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Effect of Chemical Solute Concentration Changes on Deformation Behavior of Expansive Clays

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Abstract: This study presents an investigation on the effect of the osmotic potential due to chemical solute concentration changes by the use of the net mean stress, suction and chemical concentration elastic constitutive relationship to represent the deformation behavior exhibited by expansive clays. The impact of such changes on stress/strain behavior of the soil has been accommodated by the development of a non linear elastic constitutive relationship, a state surface, which includes the effects of chemical solute concentration. In particular, it was suggested that the determination of the stiffness of the soil with respect to chemical solute concentration could be achieved via a theoretical approach. In this study, the double layer theory is investigated and the ability of the proposed numerical model to represent it is shown.

Key words: Numerical model, expansive soil, chemical solute concentration, state surface, finite element method

INTRODUCTION

In recent years, modeling of solute transport in porous media remains a key issue in the area of soil physics and hydrogeology, because anthropogenic chemicals frequently enter the soil, subsoil and aquifers, either by accident or by accepted man-agreement practices and the resulting chemical residues pose hazards to the environment.

The movement of solute in porous media is commonly describes by the Convection-Dispersion Equation (CDE) (Bear, 1972) developed and extensively applied to predict the contamination transport (Bresler, 1981; Van and Shouse, 1989; Alonso, 1998; Li *et al.*, 1999; Malusis and Shackelford, 2002; Liu *et al.*, 2005).

The presence of chemicals, in the form of solutes in the soil's pore water, can affect the deformation behavior of some compacted clays. The soil's dependency on the chemical solute concentration of the pore water therefore requires the prediction of the solute flow in unsaturated porous media.

Bear (1969) presented an equation for solute flow as:

$$\frac{\partial c_s}{\partial t} = \frac{\partial}{\partial x} \left[(D_h) \frac{\partial c_s}{\partial x} - c_s V_w \right] \quad (1)$$

where, c_s is the chemical solute concentration, V_w is the fluid velocity, D_h is the coefficient of hydrodynamic dispersion and x and t are space and time variables, respectively. This relationship ignored any physical mechanism that would cause any effective sources or sinks in the system.

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The mass balance equation presented by Bear (1969) was developed by Bear and Verruijt (1987) for partially saturated media to yield the following relationship:

$$\frac{\partial nS_w c_s}{\partial t} = \frac{\partial}{\partial x} \left[(D_n) \frac{\partial nS_w c_s}{\partial x} - c_s V_w \right] \quad (2)$$

where, n is the porosity and S_w is the degree of saturation. A similar equation was presented by Mangold and Tsang (1991).

The fate of chemicals and the representation of the relevant processes via theoretical models are beyond the scope of this investigation.

In this study, it is investigated the effect of the osmotic potential due to chemical solute concentration changes by the use of the net mean stress, suction and chemical solute concentration elastic constitutive relationship to represent the deformation behavior exhibited by expansive clays. The theoretical approach investigated here is the double layer theory. Two examples are presented in this study.

MATERIALS AND METHODS

Theoretical Formulation

Unsaturated soil is a three-phase porous media consisting of solid, liquid and air. In this study, the liquid phase is represented by the solution water-chemical solute and the air phase by the air. A coupled system of governing equations is developed to investigate the effect of chemical solute on the deformation behavior of expansive clays.

Moisture Transfer

The governing equation for moisture transfer in an unsaturated soil can be expressed as:

$$\frac{\partial(\rho_w n S_w)}{\partial t} = -\partial \rho_w \nabla \cdot V_w + \rho_w E \quad (3)$$

where, ρ_w is the density of pore water, n is the porosity, S_w is the degree of saturation of water, V_w is the total velocity of pore water, E is the sink/source term and ∇ is the divergence operator. The velocity of pore liquid is based on the generalized Darcy's law.

The inclusion of an osmotic flow term in the liquid velocity allows the representation of liquid flow behavior found in some highly compacted clay. The osmotic flow term represents the movement of water in the direction of increasing chemical solute concentration c_s . Adopting the methodology presented by Mitchell and Kenichi (2005), the total velocity of water flow can be defined as:

$$V_w = -K_w \left[\nabla \left(\frac{u_w}{\gamma_w} + z \right) \right] + K_{c_s} \cdot \nabla c_s \quad (4)$$

where, K_w is the hydraulic conductivity, K_{c_s} is the hydraulic conductivity with respect to the gradient of chemical solute concentration, u_w is the pore water pressure, γ_w is the unit weight of water, z is the reference position and ∇ is the gradient operator.

