



Unsaturated hydro-mechanical-chemo coupled constitutive model with consideration of osmotic flow



XiaoHui Chen^a, Michael A. Hicks^{b,*}

^a School of Mechanical, Aerospace and Civil Engineering, The University of Manchester, P.O. Box 88, Manchester M60 1QD, UK

^b Section of Geo-Engineering, Department of Geoscience and Engineering, Faculty of Civil Engineering and Geosciences, Delft University of Technology, P.O. Box 5048, 2600 GA Delft, The Netherlands

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ABSTRACT

Since low permeability rock has the potential to behave as an actual semi-permeable osmotic membrane, chemical osmosis may have an effect on water flow and needs to be accounted for in analysis. Hence, an advanced fully coupled formulation for modelling unsaturated hydro, chemical and mechanical effects is here presented based on modified mixture theory. Firstly, the classical Darcy's law has been modified to include the chemical potential. Secondly, the mechanical deformation, which affects the permeability, has been coupled with the water and chemical flows by using Helmholtz free energy and the Gibbs–Duhem equation. Finally, an illustrative numerical example with relevance to radioactive waste disposal has been analysed to investigate the performance of the coupled formulation and the relative influence of parameters.

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1. Introduction

The geological disposal of most low level and intermediate level radioactive waste involves shallow disposal, whereas high level waste and some long-lived intermediate level waste (e.g. from spent fuel and fuel reprocessing) is likely to be deposited in a deep geological repository [1]. The disposal system is required to provide protection to human health and the environment from the hazards of contaminant release. The sealing of the radioactive waste depends on the engineered barriers, such as the buffer clay which may be placed around the waste container, and the host rock. One of the key considerations when evaluating the viability of the host rock and buffer clay, for radioactive waste disposal, is low permeability.

Normally, the hydraulic conductivities of the host rock and buffer clay are less than 10^{-10} m/s, so that they can act as actual semi-permeable membranes to restrict the transport of solute molecules [2]. The solute molecules can either be salt, or other chemicals present during drilling, or they can be pollutants from the radioactive waste itself if leakage occurs. Thus it is very important for industry to consider the possibility and effects of chemical osmosis.

Previous researchers [3–5] have considered chemical osmosis in radioactive waste disposal, and some work has extended Darcy's

law by including chemical osmosis effects in low permeability saturated shales [6,7]. However, chemical osmosis is very complex and the capacity for osmosis generally depends on the pore size of the porous medium and the chemicals involved [8]. In biological tissues (which are a form of porous medium), the osmotic effect may be considerable; however, osmosis in rock or clay may be much more complex due to the large number of chemicals and/or presence of micro-organisms and, in such situations, the osmotic capacity of different rocks or clays to different chemicals may be unclear. Currently, most measurements of osmotic efficiency have been for a relatively small number of common non-reactive chemical elements, such as Na⁺ or Cl[−] [9]; further experimental research is needed to assess the osmotic capacity for radionuclide complexes, organic matter and gases (especially for intermediate and low level radioactive waste). For simple chemical elements (e.g. Na⁺), the influence of osmosis may be small in geomaterials; however, for more complex chemical elements, for organic matter, or due to the presence of microbial activity, the osmosis may be stronger.

For the disposal of high level radioactive waste, an important further consideration is that the waste is heat emitting; thus, for such conditions, the thermal influence needs to be considered. In contrast, for intermediate and low level waste, the heat emissions may be relatively low and the whole system may then be reasonably viewed as isothermal; however, in this case an important factor is likely to be the generation of hydrogen due to chemical reactions and micro-organism reductions. For this second scenario,

* Corresponding author. Tel.: +31 152787433; fax: +31 152783328.

E-mail address: m.a.hicks@tudelft.nl (M.A. Hicks).

unsaturated osmosis may well be important, both in the buffer that is placed in a quite unsaturated state and in the host rock, that, although unsaturated, is likely to retain a high degree of saturation. This forms the motivation behind the research in this paper, which, to simplify matters, focuses on the potential for osmotic behaviour in the host rock.

The coupled model developed herein is based on a modified form of mixture theory. Mixture theory maintains the individuality of the solid and fluid phases [10,11], but it is difficult to obtain information on the interaction between the phases. Hence, an approach that does not explicitly discriminate between the solid and the fluid phases, but views a fluid-infiltrated rock as a single continuum, here referred to as modified mixture theory, was proposed by Heidug and Wong [6]. Chen and Hicks [12] later simplified the underlying approach, before extending it to unsaturated rock [13]. This paper takes a further significant step forward by introducing chemical aspects to modified mixture theory. Specifically, chemical transport, as well as the influence of chemical transport on water flow and its consequent influence on the degree of saturation and mechanical deformation, are investigated. This has necessitated new detailed formulations incorporating chemical potential, chemical flux and chemical entropy.

