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Alternative methodology to consider damage and expansions in external sulfate attack modeling

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ABSTRACT

A diffusion–reaction numerical model is proposed to simulate the response of concrete exposed to external sulfate attack. Diffusion properties are modified based on the strain reached and the ratio of porosity filled by ettringite. A direct and intuitive approach is proposed for the consideration of the diffusion in a cracked porous media based on the constitutive law of the material. A methodology to compute expansions based on a more realistic consideration of the concrete porosimetry is presented, by which it is possible to distinguish different strain contributions from different pore sizes. The described approach also allows the consideration of different capacities to accommodate expansive product for each pore size considered and the faster filling rate existent in small pores. Critical parameters of the numerical model developed are recognized and established. Expansions obtained by the new model are in good agreement with experimental data published in the literature.

1. Introduction

Durability of concrete has become a major issue in structural engineering over the last decades. In 2012, it was estimated that 51.2% of the annual investment in the construction field in EU27 countries (excluding Cyprus, Greece, Luxembourg and Malta) plus Norway and Switzerland, was dedicated to Renovation and Maintenance (R&M), turning concrete durability into a key aspect in the industry [1]. Within this framework, restoring and management systems of existing structures gain prominence, where numerical modelization of degradation phenomena plays an essential role. It is important to highlight that in many cases, once a concrete deterioration process is detected in built structures, the only possible action is of the palliative nature, through a monitoring of the structural behavior. For this, the development of prediction models about the future evolution becomes crucial.

Degradation of concrete exposed to sulfate solutions has been of concern since the early years of the 19th century [2]. The importance of the external sulfate attack in the concrete degradation processes is usually related to the need of assessing the durability of underground nuclear waste containments, tunnel linings and dams, which may be sometimes in contact with sulfate-rich soils [3–6]. The relative significance of this phenomenon has been questioned over the last decade and, according to Neville [7], the opinion that sulfate attack is not a widespread problem in concrete structures is expressed even by those who have published extensively on the topic. The fact that there are few reported cases of structures in service damaged by sulfates in the soil or in groundwater is supported by several authors [7,8]. Despite all these opinions, most of them based on indisputable facts, now the rate of published papers dealing with the sulfate attack is greater than ever, reflecting a growing interest in the scientific community. This growing interest may be explained by the considerable controversy still existing on basic topics within the sulfate attack phenomenon and the deterioration mechanisms involved, such as the expansion mechanism and the gypsum role on the expansion process [7]. On the other hand, despite structural failures due to sulfate attack are rare, in structures that require high stability due to a small displacement tolerance, the expansive nature of the sulfate attack should be carefully assessed.

Traditionally, due to the high level of complexity of the external sulfate attack, where transport, chemical and physical processes between sulfate ions and the hydrated compounds of the cement paste are involved [9,10], unilateral efforts have been made into different specific fields to model a specific phenomenon within the overall problem. However, during the last years, a number of advanced comprehensive models have been developed [3,4,11,12], even considering a full tenso-deformational mechanical analysis through a mesostructural representation of the material, able to simulate not only crack formation and propagation, but also its influence on the diffusion-driven process [4].

Every possible mechanical framework that may be developed is based on the expansions obtained through the numerical model. Most of the models referred above [3,4,11] obtain the expansions using a simplified expression described by Tixier and Mobasher [11]. In this expression, the pore capacity to accommodate ettringite is represented by a single buffer coefficient (f). This coefficient is linearly applied to the

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overall ettringite formation and the overall porosity is considered without differentiating the size of the pores. By this consideration, all the buffer capacity of the matrix has to be filled before the expansions start to be computed. In this way, the early expansions caused by precipitation of ettringite in the small pores, where the capacity to accommodate ettringite is very limited, are neglected. As the expansions computed are the base of any future mechanical consideration, it is believed that this simplified expression is in contradiction with the sophisticated mechanical framework included in the advanced models. From this situation, the need to explore new ways to compute expansions, according to the degree of complexity and precision incorporated, is highlighted.

The objective of the present work is to present a diffusion–reaction model where a simplified approach of the chemical processes involved in external sulfate attack and the mechanical processes related to ettringite formation in the pores are considered. It is mainly based on the original proposal of Tixier and Mobasher [11], which has been significantly modified by describing a new expression for the diffusion in a cracked porous media and through a new expression to compute the expansions. This new expression is based on a more realistic consideration of the porosimetry of concrete and on the introduction of a new ettringite formation rate ($\mathcal{F}$), which quantifies and distributes ettringite precipitation. By this approach, it is able to distinguish the different strain contributions from different pore sizes. In Fig. 1, a schematic diagram of the different processes considered in this model is depicted.