Dry Air Transfer

Air in unsaturated soil can be considered to exist in two forms, bulk air and dissolved air (Fredlund and Rahardjo, 1993). The bulk air transfer is driven by a gradient of air pressure, whilst the

dissolved air transfer is coupled to the flow of pore water. Henry's law is used to define the proportion of dry air contained in the pore water.

The governing equation of dry air transfer can be expressed as:

$$\frac{\partial(S_a + H_s S_w) n \rho_{da}}{\partial t} = -\nabla \cdot [\rho_{da} (V_a + H_s V_w)] \quad (5)$$

where, ρ_{da} is the density of dry air which can be defined by Dalton's law of partial pressure and H_s is the Henry's volumetric coefficient of solubility.

Chemical Solute Transfer

The governing equation for conservation of chemical solute, where the solute is considered non reactive and sorption onto the soil surface is ignored (Yong *et al.*, 1992), can be defined as:

$$\frac{\partial(n S_w c_s)}{\partial t} = -\nabla \cdot (c_s V_w) + \nabla \cdot [D_h \nabla (n S_w c_s)] \quad (6)$$

where, D_h is the hydrodynamic dispersion coefficient defined as (Bear and Verruijt, 1987):

$$D_h = D_{mech} + D_d \quad (7)$$

which includes both molecular diffusion D_d and mechanical dispersion D_{mech} .

Stress/Deformation Relationship

In this approach the deformation and strength behavior of unsaturated soil is defined by a constitutive relationship linking stress with strain, suction and chemical solute concentration. A non linear elastic model based on a state surface presented by Thomas and He (1995) is used. The swelling behavior of the soil is represented in this approach by the inclusion of osmotic effects through chemical solute concentration term.

It is assumed here that the increment of total strain can be given as the sum of the strain increments due to changes in net mean stress, suction and chemical solute concentration, i.e.:

$$de = de_p^e + de_s^e + de_{c_s}^e \quad (8)$$

where, the subscripts p , s and c_s refer to net mean stress, suction and chemical solute concentration and the superscript e refer to the elastic component.

Based on a state surface concept, chemical solute concentration has been included as a new primary variable in the present model. Together with net mean stress and suction, the volumetric deformation of unsaturated soil is therefore defined. A new state surface of void ratio is required in the model, which should be of the form:

$$e = f(e_0, p, s, c_s) \quad (9)$$

where, e_0 is the initial void ratio and using the state surface proposed by Lloret and Alonso (1985), the new state surface can be expressed as:

$$e = e_0 + a \ln(p) + b \ln(s) + c \ln(p) \ln(s) + d_{c_s} c_s$$

where, d_{c_s} is a function relating to the chemical solute concentration.

With suitable substitution of Eq. 8 the stress-strain relationship can be expressed as:

$$\begin{aligned} d\sigma'' &= D(d\varepsilon - d\varepsilon_s^* - d\varepsilon_{c_s}^*) \\ &= D(d\varepsilon - A_s ds - A_{c_s} dc_s) \end{aligned} \quad (10)$$

Where:

$$d\varepsilon_s^* = \frac{1}{v_i} \frac{\partial \varepsilon}{\partial s} m ds = A_s ds \quad (11)$$

$$d\varepsilon_{c_s}^* = \frac{1}{v_i} \frac{\partial \varepsilon}{\partial c_s} m dc_s = A_{c_s} dc_s \quad (12)$$

D is the elastic matrix and σ'' is the net stress. For two dimensional cases $m = (1, 1, 0)$ and

$$\sigma'' = \frac{\sigma_x + \sigma_z}{2} - u_a \quad (13)$$

where, σ_x and σ_z are the stresses in the x and z directions and u_a is the pore air pressure.