Note that there is an alternative and more commonly used approach for coupled modelling in geomechanics. This is based on the classical consolidation theories of Terzaghi [14] and Biot [15,16], and is here referred to as the mechanics approach to simplify the discussion. A lot of research in coupled modelling has used this approach to provide advanced formulations. This has included hydro-mechanical coupled models [17–21], as well as more advanced models including thermal and/or chemo coupling [22–24]. However, to incorporate more complex chemical reactions in the coupling, the mechanics approach needs to borrow chemical transport and reaction formulations from geochemistry, due to the gap between geophysics and geochemistry [25]. Thus, a systematic approach for coupled modelling, which can help build coupled formulations based on a single unified theory, between geophysics and geochemistry, seems desirable. Modified mixture theory is able to give just such a smooth link [6].

Coupling may be classified into two groups: external (or structure coupling) and internal coupling. Hydro-mechanical coupling can be viewed as external coupling, because the water and rock are two distinct components and the dissolution of rock into water may be disregarded in the current application. In contrast, hydro-chemo-thermo coupling may be viewed as internal coupling, which cannot (or not easily) be separated by physical means, because chemicals dissolve in water and thermal effects stay in the body of the water or chemical as energy. For external coupling the interactive force is external, for example the water pressure causes the deformation of the rock, and so the mechanics approach may be conveniently used to analyse the force transfer. However, for internal coupling, since there are a huge number of molecules at the micro-level, even in a very small amount of material (for example, water or solid), it may be very difficult to transform the effects of the forces between the molecules for use in a macro-level force analysis, even though molecular dynamics might be involved; instead, it may be easier to consider chemical potential and thermo-potential at the macro-level. The chemical potential of a species in the mixture is defined as the change of the free energy of the system with respect to the change in the number of moles. The relationship between different types of chemical potential (including water chemical potential) and fluid pressure can be obtained by using non-equilibrium thermodynamics, so enabling a link between water/chemical forces and chemical potential.

Modified mixture theory links the force analysis for external coupling and the energy analysis for internal coupling, by using

continuum thermomechanics and non-equilibrium thermodynamics [6,12,13]. Here, it is based on the balance equation for the Helmholtz free energy of a fluid-infiltrated rock, and combines the first and second laws of thermodynamics.

In this paper, modified mixture theory has been extended to include the influence of unsaturated chemical osmosis. In particular, Darcy's law and Biot's equation have been modified by including chemical potential, and a new fully coupled formulation has been derived. The chemical osmosis has a significant influence on water and chemical transport, and on the deformation of the rock. This is illustrated by analysing a simple numerical example.

Note that the adopted sign convention is that usually used in continuum mechanics theory. Hence, positive stresses, strains and displacements are tensile, whereas, positive pore pressures are compressive [20,21].

2. Balance laws for the open system

An arbitrary sub-region V is considered in the rock or soil. S is the boundary of the sub-region and is assumed to be attached to the solid phase so that there is no solid moving across the boundary. In this study, there are two fluxes across the boundary; a water flux and a chemical flux. Moreover, two simplifying assumptions are made: (1) there is only one solute in the water and the chemical potential of the solute and water are μ^c and μ^w , respectively; (2) the gas phase is continuous in the unsaturated zone and remains at atmospheric pressure, $p_{atm} = 0$ [26,27], so that the gas transport can be ignored.

2.1. Balance equations for thermodynamically open system

The flux can be defined as

$$\mathbf{I}^\beta = \rho^\beta (\mathbf{v}^\beta - \mathbf{v}^s) \quad (1)$$

where \mathbf{I}^β , ρ^β and \mathbf{v}^β are the flux, density and velocity, respectively, of the water ($\beta = w$) or chemical ($\beta = c$) component, and \mathbf{v}^s is the velocity of the solid phase.

The balance equation for Helmholtz free energy can be obtained as

$$\frac{D}{Dt} \left(\int_V \psi dV \right) = - \int_S \boldsymbol{\sigma} \mathbf{n} \cdot \mathbf{v}^s dS - \int_S (\mu^w \mathbf{I}^w + \mu^c \mathbf{I}^c) \cdot \mathbf{n} dS - T \times \int_V \gamma dV \quad (2)$$

where ψ is the Helmholtz free energy density, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, \mathbf{n} is the outward unit normal vector, T is the constant temperature and γ is the entropy production per unit volume, and where the material time derivative is given by

$$\frac{D}{Dt} = \partial_t + \mathbf{v}^s \cdot \nabla \quad (3)$$

Since there is no solid mass flux into the sub-region, the balance equation for the solid is

$$\frac{D}{Dt} \left(\int_V \rho^s dV \right) = 0 \quad (4)$$

where the solid density is denoted by ρ^s .

Because V is open with respect to the exchange of fluid mass (water and chemical), the balance equation for the fluid can be expressed as

$$\frac{D}{Dt} \left(\int_V \rho^\beta dV \right) = - \int_S \mathbf{I}^\beta \cdot \mathbf{n} dS \quad (5)$$

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