - 131.1 + (-162G/0.2) + (-362C/0.1)$$

(27)

An illustration of the coupled hydro-mechanical behavior is made using a general case of a shallow foundation placed in a partially saturated swelling soil layer (Bentonite in this case) with initial conditions of IWC=25% and IDD=1.327g/cm³. The saturation level in the swelling soil layer is considered to increase from an initial water content of 25% to a final water content value of 35% after construction. The swell potential calculated through the swelling behavior model in ten equal increments of moisture content is presented in Table 5-4. A typical characteristic strain of 1.0% is considered for the modulus determination through Equation (2)

using the mechanical behavior model, and values are provided in Table 5-4, corresponding to each water content increment. The results are also presented in Figure 5-2, showing a decrease in CED values upon swelling and the corresponding reduction in the modulus values. The reduction in the modulus values from 0.206 GPa to 0.073 GPa against 5.13% swelling will cause additional compressive strains under the constant load from the structure. The foundation will finally be subjected to the net result of these coupled swelling and compressive strains.

The validation of coupled behavior through experimental data is also presented in Figure 5-2. The UU Triaxial Compression and swelling-potential tests (ASTM D4546) were performed on the samples prepared at an initial moisture content of 25% and then allowed to swell by adding water in increments of 1% to reach a final moisture content of 35%. The predictions of swelling percent and modulus values are in well agreement to the values obtained from test results.

The swelling behavior model proposed by Ahmed and Abduljawad (2017) has been verified using several laboratory control samples and the undisturbed samples acquired from the field in various studies carried out by Ahmed and Abduljawad (2017). This model has also been successfully used by Abduljawad and Ahmed (2017) for the prediction of swelling of field clay deposits.

Table 5-4 Coupled hydro-mechanical behavior

Sample parameters				CED			Swell behavior model				Mechanical behavior model		
Initial water content (%)	Initial dry density (g/cm ³)	Incremental Final water content (%)	Confining Pressure, P (kPa)	CED (J/cm ³)	CEDm (J/cm ³)	CEDvw (J/cm ³)	Terminal Final water content (%)	Terminal Final dry density (g/cm ³)	Incremental Final dry density (g/cm ³)	Swell (%) at P	Final CED	Strain Level (%)	E _{model} (GPa)
25	1.32	26	102	1545	1330	7	114	0.354	1.31	0.58	931	1.0	0.206
26	1.31	27	102	1505	1298	10	118	0.353	1.30	1.15	909	1.0	0.180
27	1.30	28	102	1467	1267	13	121	0.353	1.29	1.69	887	1.0	0.157
28	1.29	29	102	1431	1238	17	125	0.353	1.28	2.22	867	1.0	0.137
29	1.28	30	102	1398	1212	19	129	0.353	1.27	2.73	848	1.0	0.120
30	1.27	31	102	1367	1187	22	132	0.353	1.26	3.23	831	1.0	0.106
31	1.26	32	102	1340	1166	25	135	0.352	1.25	3.72	816	1.0	0.095
32	1.25	33	102	1317	1147	27	138	0.352	1.25	4.20	803	1.0	0.086
33	1.25	34	102	1298	1131	30	141	0.352	1.24	4.67	792	1.0	0.079
34	1.24	35	102	1283	1119	32	144	0.352	1.23	5.13	784	1.0	0.073

