



Numerical simulation of pore fluid characteristic effect on the volume change behavior of montmorillonite clays

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ABSTRACT

The aim of this paper is to analyze the association between the volume change in clayey sealing materials and pore fluid chemistry under different stresses. Montmorillonite is considered because it is commonly used as a barrier in geo-environmental projects. Microscopic observations are numerically simulated using a discrete element method (DEM). A DEM code has been developed by considering both mechanical and diffuse double layer repulsion as interparticle interactions. The results show that volume change behavior is strongly influenced by the type of the electrolyte and its concentration. An increase in the valance of exchangeable cation and electrolyte concentration cause a reduction in the thickness of DDL and soil compressibility. The DEM simulations are compared with theoretical and experimental data, and their agreements are reported. It is concluded that DEM is a virtual laboratory for simulating the microstructural behavior of clay.

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1. Introduction

Compacted active clays are used as barriers in geo-environmental projects because of their low permeability and high buffering capacity [1,2]. Although there are many benefits to use of sensitive active clays such as Montmorillonite, they are known to be problematic. Their high specific surface areas (SSA) and high cation exchange capacities (CEC) result in large amounts of surface area being exposed to water. The water absorption forms new microstructure in these soils and leads to a change in their behavior [3]. The volume change behavior in the clays due to water absorption is a challenge for soil engineers. Changes in environmental conditions and the water table, seepage and leaching activity and the stress level on the soil after a load is applied are important factors in the compression of clayey soils [4]. In contrast to granular materials, the volume change in clays is very complex and depends not only on the solid skeleton structure and pore size distribution but also on the chemical interaction between clay minerals and pore fluids [5,6], causing difficulties in predicting the behavior of clays [7].

It has also been shown that the volume change in a clay is strongly dependent on the clay's microstructure, meaning that methods for examining such structures are the best tools for predicting their behavior [8–10]. A number of recent experimental studies have reported on the influence of mineral composition and

pore fluid characteristics in the compressibility of clays [11–13]. In those studies, laboratory odometer tests were used to model the one-dimensional compressibility of clays, and verification tools such as XRD analysis and SEM photos were prepared to evaluate microstructural changes during compression [14]. The results have indicated that pore fluid chemistry, cation exchange capacity, stress history, stress state, temperature and mineral type are the most important factors controlling the volume change behavior of clays [2,15,16].

Although experimental tests provide some understanding of clay behavior, they are limited because some parameters cannot be easily controlled. In particular, pore fluid characteristics and the initial particle structure are two important factors that should be carefully controlled before beginning experimental studies. These factors are difficult or sometimes impossible to control. For example, before investigating the role of exchangeable cations in clay behavior, pure clay should be prepared by repeated washing, first with a solution with a high concentration of the appropriate cation, then with distilled water; both washes should use a centrifuge when necessary [12]. In that process, dispersed fines may be lost, which itself will cause changes in the clay behavior [17]. It is also impossible to follow changes in interparticle forces during experimental tests [4]. Because of the problems with monitoring and controlling all of the parameters affecting material behavior, researchers recently have been electing to use numerical methods instead of experimental methods to describe clay behavior [18,19].

A commonly used numerical method that can simulate material behavior at the microscopic level is the discrete element method [20,21]. The DEM has recently been used in a computerized

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“virtual laboratory” [19,22]. Molecular dynamics (MD) have also been used to simulate material behavior at the atomic scale [23,24], but the DEM is more useful than MD for engineering [25–27]. Because soils are discontinuous, many researchers have recently turned to DEM for modeling cohesionless soil behavior [28–30].

Several studies have been performed using DEM to simulate clay behavior [31,32]. The primary assumption in these studies is that the clay particles are circular or elliptical. In these previous approaches, studies were conducted at the “cluster of particles” scale because the clayey particles’ shape at that scale is similar to a disk but at a particle scale is similar to a thick line [3,5]. The mechanical force is the only interparticle force included in these studies, and only a parameter was assumed instead of interparticle physico-chemical forces. This parameter is similar to the cohesion parameter (C) in Mohr–Colomb failure criterion. Existing codes for granular materials such as PFC [33] have been used to simulate clay behavior, and the contact detection algorithms for clays are the same as for granular materials. Although these studies are useful dealing with the mechanics of cohesive materials, the approach used is not sufficient to model clayey minerals at a particle-size scale.

Anandarajah [34] assumed clay particles to be straight lines and used electrical repulsive forces based on Gouy–Chapman theory to model clay behavior using DEM. Based on that study, complementary studies have been conducted in the past decade [35–37]. These studies indicated that DEM is a powerful method for modeling clayey soil behavior [38].

