Crack Formation Modeling in Concrete Affected by Iron-Sulfide Reactions

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Abstract

Damage in concrete containing sulfide-bearing aggregates has become a critical issue in several countries such as the USA, Canada, and Ireland. This deterioration unfolds over decades and is driven by oxidation reactions in sulfide-bearing aggregates, followed by internal sulfate attack within the cementitious matrix. About 60 % to 75 % of concrete is composed of aggregates, and the oxidation of sulfide-bearing particles causes aggregate expansion, enabling sulfate release and leading to progressive cracking. This process severely impacts the mechanical and durability properties of concrete by altering its microstructure.

Pyrrhotite-related deterioration has prompted extensive research aimed at understanding the underlying chemical and mechanical mechanisms. To investigate crack formation and propagation, a quasistatic two-dimensional finite element model (FEM) was developed to simulate crack network evolution with a pixelated approach used to identify the different phases in concrete. The model provides valuable insights into the influence of microstructural characteristics on crack network formation and the role of internal phase expansion in degrading the elastic properties of concrete. A scanning electron microscopy (SEM) image of undamaged concrete from a Connecticut (CT) house that had a damaged foundation was examined, and the crack network was simulated using the developed FEM. A sensitivity analysis was performed to assess the impact of convergence criteria on model precision and computational efficiency. The model can be used to clarify damage mechanisms caused by internal chemical reactions and localized expansion.

***Keywords**: concrete degradation; crack nucleation and initiation; crack propagation; pyrrhotite*

1. INTRODUCTION

Concrete deterioration associated with the oxidation of iron sulfide minerals has been reported in several regions worldwide [1]. In Connecticut, thousands of residential foundations have been confirmed to exhibit damage attributable to pyrrhotite oxidation [2]. The observed distress typically includes whitish surface deposits, yellowish discoloration, pop-outs, and characteristic map cracking [3–5]. Pyrrhotite ($Fe_{1-x}S$) can be naturally present in aggregates. It oxidizes upon exposure to moisture and oxygen, forming iron hydroxides. During this process, sulfate ions (SO_4^{2-}) are released into the surrounding cement matrix, triggering internal sulfate attack [6, 7]. These reactions produce expansive iron corrosion products such as goethite and ferrihydrite, as well as secondary phases including gypsum, ettringite, and thaumasite. The continued accumulation of these products over time leads to progressive expansion, cracking, and deterioration of concrete foundations (see Figure 1.1).

This deterioration has motivated extensive research aimed at understanding the underlying chemical and mechanical processes driving pyrrhotite-induced damage. Studying how cracks nucleate and propagate provides important insight into the progression of damage caused by pyrrhotite oxidation. To investigate these mechanisms, a quasistatic two-dimensional finite element model was developed to simulate crack initiation and formation in concrete containing sulfide-bearing aggregates. A pixelated approach was used to capture the distinct mechanical behavior of different concrete phases such as aggregates, mortar, voids, and pyrrhotite, while expansion was applied at pyrrhotite locations to represent internal phase expansion [8]. Furthermore, the developed model in general helps in understanding damage mechanisms associated with internal chemical reactions and/or expansion and provides a foundation for future efforts to mitigate deterioration in affected structures. It can also predict elastic properties, including Young's, bulk, and shear moduli and Poisson's ratio as a function of the degree of deterioration. This extended abstract presents the model framework and its development, along with field sampling and laboratory testing. It also summarizes the model's sensitivity analysis and the preliminary simulation results.