Double Layer Theory

A number of researchers have presented formulations of double layer theory (Bolt, 1956; Van Olphen, 1977; Sridharan and Jayadeva, 1982). Van Olphen (1977) has presented the following expressions to describe the relationship defining the inter platelet half distance d for interacting Gouy double layer:

$$\int_z^u (2 \cosh y - 2 \cosh u)^{-0.5} dy = -K.d \quad (14)$$

Where:

$$z = 2 \left(\sinh^{-1} \left(\frac{\sigma}{(8\eta \varepsilon_{st} kT)^{-1}} \right) \right) \quad (15)$$

$$u = \cosh^{-1} \left(\frac{p}{2\eta kT} + 1 \right) \quad (16)$$

$$K = \left(\frac{2\eta e_c^2 v^2}{\varepsilon_{st} kT} \right)^{0.5} m^{-1} \quad (17)$$

where, σ is the surface charge density and may be defined as Mitchell and Kenichi (2005):

$$\sigma = \frac{B}{S} F \quad C m^{-2} \quad (18)$$

p is the applied pressure, B is the base exchange capacity ($\mu_{eq} g^{-1}$), S is the specific surface ($m^2 g^{-1}$), F is the Faraday constant, k is the Boltzman constant, ε_{st} is the permittivity of the medium ($C^2 J^{-1} m^{-1}$), e_c is the elementary charge, v is the valency of the ion concentration and η is the molar of ions concentration in pore fluid defined as:

$$\eta = c_s X N_A \tag{19}$$

where, N_A is the Avogadro number.

The void ratio can be defined in terms of inter platelet distance by Sridharan and Jayadeva (1982) as:

$$e = G_s \gamma_w S.d \tag{20}$$

where, G_s is the specific gravity of soil solids and γ_w is the unit weight of pore water. It is proposed here that the value of A_{c_s} can numerically be determined for a specific value of c_s by the following relationship:

$$A_{c_s} = \frac{e_2 - e_1}{c_{s2} - c_{s1}} \tag{21}$$

where, the subscripts 1 and 2 represent values of c_s and e at a chemical solute concentration of 0.1% more and 0.1% less than its actual value.

RESULTS AND DISCUSSION

Numerical Examples

A numerical solution of the four governing partial differential equations is obtained by the application of appropriate methods. For spatial discretisation the finite element method is used applying the Galerkin weighted residual approach with eight noded isoparametric elements. For temporal discretisation the finite difference method is employed with a backward difference mid interval time stepping scheme.

The examples presented here use the double layer theory described in the preceding section to predict the volume change behavior due to osmotic potential changes. The physical parameters used are shown in Table 1. The geometric configuration chosen illustrates a small two dimensional problem of size 200 by 100 mm. The spatial discretisation of the domain consists of ten eight noded isoparametric elements as shown in Fig. 1. The results of this mesh have been found to give spatially converged results.

Table 1: Material parameters used in the numerical example

Parameters	Value of function
D_h ($m^2 \text{ sec}^{-1}$)	10^{-9}
S_w	$1.0 - 0.8 \times \tanh(5 \times 10^{-6} s)$
K_w ($m \text{ sec}^{-1}$)	$10^{-15} \frac{(S_w - 0.05)^3}{0.95^3} 10^{40 \times e}$
$K_w^{c_s}$ ($m \text{ sec}^{-1}$)	10^{-14}
ρ_s ($kg \text{ m}^{-3}$)	2780
ρ_w ($kg \text{ m}^{-3}$)	1000
γ_w ($kN \text{ m}^{-3}$)	10.0
e	$5.5 - 0.4 \ln(p) - 0.25 \ln(s) + 0.02 \ln(p) \ln(s)$
S ($m^2 \text{ g}^{-1}$)	100
B ($\mu_{eq} \text{ m}^{-2}$)	400
T (K)	293
e_c (C)	1.60219×10^{-19}
F ($C \text{ mol}^{-1}$)	9.64867×10^4
k ($J \text{ K}^{-1}$)	1.38062×10^{-23}
v	1
ϵ_{st} ($C^2 \text{ J}^{-1} \text{ m}^{-1}$)	7.11×10^{-10}