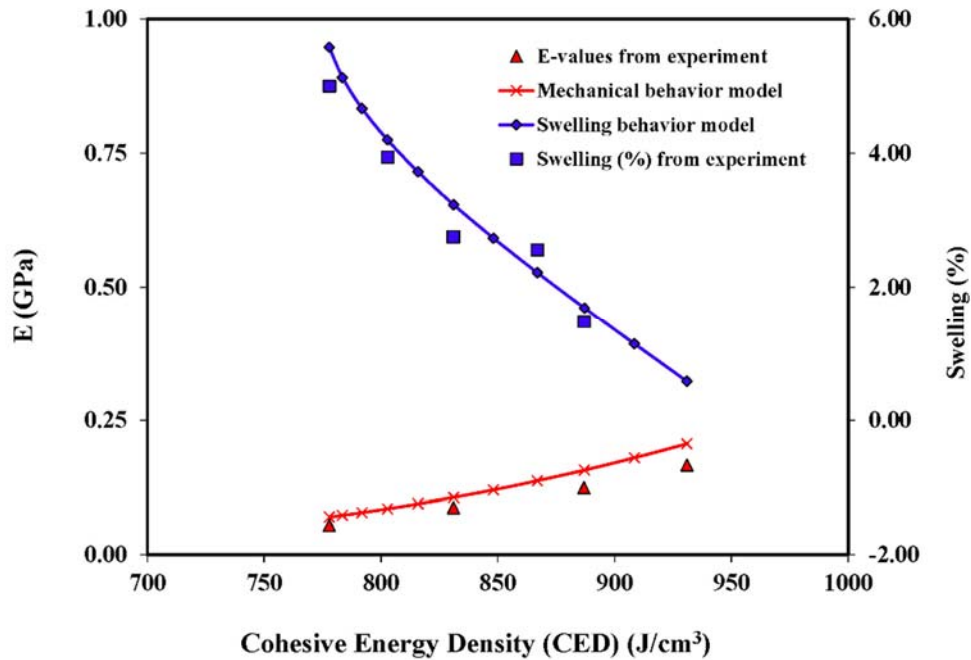
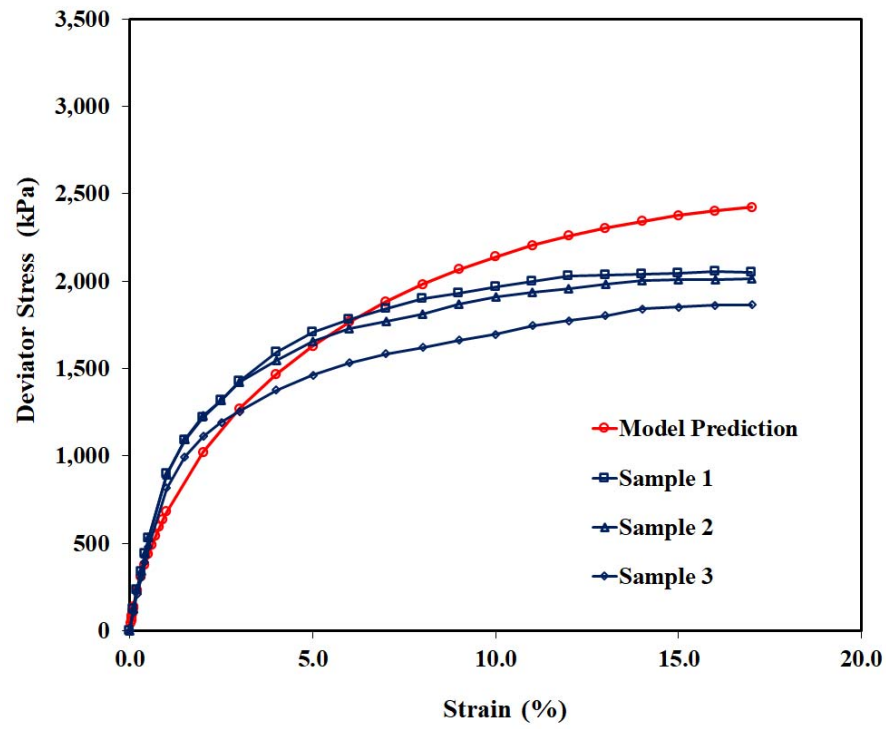


