

THERMOMECHANICAL MODEL OF HYDRATION SWELLING IN SMECTITIC CLAYS: II THREE-SCALE INTER-PHASE MASS TRANSFER: HOMOGENIZATION AND COMPUTATIONAL VALIDATION

MÁRCIO A. MURAD*[†]

Rua Getulio Vargas 333 Quitandinha, CP 95113 Petropolis, RJ Brazil

SUMMARY

In Part I¹ a two-scale thermomechanical theory of expansive compacted clays composed of adsorbed water and clay platelets was derived using a mixture-theoretic approach and the Coleman and Noll method of exploitation of the entropy inequality. This approach led to a two-scale model which describes the interaction between thermal and hydration effects between the adsorbed water and clay minerals. The purpose of this paper is twofold. Firstly, partial results toward a three-scale model are derived by homogenizing the two-scale model for the clay particles (clusters of clay platelets and adsorbed water) with the bulk water (water next to the swelling particles). The three-scale model is of dual porosity type wherein the clay particles act as sources/sinks of water to the macroscale bulk phase flow. One of the notable consequences of the homogenization procedure is the natural derivation of a generalized inter-phase mass transfer equation between adsorbed and bulk water. Further, variational principles and finite element approximations based on the Galerkin method are proposed to discretize the two-scale model. Numerical simulations of a bentonitic clay used for engineered barrier of nuclear waste repository are performed and numerical results are presented showing the influence of physico-chemical effects on the performance of the clay buffer. Copyright © 1999 John Wiley & Sons, Ltd.

Key words: swelling clay buffer; homogenization; dual porosity; mass transfer; physico-chemical effects; finite element method

1. INTRODUCTION

In a earlier paper¹ Hybrid Mixture Theory (HMT) was used to model flow, deformation and heat transfer in two-scale swelling systems such as highly compacted smectitic clays, composed of clay minerals and adsorbed (vicinal) water. By adopting a proper theory of constitution including appropriate internal variables to capture the swelling character of these systems, HMT provided a natural framework for a proper thermodynamic definition of intra-particle thermo-physico-chemical stresses. In particular, HMT provided a rational basis for a thermodynamic derivation

* Correspondence to: M. A. Murad, LNCC/CNPq, Rua Getulio Vargas 333, Quitandinha, CP 95113, Petropolis, RJ, Brazil

[†] Laboratório Nacional de Computação Científica, LNCC/CNPq, Rua Lauro Muller 455, 22290 – Rio de Janeiro, Brazil

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