Modelling the swelling and osmotic properties of clay soils. Part II: The physical approach

Andrea Dominijanni *, Mario Manassero [1]

Dipartimento d'Ingegneria del Territorio, dell'Ambiente e delle Geotecnologie [Land, Environment and Geo-Engineering Department], Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

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ABSTRACT

The increasing use of clays, with a high montmorillonite content in their mineralogical composition, as hydraulic and contaminant barriers for landfill and soil remediation applications needs to be supported by an adequate theoretical modelling of the mechanical behaviour and transport properties, in order to assess the expected performances in the long term. The framework of the thermodynamics of irreversible processes was adopted in a companion paper to derive phenomenological constitutive equations for a clay soil characterised by swelling and osmotic phenomena, without specifying any of the physical mechanisms that occur at the pore scale. In this paper, a *physical* approach is proposed in order to provide an interpretation of the phenomenological parameters, obtained from laboratory tests. The soil structure is assumed to be constituted by montmorillonite lamellae, that can be aggregated to form the so-called tactoids, which have a slit-like geometry. Chemical equilibrium is assumed to be established between the bulk electrolyte solution and the internal pore solution at the macroscopic scale, so that the hydraulic pressure and ion concentrations can be evaluated through the Donnan equations. Water and ion transport is described at the pore scale through the generalised Navier–Stokes equation and the generalised Nernst–Planck equations, respectively. Mechanical behaviour is modelled taking into account intergranular contact stresses. The approach is applied to interpret literature experimental results, showing how it can reduce the number of tests that need to be carried out and provide insight into the physical mechanisms that determine the observed phenomena.

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1. Introduction

Clay soils with a high montmorillonite content are increasingly used as hydraulic and contaminant barriers, due to their low hydraulic conductivity, k, to permeation with water and dilute aqueous solutions (k typically $\leqslant 3.0 \cdot 10^{-11}$ m/s). Bentonite, which is a clay mixture that contains about 70% of montmorillonite, is currently used in the so-called geosynthetic clay liners (GCLs), which have been proposed as an alternative to traditional compacted clay liners, due to their reduced costs and ease of installation. GCLs are factory manufactured products that consist of a thin layer of bentonite (5–10 mm thick) sandwiched between two geotextiles.

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* Corresponding author. Tel.: +39 011 090 7705, mobile: +39 3387778804; fax: +39 011 090 7699.
 E-mail addresses: andrea.dominijanni@polito.it (A. Dominijanni), mario.manassero@polito.it (M. Manassero).
[1] Tel.: +39 011 090 7705; fax: +39 011 090 7699.

Bentonite is characterised by the swelling and osmotic phenomena that are typical of polyelectrolyte gels and biological membranes, and which is attributed to the interaction between the electric charge of montmorillonite lamellae and the ions contained in the pore solution.

In order to account for these phenomena, specific theoretical approaches need to be developed to assess the long-term behaviour of barriers containing bentonite.

A first fundamental distinction can be made between *phenomenological* approaches, which only have the aim of describing *how* phenomena occur, and *physical* approaches, which, on the basis of a conceptual picture of the physical and chemical interactions between the solid and liquid phases at the soil pore scale, have the scope of explaining *why* phenomena occur.

In Dominijanni and Manassero (2012), the phenomenological approach was developed using the formalism of the thermodynamics of irreversible processes (Coussy, 1995, 2004; Eckart, 1940a, 1940b), in order to derive transport and poro-elastic constitutive equations. The analysis referred to a pore solution containing N ion species, with the following simplifying assumptions:

1. unidimensional geometry;
2. infinitesimal strains of the solid skeleton;
3. saturated porous medium;
4. incompressible solid and liquid phase;
5. infinitely diluted electrolyte solution;
6. complete dissociation of the salts in the solution;
7. absence of chemical reactions.

In order to maintain the purely phenomenological approach, i.e. without any specification of the physical and chemical phenomena that occur at the pore scale, it was necessary to refer the state variables of the system (i.e. the hydraulic pressure, the ion concentrations and the electric potential) to a virtual solution, which was considered to be in thermodynamic equilibrium with the real pore solution at any point of the porous medium. The consistency of such an approach was assured by the possibility of formulating the boundary conditions for the virtual solution, in terms of the values assumed by the state variables in the external real bulk solutions in contact with the porous medium.

The obtained constitutive equations were characterised by a defined number of parameters (called phenomenological parameters), subject to some restrictions due to the Clausius–Duhem inequality. These parameters were assumed to be measured by means of macroscopic experimental tests, without any identification of the physical mechanisms that influence them at the microscopic scale.

However, a practical shortcoming of the approach was the very high number of tests necessary to characterise a single bentonite, due to the dependency of the phenomenological parameters on the state variables.

The limitations implied by the lack of a physical interpretation of the mechanisms that generate the phenomena observed at the macroscopic scale were also emphasised.

In this paper, a theoretical model is developed following the physical approach in order to provide an interpretation of the phenomenological parameters introduced in Dominijanni and Manassero (2012).

From a historical point of view, the physical approach is older than the phenomenological one, and it dates back to the pioneering works of von Helmholtz and Smoluchowski on electrokinetic phenomena in fine capillaries (Lyklema, 2003). The aim of these eminent scientists was to explain macroscopic phenomena, such as electro-osmosis, that is, the flow of water driven by an electric potential gradient, on the basis of the electrostatic interaction between the charged wall of a capillary pore and the ions in the solution within the capillary. Their theory was later revised by Gouy (1910) and Chapman (1913), who were the first to evaluate the distribution of the electric potential in a charged pore by solving the Poisson–Boltzmann equation. The Gouy–Chapman theory represents the mathematical formulation of the simplest double diffuse layer (DDL) model, which has been named in such a way because it is based on an idealised picture of the distribution of electric charges in the pore, where the first layer of electric charges is given by the solid wall of the pore and the second layer is represented by the ions contained in the pore solution. A relevant improvement in such a model was given by Stern (1924), who accounted for the presence of a layer of specifically adsorbed ions on the pore wall surface.

Gross and Osterle (1968) coupled the Gouy–Chapman theory to transport equations in order to model the motion of electrolyte solutions through charged porous media and Groenevelt and Bolt (1969) applied this model to bentonites. In this theoretical approach, the microscopic equations are upscaled to the macroscopic scale of observation through the method of volume averaging. In such a way, a macroscopic interpretation of the transport parameters is provided, starting from the evaluation of the interaction between the solid skeleton and the pore solution at the pore scale.

Recently, Moyne and Murad (2002) extended this approach to the evaluation of the mechanical behaviour of the solid skeleton by adopting a homogenisation procedure in order to upscale the constitutive equations from the pore to the macroscopic scale.

The main difficulty involved in applying DDL is that it needs the non-linear Poisson–Boltzmann equation to be solved in the microscopic porous medium unit cell. Owing to the high non-linearity of this equation, only numerical solutions can be found and these do not provide explicit relations with the state variables.

A simpler theory, based on the approximation of considering only the equilibrium between phases at the macroscopic scale, was developed by Donnan (1911) and was applied to transport processes across membranes by Teorell (1935,