Most results reported in past studies discuss particular aspects of clay behavior, and some assumptions are based on diffuse double layer theory. The main aim of this paper is to enhance the existing method for calculating repulsive force and numerically examine the volume change behavior of clays with different pore fluid compositions and different stress levels. Simulations have been performed on pure montmorillonite with different salt concentrations, cation types and dielectric constants.

2. Simulation method

The DEM formulation is based on a group of discrete particles that are each treated as rigid elements interacting with their neighbors through interparticle forces. The three main steps in DEM calculation are the evaluation of interparticle forces, identification of contacting particles and the evaluation of Newton’s second law using the central difference method. In a DEM analysis, interparticle forces are determined based on suitable particle–particle interaction equations. Newton’s second law is then applied to find the acceleration of particles. The acceleration is then integrated twice to obtain a new estimate for the relative displacement of particles [20].

Defining the inter-particle interactions and forces is an important step in the DEM. In clay minerals, there are not only the mechanical forces but also physico-chemical interactions between the particles. Double layer repulsive forces and Van der Waals attractive forces are the main forces acting between clay particles. The magnitudes of these forces are based on the specific surface area (SSA), cation exchangeable capacity (CEC) of the clay particles and pore fluid chemistry [39,40].

The repulsive forces for some clayey minerals are more important than the attractive forces. The mass of the clay and the pH of the electrolyte are two major factors affecting the magnitude of the attractive forces [5,8,40]. Montmorillonite has a high SSA and CEC as well as a pH-independent behavior, so the repulsive forces between montmorillonite particles are larger than the Van der Waals attractive forces. Therefore, in this study, attractive forces have been neglected [6]. Details of the double layer repulsion and the mechanical forces are addressed below.

2.1. Double layer repulsive force

2.1.1. Theory

Clay particles behave electrically like plate capacitors. The plates, i.e., the clay crystal faces, are considered to be uniformly negatively charged over their surface. When they are located in a fluid, these charges are counterbalanced by positive ions and an electrical field is developed locally. As a result, the cation concentration decreases with increasing distance from the clay particles [41]. The clay surface and the distributed charges adjacent to it are called the diffused double layer (DDL) [3,5,11]. The Gouy–Chapman diffuse double layer theory has been used in many studies to model the interaction between clay particles and pore fluids [11,40,42]. The double layer repulsive force is a function of system variables, the static dielectric constant (ϵ) of the medium, the concentration and the valance of the cation (n, v), the intensity of the surface charge based on the surface potential (ψ_0) and the charge density (ρ), the temperature (T), and the distance between two particles.

Based on this theory, Langmuir’s Eq. (1) is used to calculate the double layer repulsive force between parallel infinite clay plates [40].

$$P = 2nkT[\cosh(u) - 1] \quad (1)$$

$$u = \frac{ve\phi}{kT} \quad (2)$$

$$z = \frac{ve\phi_0}{kT} \quad (3)$$

$$K = \sqrt{\frac{8\pi nv^2 e^2}{\epsilon kT}} \quad (4)$$

where “ u ” is the non-dimensional potential between two parallel particles at any distance as calculated using Eq. (2), “ z ” is the non-dimensional potential on the clay surface, “ k ” is Boltzmann’s constant ($=1.38 \times 10^{23}$ J/K), “ ϕ ” is the electric potential at a distance “ x ” from the clay surface, “ ϕ_0 ” is the electric potential at the clay surface and “ e ” is the charge on an electron ($=4.8 \times 10^{-10}$ esu).

Eq. (1) is valid for an ideal infinite parallel particle model. In reality, clay particles not only have limited lengths but are also located in random positions based on their degree of compaction and pore fluid chemistry [3,8]. Although there is no closed form solution for calculating repulsive forces between small particles, Lu and Anandarajah [44] developed an approximate method for calculating the repulsive force between two finite parallel particles [43]. This force is given by Eq. (5), where “ K ” is the reciprocal of the double layer thickness [40] as obtained using Eq. (4).

$$P = 2nkTK[\cosh(u) - 1] \quad (5)$$

2.1.2. Calculation electrical potential (u)

The non-dimensional electric potential (u) at the distance of interest is required to compute Eq. (1). Methods commonly used to calculate u can be grouped into three categories:

1. *Use of tabulated literature values.* Values for u derived from Gouy–Chapman theory were tabulated and presented by Van Olphen [40] for particular configurations. Although the use of tabulated values is suitable for estimating the repulsive force, tabulated values cannot be used easily in numerical simulations of particle interaction because of the need to interpolate between table entries.
2. *Use of semi-empirical equations.* Eq. (6) provides an example of a relationship for “ $u-Kd$ ” that was proposed by Sridharan and his coworkers [45,46] and Tripathy et al. [42] based on experimental data. In Eq. (6), “ Kd ” is a dimensionless parameter used

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