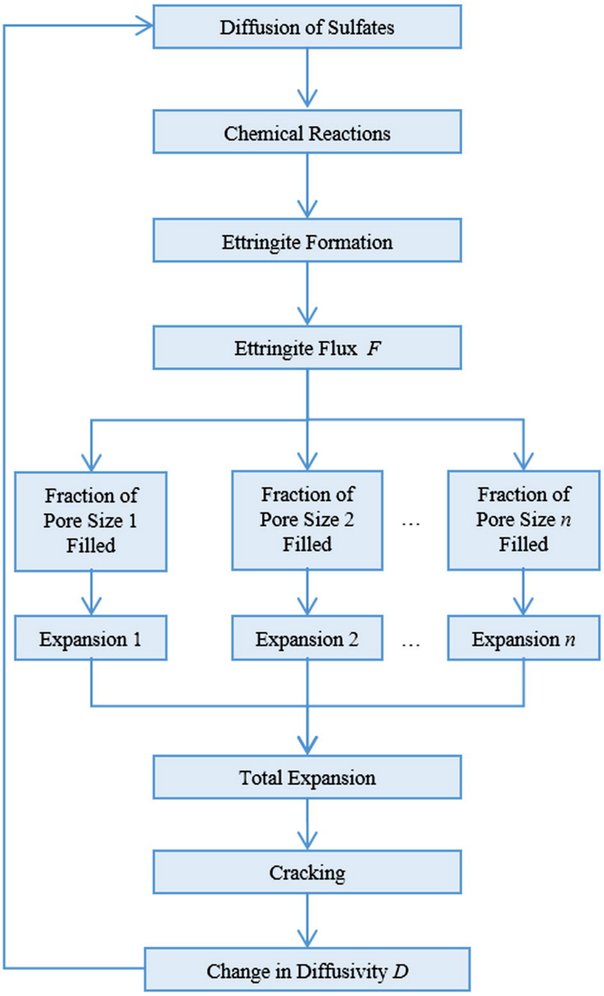

Fig. 1. Processes considered in the model.

Critical parameters of the numerical model developed will be recognized and established. Finally, expansions obtained by the new model will be compared to experimental data by Brown [13] and Ferraris et al. [14].

2. Description of the chemo-transport model

2.1. Chemical reactions considered

In this model, it is considered that the deterioration process related to external sulfate attack is caused by the potential volume expansions associated to the chemical reactions of sulfate ions with the unreacted hydration compounds of the cement paste. Eqs. (1)–(4) describe the series of reactions considered to take place when the sulfate ions penetrate a cement based structure. This process is initiated by the reaction of sulfate ions (SO_4^{2-}) with calcium hydroxide (CH) to form gypsum ($C\bar{S}H_2$) (Eq. (1)).

$$CH + SO_4^{2-} \rightarrow C\bar{S}H_2 + 2OH^- \tag{1}$$

Gypsum formation is considered as an intermediate phase that later may react with the aluminate phases to form secondary ettringite ($C_6A\bar{S}_3H_{32}$) [11,15–17]. Three calcium aluminate phases are considered as described in Eqs. (2)–(4): tricalcium aluminate (C_3A), tetracalcium aluminate (C_4AH_{13}) and monosulfate ($C_4A\bar{S}H_{12}$). Note that no direct reactions between the sulfate solution ions and aluminate phases are contemplated, since it is assumed that all ingressing sulfates react first with calcium hydroxide to form gypsum.

$$C_3A + 3C\bar{S}H_2 + 26H \rightarrow C_6A\bar{S}_3H_{32} \tag{2}$$

$$C_4AH_{13} + 3C\bar{S}H_2 + 14H \rightarrow C_6A\bar{S}_3H_{32} + CH \tag{3}$$

$$C_4A\bar{S}H_{12} + 2C\bar{S}H_2 + 16H \rightarrow C_6A\bar{S}_3H_{32} \tag{4}$$

It is assumed that the expansions are caused only by the formation of secondary ettringite. The role of gypsum in the expansion mechanism is still far from clear [7], so in this study, the expansive nature of gypsum formation is not considered.

As previously proposed by Tixier and Mobasher [11], and afterwards used by other researchers [4,17], Eqs. (2)–(4) are lumped in a single expression to simplify the numerical treatment (Eq. (5)). It should be noticed that by this simplification, one single chemical reaction rate will be used to define the kinetics of the reactions between the three calcium aluminate reactive phases and the gypsum formed.

$$CA + qC\bar{S}H_2 \rightarrow C_6A\bar{S}_3H_{32} \tag{5}$$

In Eq. (5), CA refers to the equivalent calcium aluminates (see Eq. (6)) and q represents the stoichiometric weighted coefficient of the sulfate phase (see Eq. (7)).

$$CA = \gamma_1 C_3A + \gamma_2 C_4AH_{13} + \gamma_3 C_4A\bar{S}H_{12} \tag{6}$$

$$q = 3\gamma_1 + 3\gamma_2 + 2\gamma_3 \tag{7}$$

In Eqs. (6)–(7), the coefficients γ_i used are defined as the proportion of each aluminate phase to the total aluminate content.

2.2. Diffusion–reaction model

The deterioration processes defined by the chemical reactions take place depending on the availability of sulfate ions and calcium