Computers and Geotechnics 69 (2015) 272–278

Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Research Paper

Calculation of the repulsive force between two clay particles

Xiangyu Shang [a,b,*], Nian Hu [c], Guoqing Zhou [a]

[a] State Key Laboratory for Geomechanics and Deep Underground Engineering, China University of Mining & Technology, Xuzhou 221008, Jiangsu, China
[b] School of Mechanics & Civil Engineering, China University of Mining & Technology, Xuzhou 221116, Jiangsu, China
[c] Faculty of Engineering, The University of Nottingham, NG7 2RD Nottingham, UK

ARTICLE INFO

Article history:
Received 24 December 2014
Received in revised form 11 May 2015
Accepted 31 May 2015
Available online 16 June 2015

Keywords:
Clay particle
Electrical repulsion
Excess osmotic pressure
Maxwell's stress

ABSTRACT

Calculation of repulsive force between clay particles is important for discrete element simulations of clays. This paper discusses the repulsive forces between two clay particles on the basis of the model in which two identical plates with finite length are symmetrically placed about a mid-plane. It is proven that the electrical repulsion calculated by the method commonly adopted in the literature is actually the osmotic repulsion, which only considers the contribution from excess osmotic pressure but ignores the contribution from Maxwell's stress. A formula, which includes not only potential itself but potential gradient terms, is proposed to determine the total repulsive force between two clay particles. Finally, numerical calculations show that the errors due to neglecting the potential gradient terms can be up to over 25%.

1. Introduction

It is well known that clay particles carry charges on their surfaces. There are two typical types of charges: structural and surface. The structural charge is usually due to ion substitutions, although it can also be caused by structural imperfections of clay structure. The surface charge is usually due to chemical reactions that occur at the surface of clay minerals, but it can also be caused by adsorption of surfactant ions [1]. The existence of the charge results in the physico-chemical interaction forces between clay particles which significantly affect the macro mechanical properties of clayey soils such as compressive behaviour of clays under high pressure [2] and expansion process of expansive soils [3]. To understand these behaviour is of particular interest to engineers in field of mining, road and railway engineering.

As saturated clay is considered, it can be recognised that clays particles are charged particles in a dielectric fluid. When two charged particles are approaching each other in an electrolyte solution, there are two main inter-particle forces: electrostatic double-layer force and van der Waals force. Micro–macro links in mechanical behaviour of soils including clays have been an active research field over the last several decades. In order to investigate the above links, discrete element method (DEM) has been developed and widely used in the field of soil mechanics [4]. However, until now the application of DEM in non-cohesive granular materials is more successful than in clayey soils. One main reason is that the interaction between clay particles is more complex than that of granular grains. In sands, the contact force is most significant and electrostatic forces can be ignored. However, the calculation of physic-chemical interaction force between clay particles is of critical importance in DEM simulations of clays. Anandarajah and coworkers developed a series of calculation methods for repulsive and attractive forces between clay particles [5,6], and incorporated them into discrete element method [7,8]. By means of their DEM codes, they simulated macro mechanical behaviour of clays under one-dimensional compression [9] and triaxial shear [10,11]. These results demonstrate the great potential of DEM to disclose the macro–micro mechanical links of clays.

The interaction between two charged particles in electrolyte can be dated back to the problem of stability of colloidal suspensions. This problem has been investigated by Derjaguin and Landau [12] and Verwey and Overbeek [13] and their theory is called the DLVO theory. To determine the electrical force between clay particles using DLVO theory, it is necessary to simplify the shape of clayed particles and relative location of two particles based on the concept of electrical double layers. As early as in the 1950s, two infinite parallel charged plates with a separation were used as the model to calculate the electrical force, and it was shown that the results obtained from this simple model are consistent with the one-dimensional compressibility of clays from

* Corresponding author at: State Key Laboratory for Geomechanics and Deep Underground Engineering, China University of Mining and Technology, 1 Daxue Road, Xuzhou 221008, Jiangsu, China. Tel./fax: +86 516 83995678.

E-mail addresses: xyshang@cumt.edu.cn (X. Shang), evxnh4@nottingham.ac.uk (N. Hu), gqz@cumt.edu.cn (G. Zhou).

http://dx.doi.org/10.1016/j.compgeo.2015.05.017
0266-352X/

laboratory test [14]. This model is essentially one-dimensional (1D) and was used widely due to its simplicity since the analytical results can be obtained. Anandarajah and Lu [5] firstly calculated the repulsive force between two inclined charged platy particles with finite length which are symmetric about a mid-plane in a dielectric medium. It is evident that this two-dimensional (2D) model is more reasonable because actual clay particles are finite in length and non-parallel in general. They also argued that the repulsive force between two symmetrical charged platy particles depends only on the electrical potential along the mid-plane. This result is widely used in DEM simulations of clays up to now [3,8,9–11,15,16]. However, it is shown in this study that the repulsive forces between two clay particles with finite length not only depends on the potential itself but also on the potential gradient along the mid-plane. The main purposes of this paper is to propose a formula to accurately calculate the total repulsive inter-particle force based on this 2D model.

The outline of this paper is summarised as follows. Firstly, we introduce the basic conceptual model of clayey particle interactions and the general expression for calculating repulsive force, and the governing equations for electrical potential, i.e. Poisson–Boltzmann equations. Then we present a formula to more accurately calculate the total repulsive inter-particle force, and compare the calculated repulsive forces based on the proposed formula and those reported in the literature by means of numerical simulation.

