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Research Paper

Compressibility of montmorillonite/kaolinite mixtures in consolidation testing using discrete element method

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ABSTRACT

In this study, the investigation of volumetric changes in soil containing montmorillonite and kaolinite and mixtures of the two has been carried out using the discrete element method (DEM). In order to achieve this goal, seven clay samples containing montmorillonite and kaolinite were prepared using the DEM by modeling all physicochemical forces between particles during consolidation testing. Particles were simulated in both flexible and non-flexible modes. The consolidation coefficients along the loading and unloading paths were found to be dependent upon the montmorillonite content of a given mixture. The results of analysis were then compared with those from laboratory testing.

1. Introduction

Clay can contain a variety of minerals and the behavior of saturated clay is dependent upon the types of mineral. Three common types of minerals found in clay soil, montmorillonite, kaolinite and illite, have been frequent topics of discussion in the technical literature. Under saturated conditions, each of these minerals exhibits a distinct type of volume change. Therefore, the behavior of saturated clay should be investigated separately for each mineral. Under natural conditions, it is evident that clay rarely contains one pure mineral and geotechnical projects are mainly performed on clay that is a mixture of several minerals. As such, determining the volume change of clay minerals and their mixtures for geotechnical projects such as the loading of foundations is very important.

Several laboratory studies have examined volume change in saturated clay, mainly through consolidation testing at different stress values. Also detailed experimental studies have been conducted on the different mixtures of clay minerals [1–3]. Tiwari and Ajmera [4] examined 36 samples, including montmorillonite, illite, kaolinite and quartz to characterize the volume change under different conditions. Hammad et al. [5] also carried out consolidation testing on a mixture of montmorillonite and kaolinite and found a correlation between the montmorillonite content and the volume change parameters. In recent years, XRD analysis and SEM images have aided identification of the microstructural characteristics of clay [6].

As stated, studies on clay mainly have been carried out in the laboratory. However, micromechanical and numerical methods offer distinct advantages for the study of the clay fabric and microstructural properties such as inter-particle forces, deformation and bending deflection of particles. One of the best micromechanical methods for such studies is the use of the discrete element method (DEM) [7]. Initially, Cundall and Strack [7] simulated disc-shaped particles and compared the results with investigations done by De Josselin de Jong and Verruijt [8] on photoelastic disks. DEM has been used mainly for the study of granular soil. In recent studies, various particle shapes, the development of contact law and fracture of particles have been investigated using DEM [9–13].

In some DEM studies on clay, the shape of the particles is assumed to be circular and motion law has been introduced as for sand. Andersson and Lu [14] investigated the effect of the chemical characteristics of pore fluid and clay minerals on the sedimentation and swelling behavior of clay and compared them with laboratory results. Lu et al. [15] then investigated the sedimentation and sedimentation velocity of kaolinite. In their study, the clay clusters were assumed to be circular and, when two particles were closer than a set minimum distance, they were assumed to act as a single particle.

In recent years, DEM researches have been carried out on plate-like clay particles. Anandarajah [16] simulated consolidation testing for plate-like particles of clay in which a diffuse double layer force of clay was implemented in addition to mechanical contact forces.

Abbreviations: CEC, cation exchangeable capacity; DDL, diffuse double layer

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Anandarajah modeled one-dimensional (1D) consolidation testing of kaolinite by implementing the physicochemical forces between particles as diffuse double-repulsion forces, Van derWaals attraction forces and mechanical forces [17]. Three-dimensional (3D) modeling of clay particles has been carried out using DEM in which clay particles were considered to be square-shaped and the electrostatic diffuse double-repulsion forces, Van derWaals attraction forces and mechanical forces are considered [18,19]. The effect of particle subdivision (clay particles separating into a number of individual particles) on swelling potential has been investigated in 3D simulations [20]. The results showed that particle subdivision results in significant increase in swelling.

Bayesteh and Mirghasemi have used DEM to investigate the properties of clay particles for 1D consolidation testing [21–23]. The results show that volume change is strongly influenced by the types of electrolyte and their concentrations. They found that, as the cation valance and electrolyte concentration increase, the thickness of the double layer decreases and, as a result, clay compressibility decreases [22].

All DEM studies carried out thus far have been done on a pure mineral; however, in engineering projects, clay is generally formed of a mixture of several minerals. This means that the behavior of a clay mass that includes several mineral types must be investigated. Clay minerals have different characteristics, including the specific surface, cation exchange capacity (CEC), thickness and thickness of the double layer. Therefore, a new method should be used to calculate the inter-particle forces of clay mineral mixtures.