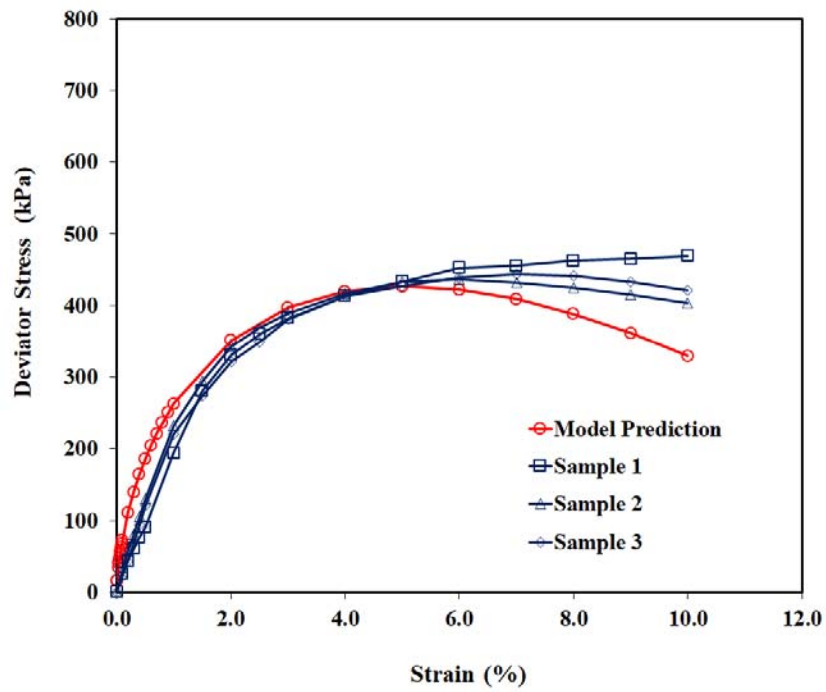
Figure 5-2 Coupled hydro-mechanical behavior and its validation

5.2 Stress-strain behavior prediction

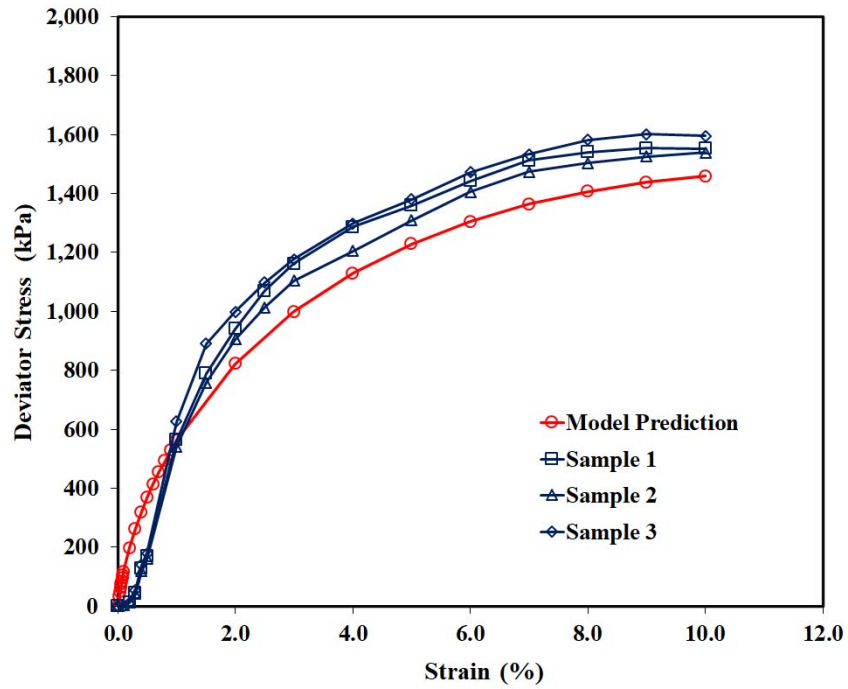
The model has been successfully applied to predict stress-strain curves for swelling soils. Figure 5-3 shows the stress-strain curves predicted from the model compared with the experimental curves generated from UU Triaxial Compression tests on both natural and controlled samples. The stress-strain curves predicted from the mechanical behavior model successfully captured the main features of the stress-strain response of swelling soils, including the initial elastic response, plasticity, peak strength, and post peak behavior. The experimental curves were obtained for three (03) replicated specimens of each set of four (04) different conditions to observe the variation in the stress-strain behavior among the tested specimens. The tests on reconstituted replicated specimens have resulted in similar stress-strain plots due to controlled sample parameters i.e., same sample constituents, initial dry density, and moisture conditions. The natural soil samples, however, have shown little variation in the peak stress and the corresponding strain values. This variation in peak stress is associated with the natural variation of several minerals quantified in the field samples of the Qatif clay. The variation in mineralogy is reflected by upper and lower bound model predictions against maximum and minimum gypsum content of 12% and 9% in the field samples, respectively.