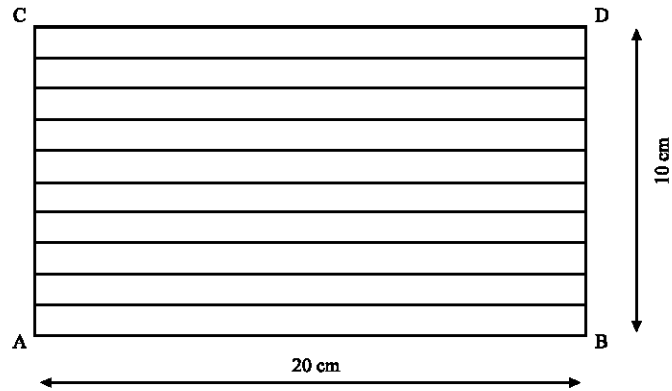


Fig. 1: Finite element mesh

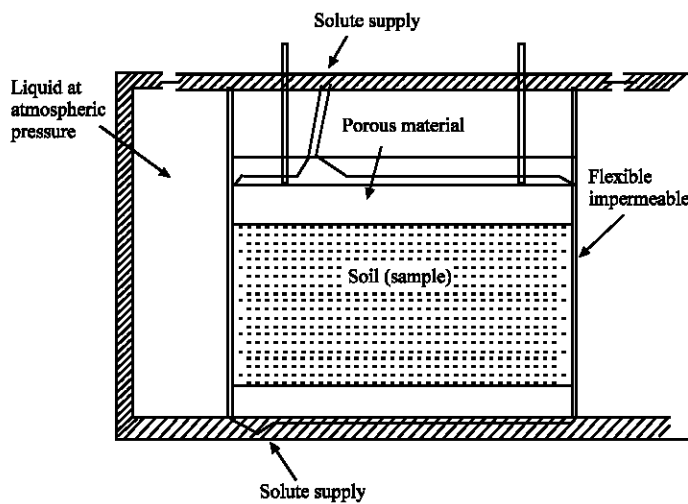


Fig. 2: Schematic representation of the problem

Example 1

The soil represented in these examples is an illite fraction of the same type as the soil described by Bolt (1956). The parameters relating the diffusivity and the permeability with respect to the solute phase are typical values for a clay type soil (Mitchell and Kenichi, 2005). The suction versus degree of saturation relationship is assumed as typical for clay type soil. The specific surface and base exchange capacity for an illite are taken as an average of published results, (Mitchell and Kenichi, 2005). The relationship for void ratio used is taken to describe the typical behavior of a clay type soil under low suction conditions (Thomas and He, 1995).

The example shows the model simulating the swelling characteristics of an illite under osmotic potential gradients. Physically the problem can be considered to be a soil sample placed in a flexible impermeable membrane with a porous material at the top and bottom of the sample. Figure 2 shows a schematic diagram of an experimental set-up. The sample is assumed to have an initial degree of saturation of 100% and an initial void ratio of 2.18, this corresponds to an initial pore water pressure of 0 kPa. An initial solute concentration of 100 mol m^{-3} is assumed, this is equivalent to a 0.1 M solution.

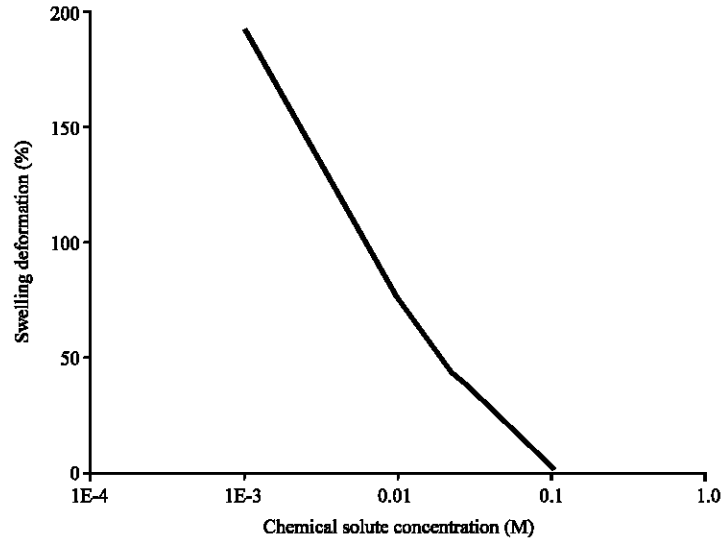


Fig. 3: Chemical solute concentration versus swelling strains

Suction is controlled on the boundary by applying a constant pore water pressure of 0 kPa on the surfaces AB and CD. This numerical condition was applied so that only strain due to osmotic potential changes was produced. A solute concentration gradient is applied by a fixed boundary condition on the surfaces AB and CD, with the applied c_s decreasing from 100 to 1 mol m^{-3} . Surfaces AC and BD are considered to be impermeable. The soil rests on a fixed base AB and is allowed to swell freely.