Most studies have included non-flexible clay particles. In other words, deflection and flexibility of clay particles has not been considered in most studies despite the fact that XRD analysis and SEM images show that clay particles, especially at low porosities, exhibit flexibility. Deflection is more evident in smectite minerals than in other types [24]. It is therefore necessary to consider flexibility of clay particles in DEM simulations [17]. New inter-particle forces should be defined to maintain consistency between the segments of a particle.

In the present study, montmorillonite particles are modeled under flexible and non-flexible conditions and the results are compared with those from laboratory testing. Next, mixtures of montmorillonite and kaolinite are simulated and volume changes in the samples under 1D consolidation testing are investigated using a novel method to incorporate diffuse double-layer forces.

2. Theory

DEM involves a group of independent particles interacting through inter-particle forces. The main steps in this method are evaluation of inter-particle forces, identification of particles subjected to mechanical or physicochemical forces and the use of Newton's second law to determine the particle acceleration. By the double integration of acceleration in small time steps, the new position of each particle can be obtained. By knowing the new position of each particle in the particle assembly, the three steps can be repeated until they reach the desired state. The inter-particle forces include mechanical and physicochemical forces in which the physicochemical force is dependent on the specific surface of each particle, the cation exchange capacity (CEC) and the chemical characteristics of the pore fluid [25,26].

When a clay particle contacts an electrolyte, its active surface begins to interact with the cations and soluble chemicals in the electrolytes. The negative charge of the clay particles in the space between the plate-like particles causes ion distribution which generates an electrical double layer (EDL). The surface of the clay plates that contains the negative charge and ions that are released into the space adjacent to the particle is known as the diffuse double layer (DDL) [27]. Between clay particles, the DDL force is effectively applied as a repulsive force.

2.1. Calculation of DDL forces between clay particles

In the followings, the calculation of the DDL forces and associated equations are first done for a pure mineral type. Then calculations are made on montmorillonite and kaolinite mixtures. The method of calculating and applying the DDL force has been expressed for each case separately. Generally, there are three cases of applying DDL forces between particles in a mixture of montmorillonite and kaolinite such as montmorillonite - montmorillonite, kaolinite - kaolinite and kaolinite – montmorillonite particles. In the first and second cases, DDL forces are applied as for pure minerals that is described in Section 2.1.1. Section 2.1.2 discusses the way that kaolinite – montmorillonite repulsive DDL forces are calculated.

2.1.1. Repulsive forces between pure mineral particles

DDL forces are the most important physicochemical forces between clay particles, especially between montmorillonite particles [17]. In this study, the zone of DDL force effect (area of repulsion) was determined using the method developed by Bayesteh and Mirghasemi [22]. Langmuir's equation was used to calculate the DDL force between two infinite parallel particles of a pure mineral as shown in Eq. (1) [26]:

$$P = 2nkT \times [\cosh(u) - 1] \tag{1}$$

In this equations, u is the dimensionless potential between two parallel particles at any distance from the particle and is calculated using Eq. (2) as:

$$u = \frac{ve\phi}{kT} \tag{2}$$

$$z = \frac{ve\phi_0}{kT} \tag{3}$$

$$K = \sqrt{\frac{8\pi nv^2e^2}{\varepsilon kT}} \tag{4}$$

in which Z is the dimensionless potential on clay surface, k is the Boltzmann constant, ϕ is the potential at a distance of x from the surface of the clay particle, ϕ_0 is the potential on the surface of the clay particle and e is the charge of an electron. Anandarajah's experimental coefficients can also be used to obtain the repulsion force between the non-parallel finite particles of a pure mineral and its application point on each particle [16,28].

2.1.2. Repulsive forces between particles in a specimen with mixture of two minerals

As is known, the forces between clay particles include the DDL force, Van der Waals attraction force and mechanical force. The DDL force, especially in montmorillonite, has a greater effect than other forces. Thus, the DDL force between various mineral particles is introduced and the mechanical and Van der Waals attraction forces are calculated as has been done for particles of pure minerals. Given that this force is dependent upon the intrinsic properties of minerals, its magnitude will vary according to the type of mineral. The thickness of the DDL and the distribution of the electrical potential are a function of mineral type. The thickness of each particle can be calculated using Eq. (5) [17]. In Eq. (5), S and G_s are specific surface and specific gravity of clay mineral, respectively.

$$h = \frac{2000}{SG_s}\,(nm) \tag{5}$$

The dimensionless electrical potential (ϕ_0) can be calculated for each mineral as determined in Eq. (6). Then, assuming that the dimensionless electrical potential is equal to its maximum value for adjacent dissimilar minerals, the minimum potential between them can be obtained using Eq. (7). In these equations, ρ is the charge density, ε is the di-electric constant, n is the electrolyte concentration and T is the temperature.

$$\phi_0 = 2\sinh^{-1}\left(\frac{\rho}{230\sqrt{n.\ \varepsilon.\ T}}\right) \tag{6}$$