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Numerical simulation of fly ash concrete under sulfate attack

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HIGHLIGHTS

- An existing numerical model was extended to accommodate fly ash effects.
- Pozzolanic and hydration reactions were included in the extended model.
- The extended model was validated with observation data from literature.
- Sulfate resistance of fly ash concrete was simulated using the extended model.
- Critical factors affecting concrete sulfate attack were explored.

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ABSTRACT

Portland cement concrete (PCC) suffers sulfate attack in sulfate-rich environments. On the other hand, industrial by-products such as fly ash and slag are routinely added to PCC to improve its properties. However, the impact of fly ash on concrete durability is not always conclusive and it is time- and energy-consuming to test concrete durability in the laboratory or through field observation. This study presents a numerical simulation of the durability of Portland cement concrete made with fly ash. The simulation of sulfate attack on fly ash concrete was performed based on ion transport mechanism. The chemical reactions among chemical compounds of hydrated cement paste and sulfate ions were considered. Additionally, the pozzolanic and hydration reactions of fly ash were incorporated as well to incorporate the impact of fly ash. The pozzolanic and hydration reaction were simulated through the extended version of an existing numerical procedure. Field observation data from the United States Bureau of Reclamation (USBR) was employed to validate the extended simulation program. After pozzolanic and hydration reactions of fly ash were incorporated, the prediction agreed well with the field measurements. The simulation shows that pozzolanic reaction of fly ash can significantly slow down sulfate attack on concrete, thus increasing the sulfate resistance of PCC and extending the service life of concrete infrastructures. The major factors that affect the sulfate resistance of concrete were explored through the numerical simulation as well.

1. Introduction

When Portland cement concrete (PCC) is exposed to sulfate salts, the sulfate ions move through pore system, reacting with chemical compounds of hydrated cement paste, producing expansive products, and causing damages such as spalling and cracking. The mechanisms in sulfate attack on concrete are always complicated and confusing [1]. Neither experimental nor numerical approaches can thoroughly explain this phenomenon. A typical test, which is aimed to describe the sulfate attack, usually does not duplicate the field conditions that concrete infrastructures are confronted with. The temperature is usually fixed and the specimens may be partially or continuously immersed in a specific sulfate salt, such as Na_2SO_4 or $CaSO_4$. Also usually only the macroscopic deterioration is measured over a defined period, such as expansion, mass loss, or strength decrease. When the field condition is not identical with the standard test, a sulfate resistant concrete defined by such standard test might not perform well in the field. On the other hand, although the field observation, for instance the one located at Sacramento, California [2], can "precisely" give the sulfate resistance of concrete in a specific area, it

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takes a very long period to get such feedback. Additionally, when concrete with poor sulfate resistance is casted in the field, field observations can merely report that such concrete is not appropriate in a specific area while it is not able to guide the concrete mix proportion design in the first place.

Distinct from laboratory test and field observation, numerical analysis can conveniently simulate various field conditions, including ion type and concentration, temperature, etc. More importantly, numerical analysis focuses on the mechanism of sulfate attack, reveals the change of chemical components inside cement paste/concrete and the mechanical degradation of concrete from a microscopic viewpoint. Additionally, such an alternative can quickly assess the sulfate resistance of concrete without consuming lots of energy.

Neville [3] described three approaches to mitigate sulfate attack, including using cement with low C_3A content, reducing $Ca(OH)_2$ content in the hydrated cement paste by using cements that contain supplementary cementitious materials (SCMs), and making concrete as dense as possible to prevent the ingress of sulfate solutions. The blended cements or cements added with mineral admixtures are widely used in concrete construction. There is no conclusive conclusion on the issue that whether the addition of mineral admixtures is helpful in improving the sulfate resistance of cement concrete. The sulfate resistance of blended cements depends on the cement-fly ash interaction products rather than on any arbitrary factor based on the fly ash chemistry alone [4]. Based on 24 months laboratory sulfate attack experiments, Al-Dulaijan et al. [5] claimed that the fly ash they used can improve sulfate resistance of concrete. Similar conclusion was drawn by Nie et al. [6]. Field observation on the sulfate attack on concrete by the US Bureau of Reclamation (USBR) [7] demonstrates that 30% low-calcium fly ash can greatly improve sulfate resistance in a standard Na_2SO_4 solution while the high-calcium fly ashes generally reduce the sulfate resistance of concrete, which is due to its rich contents of C_3A and $C_4A_3\hat{S}$. Similarly, Mather [8] and Tikalsky and Carrasquillo [9] reported that a high lime Class C fly ash may decrease sulfate resistance of concrete. The sulfate exposure test is suggested when fly ash containing more than 10% calcium oxide is added into concrete [10]. Several empirical models were developed to compare the contents of calcium, aluminate, and silicon oxides in fly ash, in which some thumb-up rules were recommended to determine whether a specific type of fly ash is beneficial to sulfate resistance of concrete [11,12]. According to Liu et al. [13], when cement paste was partially exposed to high concentrated sulfate solutions, the addition of fly ash can accelerate the sulfate ions penetrating into paste by capillary sorption due to pore size refinement, causing a higher concentration of SO_4^{2-} pore solution in the upper part of paste in contact with air but also in the saturated part in a shorter time than the pure cement paste. Due to such a higher concentration of SO_4^{2-} pore solution, pozzolanic activity of fly ash can be activated, generating more ettringite and gypsum, causing worse deterioration of cement-fly ash paste.