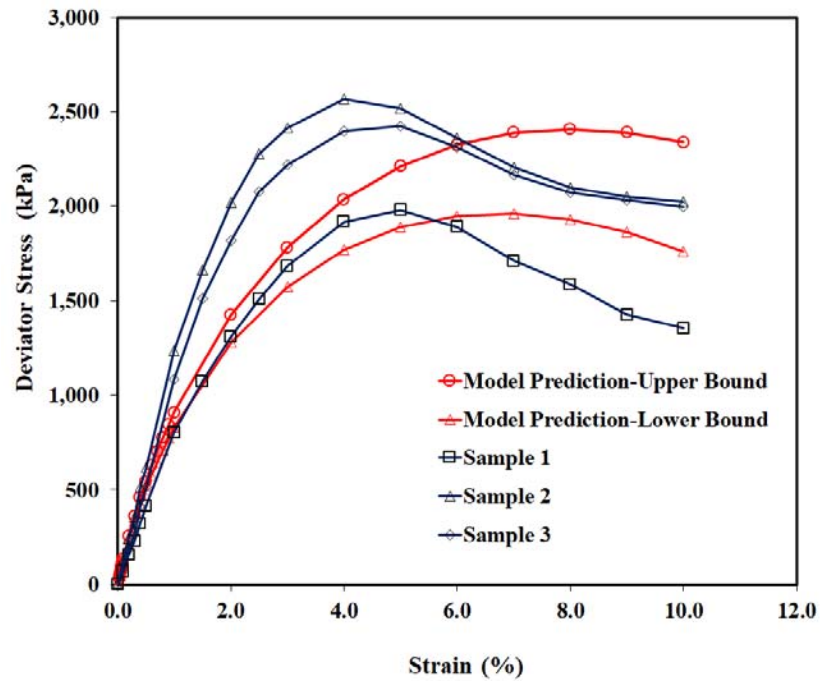
(a)



(b)



(c)



(d)

Figure 5-3 Model predictions of stress-strain plots; (a) Bentonite samples on dry side of optimum, (b) Bentonite samples mixed with 20% sand at optimum moisture content, (c) Bentonite samples on wet side of optimum, (d) Swelling clay samples of Qatif at natural moisture content

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The nano-level constitutive model presented in the previous chapters provides a state-of-the-art technique at the molecular level for modeling the swelling soils to predict the stiffness moduli and stress-strain response. This chapter provides a summary of the conclusions of this study and further recommendations for future research.

6.1 Conclusions

(i) In the molecular-level simulations, a swelling soil matrix constituting both clay and non-clay particles, pore water, and dissolved salts was created to model interactions among these particles. The results of molecular-level simulations were compiled to develop a hydro-mechanical model that can be utilized to predict the swelling-mechanical behavior of the swelling soils. The model can be applied to all possible combinations of clay and non-clay minerals with cementing agents.

(ii) The proposed model can be effectively used to predict the overall material behavior of the expansive soils, covering all possible variations in the structure and fabric of clay-bearing soils/rocks having nano, micro and macropores.

(iii) The model is characterized by a set of few parameters only, including cation exchange capacity, density, moisture content, and cohesive energy density, along with field stress conditions. These parameters can be determined from the basic characterization tests on the representative samples with great accuracy.

(iv) The predictions of stiffness moduli and stress-strain plots from the proposed model have been found to be in well agreement with the results obtained from the macro-level tests on the field and laboratory samples. Since the model is developed from the realistic simulations of the interaction between clay and non-clay minerals, pore water, and dissolved salts, it results in the stress-strain plots which constitute, by default, the elastic and elastoplastic behaviors.

(v) The coupled hydro-mechanical response under any given loading conditions can be well assessed through the coupling of the mechanical behavior model developed in this study with the existing nano-level swell behavior model by Ahmed and Abduljawad (2017).

(vi) The developed model has also been successfully validated from the existing literature using the data from two (02) swelling clays (MX-80 and FEBEX Bentonite). This suggests that the model can be used in all fields, such as civil engineering, agriculture in addition to the petroleum industry and waste management.

