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A MICROMECHANICAL MODEL FOR CEMENT PASTE WITH EFFECTS OF CARBONATION

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Cement-based materials have a complex behavior, such as mean stress dependency, plastic deformation, volumetric compressibility and dilatancy, etc.. In many engineering structures, this material is subjected not only to mechanical loading, but also to moisture transfer, variation of temperature and chemical degradation. The mechanical behavior of cement-based materials is inherently related to the chemical composition and mechanical properties of constituents. The durability analysis of such structures requires the consideration of such multi-physical coupling phenomena. Based on the standard framework of thermodynamics, many phenomenological elastoplastic and damage models have been proposed for modeling cement-based materials. But these phenomenological models can not properly take into account the relationships between microstructure (such as change of porosity, inclusion, physical and chemical reactions, etc.) and macroscopic behavior of the studied material. The purpose of this study is to propose a micromechanics-based approach for the modeling of elastoplastic behavior of cement-based porous materials considering the effects of mechanical loading and chemical reaction called carbonation.
The carbonation of a cement paste corresponds to physical and chemical mechanisms which result from the instability of portlandite ($Ca(OH)_2$) and calcium silicate hydrate (C-S-H) phases in cement-based material under the influence of carbon dioxide CO_2. The dissolution of CO_2 in interstitial fluid cause a global reaction which can be written as follows:

$$Ca(OH)_2 + CO_2 = CaCO_3 + H_2O \tag{1}$$

The carbonation leads a drop of porosity in cement-based material with the generation of calcite ($CaCO_3$) whose size is much smaller than the one of pore. Due to the carbonation, the constituents of the studied cement paste will be changed. With this procedure, the studied material can be seen as a "effective" porous medium composed of spherical pores and solid matrix which is reinforced by the small grains of calcite generated during the chemical reaction (see Figure 1), here the solid phase is described by a pressure sensitive plastic model.

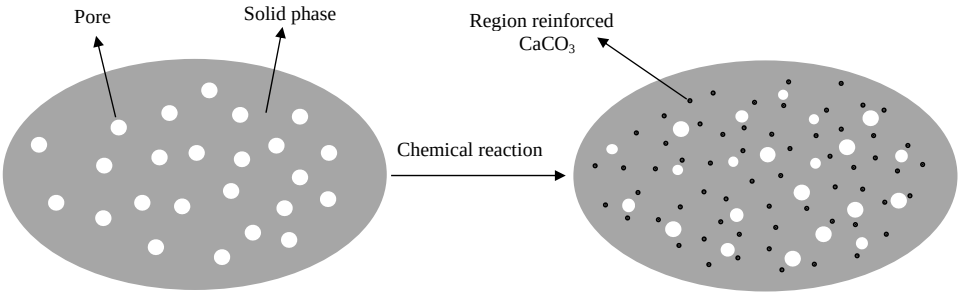

Figure 1: Schematization of the chemical reaction

Based on [1] [2], a two-step homogenization procedure (from micro to meso and from meso to macro) is proposed to formulate a macroscopic plastic criterion for the macroscopic elastoplastic behavior of the studied cement-based materials, considering the effects of porosity f and the volume fraction ρ of calcite generated during the chemical reaction. Then the proposed micromechanical model is implemented in a Finite Element code Abaqus via a UMAT subroutine. A good agreement is found between numerical simulations and experimental data (Figure 2) for different confining pressures and different states of carbonation. The main features of macroscopic behavior of the studied material are well predicted.

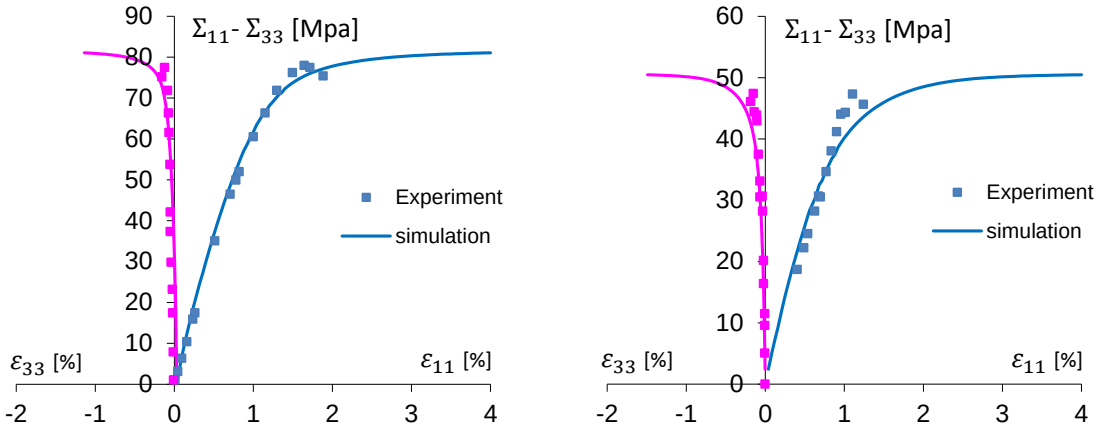

Figure 2: 3mm carbonated samples with 17.5 MPa confining pressure and 6mm carbonated samples with 0.5 MPa confining pressure

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