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Numerical modelling of mechanical deterioration of cement mortar under external sulfate attack

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HIGHLIGHTS

- An analytical model to estimate the flexural strength of composite is developed.
- The proposed method is applied to investigate the external sulfate attack.
- Internal pressure is a critical factor for evaluating the flexural strength.
- An empirical model is proposed to estimate the degradation of flexural strength.

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ABSTRACT

An integrated numerical method is developed to model the deterioration of mechanical properties of cement mortar under external sulfate attack (ESA). The proposed method is module-oriented, which includes three modules, i.e. an ionic diffusion module, a chemical reaction module and a mechanical module. In the mechanical module, an analytical model is developed for evaluating the variation of flexural strength under ESA. The development of internal pressure obtained from numerical computations and the degradation of elastic property estimated using the conventional Mori-Tanaka (MT) method are both considered in the proposed analytical model. Ionic diffusion and chemical reactions during the ESA are solved by the modified Poisson-Nernst-Planck (MPNP) model and chemical thermodynamics in the ionic transportation and the chemical reaction modules respectively. The developed method is validated against the reported ESA experiments in terms of the deterioration of both the elastic modulus and the flexural strength. Furthermore, the key factors governing the mechanical deterioration of cement mortars under ESA are discussed in details, and an estimation model is developed.

1. Introduction

External sulfate attack (ESA) is a critical durability concern for cementitious materials, which may lead to destructive action [1–3]. During the ESA, the ingress of sulfate ion causes massive precipitations of the expansive hydration products, i.e. gypsum and ettringite (AFt), resulting in propagation of microcracks [4]. In addition, calcium leaching generally occurs along with the ESA, and the collective effects would cause degradations of mechanical properties, such as elastic modulus and strength. Studies on the sulfate resistance of cementitious materials have been carried out for decades. In the early studies [5,6], flexural strength was regarded as an indicator to assess the potential sulfate resistance, mainly because the flexural strength is a more sensitive parameter comparing to other properties, such as compressive strength, expansion or elastic properties. On the other hand, as an important parameter in structural design, the degradation of flexural strength under the ESA has yet been thoroughly investigated. Many researchers studied the degradation of the elastic modulus and compressive strength [7,8], but very few addressed the topic of flexural strength degradation. Actually, the degradation mechanism of flexural strength was found to be very different from the other properties due to the development of internal pressure during the ESA [9].

According to experimental studies, the overall degradation extent of a material is closely related to the size of the specimen as the chemical attack is progressive. In addition, the size of the test specimen also plays an important role in controlling the efficiency of the experiment. In order to achieve significant ESA corrosions within an acceptable testing duration, the method of using small mortar specimens tested under sodium sulfate (Na_2SO_4)

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solutions [10] were thus widely adopted. Comparing to concrete, mortar possesses the similar microstructures but can generally be prepared in a much smaller size due to the fine aggregate distribution, such as 10 mm × 10 mm × 60 mm [9] and 40 mm × 40 mm × 160 mm [11]. Aköz et al. [5] measured the variation of flexural strength of cement mortars under the ESA with different sulfate strengths. Zhang et al. [9] carried out several similar ESA experiments, where the exposure time, concentration of Na_2SO_4 and water-to cement ratio (w/c) were found to be the main influential factors. Some other researchers [12,13] studied the durability of mortar and concrete subjected to the combined ESA and flexural loading, but their experimental measurements were focused only on the variation of elastic modulus instead of flexural strength.

Modelling investigations on the degradation of the flexural strength of cementitious materials under ESA were very limited in the literature [9,14], and mainly the empirical methods were reported. Schneider and Chen [14] proposed an empirical model to study the degradation of flexural strength under ESA, and the mutual influences of mechanical and chemical actions on the flexural strength were taken into account. The parameters adopted in their model must be calibrated from specific experiments [14], which confines the scope of the application. Zhang et al. [9] developed an analytical model based on micromechanics to evaluate the variation of flexural strength of mortars under the ESA. However, their model also used the parameters determined directly from experiments, including the parameters for evaluating the degradation of elastic modulus and the development of internal pressure [9]. Therefore, a more advanced method that is independent of the experimental data is highly demanded.