6.2 Future research recommendations

Following are the suggestions for future research through molecular-level modeling of swelling soils:

(i) The hydro-mechanical model developed in this study could be formulated into a numerical model using Finite Element Method (FEM) technique.

(ii) The developed model can further be extended by coupling the hydro-mechanical behavior model developed in this study with the other molecular-level swell behavior models for swelling soils.

(iii) The model can be extended to hydro-thermo-mechanical model for nuclear waste repositories.

(iv) The model application can also be extended to determine the mechanical properties of oil-contaminated clays and gas shales.

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VITAE

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Academic Background: |B.Sc. in Civil Engineering and M.Sc. in Geotechnical Engineering |

- More than **Fifteen (15) years** of **multinational experience** in the fields of geotechnical and geophysical explorations, engineering, design, and construction.
- April 2010 to date: **Technical / Regional Manager at Riyadh Geotechnique & Foundations (RGF) Co., Al-Khobar, Saudi Arabia.** Review and preparation of geotechnical (*Onshore & Offshore*) and geophysical (*Onshore*) investigation reports including the assessment of the adequacy of the scope of work, authenticity of the field and laboratory investigations, and the accuracy of the geotechnical data analysis and design. Design and review of the geotechnical designs including shallow and deep foundations, and soil-structure interaction problems.
- September 2007 to April 2010: **Geotechnical Engineer at NESPAK (Pvt.) Limited, Pakistan** and remained involved in the analysis, design, and report writing for the geotechnical investigation of various projects.

- ***Engineering/Computation Capacity***

Well-versed with *state-of-the-art* geotechnical analysis, design and evaluation softwares such as **Materials Studio, Plaxis 2D/3D, Allpile, LPile, APile, GRLWEAP, GEO Studio (Slope/W, Sigma/W), Settle 3D, RocPlane, RocFall, RocTopple, Slide, Pdisp, gINT, RES2DINV, RES3DINV, GEO-5** and others.

- ***Short Courses / Workshops***

- Workshop on Soil Stabilization and Ground Improvement, 2008, organized by Geotechnical Engineering Department, UET, Lahore.
- Workshop on Assertive Client Handling, 2009, organized by Human Resource Unit, NESPAK, Pakistan.
- Range of lectures on Plaxis 2D/3D by Bentley Institute.
- Attended various lectures on different dimensions of Geotechnical Engineering.
- Training and implementation of **ISO 17025** in various field and laboratory geotechnical tests.
- Remained involved in projects with **Key Clients, Consultants and Contractors** including Saudi Aramco, SEC, Royal Commission (RC) in Jubail, NEOM, Ma'aden, KJO, Municipalities, AECOM, Bechtel, Parsons, Jacobs Zate, Worley Parsons, SLFE, AMFW, KBR-AMCDE, Khatib & Alami, Saudi Oger, NESMA, Tamimi, JGC, Larsen & Turbo, Sepco, Saipem etc.
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- [1] **Muhammad Abdul Waheed**, Omar S. Baghabra Al-Amoudi, Mohammed A. Al-Osta, Habib-ur-Rehman Ahmed, “A universal hydro-mechanical coupled behavior model for clay-bearing strata – Molecular-level simulation approach”, 2023, Scientific Reports, 13:19925. <https://doi.org/10.1038/s41598-023-47402-3>.
- [2] **Muhammad Abdul Waheed**, Omar S. Baghabra Al-Amoudi, Mohammed A. Al-Osta, Habib-ur-Rehman Ahmed, “Molecular-level behavior induction in the constitutive modeling of swelling clayey soils – A review”, 2023, Transportation Geotechnics, 39 (2023) 100947.
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- [5] E. Spyropoulos, B Nawaz, A Ojo, H R Ahmed and **M A Waheed**, “Stability assessment of obliquely-bedded rock cuts using multi-prong procedures – case study”, EUROCK – Torino (Italy), 2021.
- [6] Emmanouil Spyropoulos, John Fahd Touma, Habib-ur-Rehman Ahmed and **Muhammad Abdul Waheed**, “CPT and SPT as complementary tests for the formulation of Geotechnical Design Profiles”, GeoChina 2021 International Conference.