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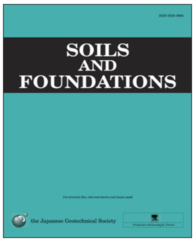

Numerical simulation of porosity and tortuosity effect on the permeability in clay: Microstructural approach

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Abstract

This study presents an analysis of the association between the coefficient of permeability of active clays and their porosity and tortuosity. Montmorillonite was selected because it is used as a barrier in geo-environmental projects and its sensitive structure results in wide variations in permeability when in contact with pore fluids. The microstructural approach was selected for a numerical simulation using the discrete element method (DEM). A DEM code was developed by considering the mechanical force, diffuse double-layer repulsion, and van der Waals attraction as the inter-particle interaction. The coefficient of permeability was calculated by simulating consolidation tests, and the DEM simulations were compared with the experimental data. The results show that the coefficient of permeability decreased as the void ratio decreased. At the same void ratio, there was a deviation between the coefficient of permeability for clay–electrolyte systems caused by the micro-fabric and variations in tortuosity. Micro-fabric evolution during loading showed that increasing the stress state caused a reorientation of the particles perpendicular to the direction of loading and increased the anisotropy of the particle orientation, increasing the tortuous flow path. A dispersed or oriented structure can occur at the same void ratio for different clay–electrolyte systems, causing variations in the coefficient of permeability.

Keywords: DEM; Tortuosity; Permeability; Clay microstructure; Numerical simulation; Montmorillonite

1. Introduction

Compacted active clays are used as barriers in geo-environmental projects because of their low permeability and high buffering capacity (Komine, 2008). In spite of the benefits of these active clays, they are known as problematic soils. The high specific surface area (SSA) and high cation exchange capacity (CEC) of clay cause more surface area to be exposed to pore fluid following the formation of the new fabric (Mitchell, 1993). The chemical compatibility of compacted soil has been of concern to geotechnical engineers and soil scientists since the early 1980s when the serious leakage of hazardous chemicals was discovered in underground burial facilities (Xu, 1994).

Changes in hydraulic conductivity are usually postulated to be the result of micro-fabric changes caused by pore fluid chemistry. For example, calcium montmorillonite has higher permeability than sodium montmorillonite (Mitchell, 1993). Thermodynamically, clay has a greater affinity for high concentrations of sodium and divalent cations (such as calcium) than lower concentrations. The tendency of clay to exchange a cation leads to the rearrangement of the particles, potentially changing the permeability (Guyonnet et al., 2005).

A number of studies have examined the permeability of clay in contact with various pore fluids (Petrov and Rowe, 1997;

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Notations

ε	static dielectric constant
n	concentration of cations
ν	valance of cations
$\psi 0$	surface potential
T	Temperature
l	particle length
H	Hamaker constant
α	angle between pair particles
Ks	shear stiffness coefficient
KN	normal stiffness coefficient
W	particle width
γ	fluid density
η	fluid viscosity
S	specific surface area
τ	Tortuosity
e	void ratio
Le	effective (or actual) length
θ	angle between flow direction and particle orientation
CEC	cation exchangeable capacity
Cv	coefficient of consolidation
mv	coefficient of volume compressibility
Aij	fabric tensor
M	anisotropy of the particle orientation

Siddiqua et al., 2011). These and other studies (Olsen, 1960; Mesri and Olson, 1971a) investigated the effect of the pore fluid, the stress level and the void ratio on the hydraulic conductivity of clay. The studies showed that increasing the stress level decreased the permeability as a result of a reduction in porosity. Mesri and Olson (1971a) showed that hydraulic conductivity varies for different pore fluids at the same void ratio. The effect of particle rearrangement on permeability was not investigated in these studies.

It has been shown that the hydraulic conductivity of clay is strongly dependent upon the type of particle fabric (Mitchell, 1993; Olsen, 1960). The rearrangement of the particles affects the tortuosity and porosity, two important microstructural parameters in the evaluation of permeability. This means that microstructural methods are the best approach for monitoring their behavior (Ichikawa et al., 2004). Experimental studies have traced variations in hydraulic conductivity at the microscopic scale using SEM and XRD analyzes (Melchior et al., 2002; Egloffstein, 2011).

Although experimental methods enhance the understanding of clay behavior, there are limitations to controlling all the parameters that could influence the results, especially since experimental tools cannot systematically evaluate the microfabric or the particle rearrangement. The pore fluid characteristics and the initial fabric of the samples should be prepared in the first stage of any experimental study (i.e., homoionic or disperse montmorillonite) (Mesri and Olson, 1971a). These processes are sensitive and occasionally inaccessible. Limitations to controlling and monitoring the parameters that affect the clay behavior have led researchers to use numerical methods in place of experimental methods (Zdravkovic and Carter, 2008).

A common numerical procedure for simulating soil behavior at the microscopic level is the discrete element method (DEM) (Cundall and Strack, 1979; Zhu et al., 2008), which has been used as a virtual laboratory (Zdravkovic and Carter, 2008; Munjiza, 2004). Due to the discontinuous nature of soil, researchers have tested the use of DEM models to simulate non-cohesive soils (Zhu et al., 2008; Liu et al., 2003) and cohesive soils (Anandarajah, 1994). The good agreement between DEM simulations and experimental results indicates that DEM models are powerful tools for modeling clay behavior (Anandarajah, 2003). The authors recently used DEM models to simulate one-dimensional compression behavior in montmorillonite (Bayesteh and Mirghasemi, 2013a; Bayesteh and Mirghasemi, 2013b). The results indicated compatibility between theoretical and existing experimental data.

Past studies quantified the effect of the void ratio and the stress level on clay hydraulic conductivity in contact with pore fluid (Yu and Li, 2004). Differences in permeability at the same void ratio in the results have been explained by the differences in particle arrangement and tortuosity; however, particle rearrangement and the variation in their tortuosity due to changes in pore fluid characteristics have not yet been quantified. To attain this goal, the present paper used DEM to systematically examine changes in the coefficient of permeability of montmorillonite at different pore fluid compositions and stress levels. A DEM model was used to investigate the anisotropy of a particle orientation and to evaluate the variations in microstructural parameters affecting the coefficient of permeability, such as tortuosity. Simulations were done on pure montmorillonite with different salt concentrations and cation types. The results indicate that, at the same porosity, the difference in permeability for montmorillonite at two pore fluid compositions depends on the variations in particle anisotropy and tortuosity. The main limitation of this study is the 2D modeling, considering the saturated media and the simulation behavior at high void ratios.

2. Theoretical background

The Kozeny-Carman (KC) equation is a widely-used relationship between the physical properties of a fluid, namely, the soil mass and the saturated hydraulic conductivity (Scholes et al., 2007), as shown in Eq. (1):

$$K = \frac{\gamma}{\eta}\frac{1}{\tau^2 S^2}\frac{e^3}{1+e} \tag{1}$$

where γ is the fluid density, η is the fluid viscosity, S(or SSA) is the specific surface area, τ is the tortuosity and e is the void ratio. Laboratory studies have shown that the KC equation can