Numerous numerical simulations were conducted to investigate the consequent products, decalcification, and deterioration of mechanical properties of concrete under sulfate attack. Geospodinov et al. [14] proposed a mathematical model to outline how capillary filling with chemical products affects the process of ion penetration from the surrounding sodium sulfate solution and into the cement stone. The mathematical model can consider the multiple connected areas consisting of cement stone matrix and inclusions. However, the liquid in the capillaries is assumed to be immovable. Therefore, a further improved mathematical model was proposed by Mironova et al. [15], in which the subsequent liquid was considered to be pushed out due to the fact that the capillary was filled with products of chemical reactions in sulfate attack. The liquid push out effects was found to strongly influence sulfate ion diffusion. Marchand et al. [16] utilized a numerical model to investigate the influence of weak sodium sulfate solution on the durability of concrete, in which the coupled transport of ions and liquid and the chemical equilibrium of solid phases within the saturated system were taken into account. It was found that exposure to weak sodium sulfate solutions, a significant reorganization of the internal microstructure of concrete occurred, and the dissolution of calcium hydroxide and the decalcification of C-S-H were presented. Santhanam et al. [17] placed cement concrete into sodium and magnesium sulfate solutions and measured the expansion of concrete and observed the microstructure change. They reported two stages of expansion for concrete in sodium sulfate solution, i.e., little expansion stage and rapid expansion stage, as well as a steady expansion for concrete in magnesium sulfate solution. Based on microstructure observation during sulfate attack, the mechanism of sulfate attack on concrete from the two different sulfate solutions were simulated in developed models [18]. Zuo et al. [19] used Fick's second law and reaction kinetics to establish a nonlinear and non-steady equation for the diffusion–reaction behaviors of sulfate ions in the concrete plate. The sulfate and calcium aluminate concentrations and the expansive strain due to sulfate attack in concrete were investigated. The sulfate-induced damage can significantly affect the pore structures and therefore the transport of ions in concrete. Sun et al. [20] proposed a diffusion model of sulfate ions in which the evolution of sulfate-induced damage was taken into account. They used ultrasonic tests to determine the evolution of damage related to immersion time and concentration of sulfate ions.

Nevertheless, the influence of the addition of fly ash on the sulfate resistance was rarely investigated at the microstructure level. Due to chemical reactions introduced by fly ash, such as pozzolanic reaction, the microstructure of fly ash concrete and the pore system in it will be different from those of plain cement concrete, which will result in different sulfate resistance. It is well known that the pozzolanic reaction consumes calcium hydroxide, making the concrete denser while the product of sulfate attack, ettringite, hard to form. However, fly ash rich in calcium oxide may accelerate the sulfate attack.

2. Objective and scope

The objective of this study is to extend a numerical model by incorporating the effects of fly ash and to employ the extended model to numerically simulate sulfate attack of fly ash concrete. In order to fulfill this target, the chemical reactions caused by fly ash, including pozzolanic and hydration reactions, were taken into accounts along with the regular chemical reactions occurring prior to sulfate attack. The Mobasher–Tixier Model [21,22] was extended by incorporating the chemical reactions related to the addition of fly ash using a finite difference method. The simulation procedure on the sulfate attack was shown in Fig. 1. The modified model was validated with the field observation data obtained from the United States Bureau of Reclamation (USBR) before it was used to explore the main factors affecting the durability of fly ash concrete.

3. Chemical reactions in concrete under sulfate attack

When fly ash is added into cement paste, pozzolanic reaction might occur depends on its chemical components. Assume that the reaction of pozzolan and lime produces the same hydration products as cement as following reaction:

$$3CH + 2S = C_3S_2H_3 \qquad (1)$$