Based on the previous study [3,15], the module-oriented numerical method is further developed in this paper to study the mechanical degradation of cement mortar under the ESA. The method consists of an ionic transportation module, a chemical reaction module and a new mechanical module. In the mechanical module, an analytical model is proposed to calculate the flexural strength for a composite medium with internal pressure, which simulates the case of cementitious materials subjected to the ESA [3]. Only the basic properties, such as cement composition, physical and mechanical properties of the cement constituents as well as the immersion conditions, are required for the modelling. To fully demonstrate the influence of internal pressure on the flexural strength, the reported ESA tests on the mortars prepared from both the sulfate-resisting cement (low in C3A) [16] and ordinary Portland cement (high in C3A) [9,11] are modelled. Furthermore, by using the proposed numerical method, the governing factors for the mechanical deterioration of cement mortars under ESA are investigated, and an estimation model is developed for evaluating the mechanical deterioration of OPC mortars during the ESA, including the variations of both the elastic modulus and the flexural strength.

2. Numerical framework

The present numerical framework is module-oriented, consisting of three main modules. Operator splitting approach (OSA) is adopted for modelling the reactive transportation during the ESA [17,18], so that the simultaneous process can be separated and modelled in the ionic transportation module and the chemical reaction module respectively. The damage evaluation module as developed in the previous studies [3,15] is further expanded into a mechanical module, where the accumulation of damages and deterioration of mechanical properties are evaluated. An overview of the proposed numerical framework is shown in Fig. 1.

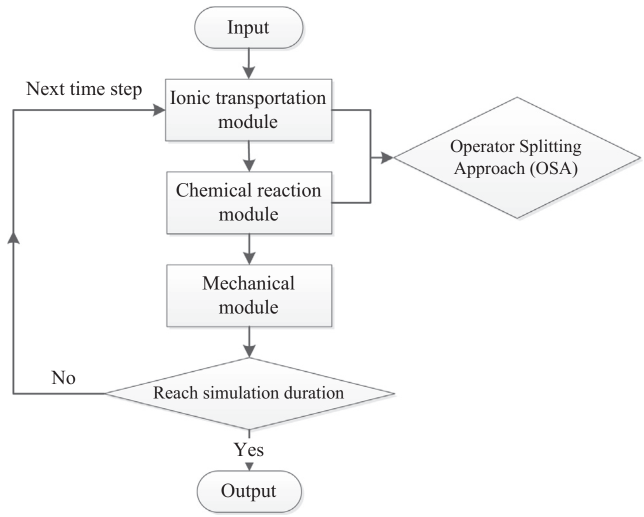

Fig. 1. Numerical framework.

The validity of applying the OSA in modelling the chemical degradation of cementitious materials has been demonstrated based on the local equilibrium assumption (LEA) [3,15,19]. As shown in Fig. 1, the ionic transportation module and the chemical reaction module are modelled sequentially, and the degrees of freedom (DoFs) are thus classified into two categories, i.e. primary and secondary DoFs, which can significantly reduce the computational effort. The diffusive species and the variables related to the ionic transportation are the primary DoFs, and the solid contents of cement hydrates are the secondary DoFs associated to the chemical reaction module. Within each time step, the ionic transportation module is first executed based on the modified Poisson-Nernst-Planck (MPNP) model, which has been demonstrated by the authors [3] to generate accurate simulations on the ESA. The chemical reaction module is carried out subsequently using chemical thermodynamics to evaluate the chemical reactions caused by the transportation of multiple ions [20]. The damages and deterioration to the material resulted from chemical reactions are then evaluated in the following mechanical module. All three modules are coded and run in MATLAB, and each module is carried out using as independent solver. Finite element method is applied to solve the complex partial differential equation (PDE) system, i.e. the MPNP model [3], in the ionic transportation module. By using chemical thermodynamics, the chemical equilibrium are forced on each finite element node and calculated algebraically. In the mechanical module, the empirical models, as reported in the literature [3,19], are adopted to estimate the material damages and the deterioration of physical properties. Mori-Tanaka (MT) method [21,22] is implemented to assess the degradation of elastic properties caused by the chemical reactions and the corresponding damages. Furthermore, an analytical model is developed to evaluate the deterioration of the flexural strength of cement mortar under the ESA, which is presented first in the following section.

3. An analytical model for evaluation of flexural strength

Herein, an analytical model is developed for evaluating the flexural strength of a composite medium with internal pressure. The proposed model can function as a part of the mechanical module to be coupled with the reactive-transportation modules, as introduced in Section 4, to model the deterioration of flexural strength of cementitious materials under the ESA. The present analytical model can also be standalone for evaluating the initial flexural