2. Conceptual model

2.1. Excess osmotic pressure and Maxwell's stress

In an electrolyte solution, hydrostatic pressure and osmotic pressure of electrolyte ions are acting on an uncharged clay particle. When the particle gets charged, an electrical double layer (EDL) around the particle will be formed by the particle charge and electrolyte ions, as shown in Fig. 1. Whithin the EDL, the number of counter ions are much larger than that of co-ions. Thus electrolyte ions (mainly counterions) in the EDL exert an excess osmotic pressure on the particle, which is the difference in the local osmotic pressure between the EDL and the bulk electrolyte solution. Meanwhile, Maxwell's stresses acting on the charged particles shown in Fig. 1 mainly result from the coulomb attraction between the charges on the particle surface and the counterions within the EDL. It is noteworthy that direction of Maxwell's stress is opposite to that of excess osmotic pressure. Thus the electrical double layer induces two additional stresses on the charged particle: the excess osmotic pressure and Maxwell's stress.

2.2. Interaction between the electrical double layers

When two clay particles get closer, the overlap between their electrical double layers results in the interaction forces between them. This reaction force becomes repulsive for the cases of two particles with charges of the same sign. As shown in Fig. 2, the excess osmotic pressure increases due to the further increasing concentration of counterions in the zone between two particles. Meanwhile, the Coulomb attraction induced by the counterions also increases. However, the Coulomb repulsion induced by the charges on the other particle also increases. Thus the net Maxwell's stress on particle is reduced. For two identical particles with charges of the same sign, the electrostatic interaction is always repulsive.

2.3. Electrostatic force on a charged particle

The general electrostatic force acting on a charged particle can be obtained equivalently by integrating electrostatic stress field on any closed surface including the charged particle [12,13,17,19]. As shown in Fig. 3, for any closed surface Σ enclosing particle 1, the interaction force acting on particle 1 is equal to the total force acting on Σ. Thus the interaction force acting on particle 1 can be determined by integrating Maxwell's stress and excess osmotic stress on closed surface Σ as follows [17]

$$f_i = \oint\!\!\!\oint_{\Sigma} (\Delta\Pi n_i - \sigma_{ij} n_j) dS \tag{1}$$

where $\Delta\Pi$ is the excess osmotic stress and σ_{ij} is Maxwell's stress:

$$\sigma_{ij} = \varepsilon\left(E_i E_j - \frac{1}{2}E^2\delta_{ij}\right) \tag{2}$$

where ε is the constant permittivity in the electrolyte and E_i is electric vector field with magnitude E. According Faraday's law, the electric vector can be related to the electric potential ψ as follows:

$$E_i = -\nabla_i \psi \tag{3}$$

The osmotic repulsive force between clay particles arises from the non-uniform counterion concentration in the clay–electrolyte solution system. The local excess osmotic stress is

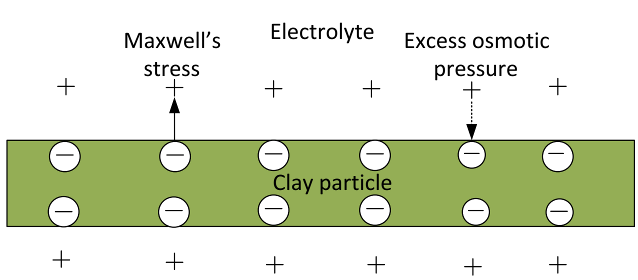

Fig. 1. Electrical double layer around a charged clay particle.

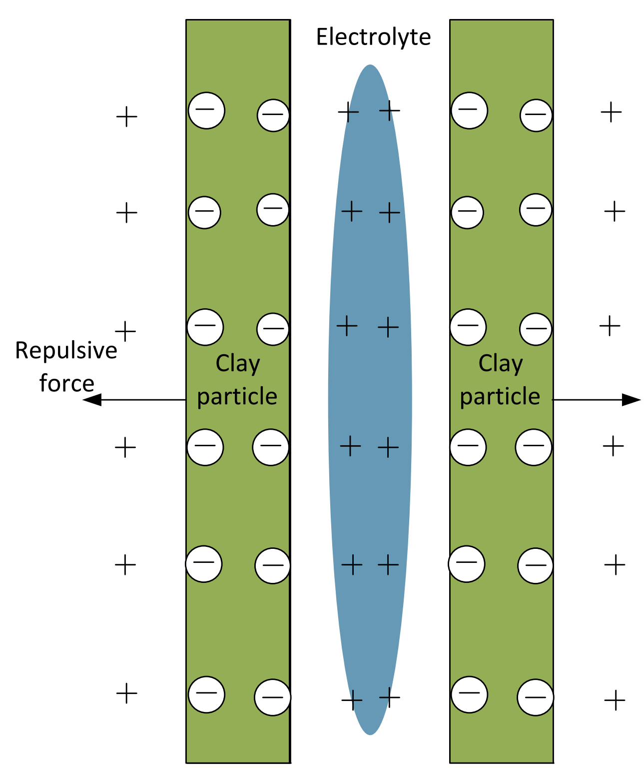

Fig. 2. Interaction between two charged clay particles.