Within the soil sample, the applied chemical solute concentration on the boundaries AB and CD lead to a gradient of chemical solute concentration. This gradient induces liquid flow in the direction of increasing concentration. The chemical solute concentration decrease results in a change in the double layer forces, causing an increase in the inter platelet distance thereby producing a swelling strain.

Figure 3 shows the swelling strain versus chemical solute concentration of the sample. At higher chemical solute concentration the amount of swelling due to a unit change in chemical solute concentration is lower than at more dilute concentrations. This reflects the physical fact that when diluting a solution to half of its original concentration the volume of additional liquid required for each subsequent dilution follows an exponential type increase.

A final strain of 190% in the sample is produced when the chemical solute concentration has reached a value of 1 mol/ m^3 throughout the soil. These results can be compared to the results obtained by Sridharan and Jayadeva (1982) from a similar double layer formulation. These results presented by Sridharan and Jayadeva (1982) also show a strain of 190% being predicted by double layer theory. This comparison verifies that the correct numerical solution of Eq. 14 has been achieved.

Example 2

This example shows the model simulating the swelling characteristics of an unsaturated illite under osmotic potential gradients. Again, physically the problem can be considered to be a soil sample placed in a flexible impermeable membrane with a porous material at the top and bottom of the sample Fig. 2. The sample is assumed to have an initial degree of saturation of 95% and initial void ratio of 0.7. This corresponds to an initial pore water pressure of -100 kPa. An initial solute concentration of 100 mol m^{-3} (0.1 M) is assumed.

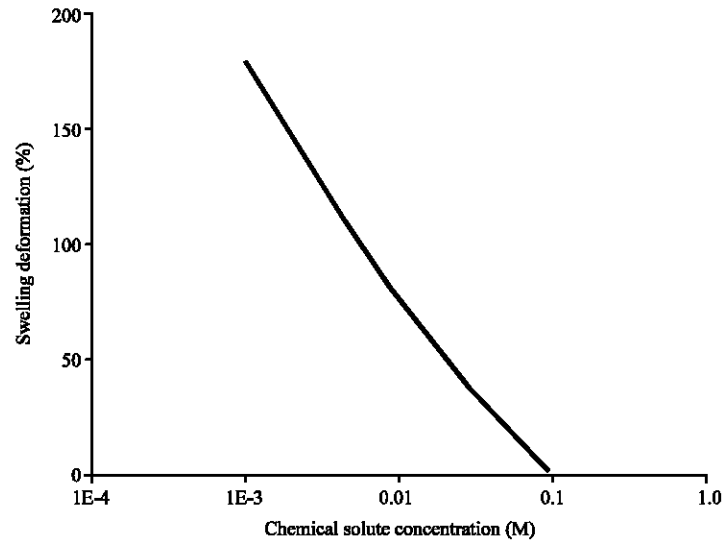


Fig. 4: Chemical solute concentration versus swelling strains

The load path considered in this example again follows a decrease in solute concentration to a value of 1 mol m^{-3} (0.001 M). The pore water pressure held at its initial value of -10 kPa keeping the sample in the unsaturated zone. The boundary conditions in this example are applied in the same manner described in example 1.

Figure 4 shows the swelling strain versus chemical solute concentration of the sample. Again, it can be observed that as the chemical solute concentration decreases the soil exhibits a swelling deformation response. In this case, the quantity of strain produced is reduced in comparison to that achieved in example 1. The reason for this is that the amount of swelling strains produced by the change in chemical solute concentration are reduced by a factor applied to A_{cs} . This example shows the effect of factor applied to the stiffness of the soil with respect to chemical solute concentration.

CONCLUSION

The objective of this study was to investigate the effect of chemical solute concentration changes on the deformation behavior exhibited by expansive clays by the proposed numerical model. The determination of the stiffness of the soil with respect to chemical solute concentration has been represented by the double layer theory. While it is recognised that further experimental work is required to develop more sophisticated models and produce qualitatively accurate numerical results, the study presented demonstrates the ability of the proposed model to represent an important aspect of the physical behavior of expansive clays. The numerical analysis presented here is an initial attempt at the modelling of unsaturated expansive soils.

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