Figure 1.1: Deterioration of concrete foundation due to pyrrhotite

2. QUASISTATIC NUMERICAL MODEL

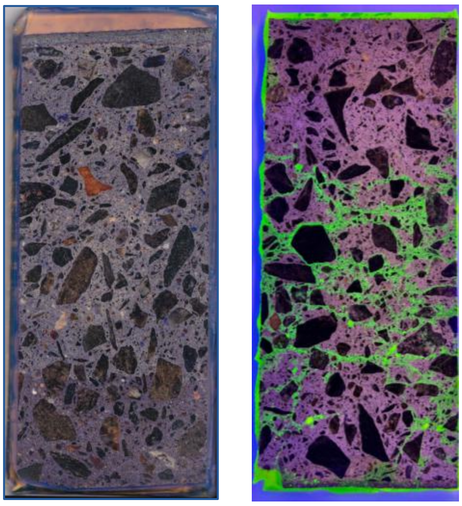
2.1 Model Development

The model represents concrete microstructures by discretizing a 2-D image into pixels with each pixel assigned material properties corresponding to its phase. Chemically driven expansion associated with pyrrhotite oxidation is introduced through an intrinsic strain applied to the relevant phases. When the stress (or strain) at a given pixel exceeds a predefined critical stress (or strain), it is converted into a crack pixel with zero stiffness [9]. Following each cracking event, the stress field is recalculated, and the procedure is repeated iteratively to simulate the progressive development of crack networks. Additional details are provided in [8, 10].

Concrete behaves as a quasi-brittle material; therefore, a quasistatic, linear-elastic framework is adopted to capture its crack-formation mechanics. The stress field is obtained by minimizing the elastic potential energy with the governing equations discretized using bilinear four-node quadrilateral finite elements. Previous evaluations of this formulation have demonstrated that it yields reliable elastic properties [11]. The elastic modulus and Poisson's ratio are assigned to the various concrete phases such as aggregate, mortar, and voids, while the pyrrhotite-bearing phases are assigned a predefined intrinsic strain of 0.01 to promote crack initiation at those locations under the adopted failure criterion [8]. Additionally, the number of cracks permitted per iteration, N, can be specified to control how many pixels are converted into crack pixels during each iteration.

2.2 Field Sampling and Laboratory Testing

Cores were collected from a deteriorated foundation in Stafford Springs, Connecticut, scheduled for full replacement due to pyrrhotite-related deterioration. Samples were obtained from multiple structural elements, including walls, slabs, and foundation. The specimens were tested for elastic properties via resonance frequency testing (RFT), as well as for compressive strength [12]. Moreover, selected cores were sliced into 10.8 cm by 25.4 cm sections, Figure 2.2 (a), for further evaluation, including carbonation assessment and UV epoxy impregnation to highlight internal crack networks, see Figure 2.2 (b). The sliced sections were further divided into smaller sections and carbon-coated for SEM analysis. Selected undamaged regions i.e., areas without visible cracking were then extracted from the SEM images and used as input microstructures for the model, see Figure 3.2 (a).



(a) (b)

Figure 2.2: Field sample preparation: (a) sliced section; (b) cracked sample

3. RESULTS AND DISCUSSIONS

3.1 Sensitivity Analysis

As with any numerical model, computational time becomes an important factor especially when the system includes very large pixel counts, as is the case here. In addition, the distribution of pyrrhotite within aggregates is heterogeneous: some aggregates contain no pyrrhotite, while others contain varying amounts. To control computational time, a sensitivity analysis was performed focusing on two key parameters: the convergence criterion and the number of cracks allowed per iteration, N [8]. A very small convergence threshold improves numerical accuracy but also leads to longer run times. Similarly, reducing N yields a more realistic representation of crack evolution in concrete, yet it also requires substantially higher number of iterations. The goal of this analysis is to identify parameter values that balance physical realism with practical computational efficiency. In these simulations, N = 400 cracks per iteration was selected, which is sufficient for expediting the study, while creating a representative crack map pattern of the damaged concrete [8].

Two main parameters were examined for the convergence criteria: (1) the elastic modulus and (2) the cracking pattern. In FEM, consistent output is essential to ensure that the numerical approach is reliable. First, the elastic modulus should stabilize as the solution approaches convergence. An initial convergence threshold of 10^{-14} was selected, as this level has been shown to produce reliable results [11]. To assess the effect of higher convergence thresholds, the elastic modulus obtained at each level was compared to the 10^{-14} reference solution. The percent error was approximately 23.3 % at 10^{-6}, but dropped sharply to 0.37 % at 10^{-8}, 0.62 % at 10^{-10}, and 1.63 % at 10^{-12}. The results show that a convergence level of 10^{-8} or lower yields accurate elastic properties, with errors below 2 %. Second, the crack formation pattern was examined. The crack networks were consistent when convergence criteria of 10^{-10} or lower was selected. Based on these observations, a convergence criterion of 10^{-10} was selected. This choice provides reliable results while requiring less computational time compared to the 10^{-14} case. Higher resolution reduces anisotropy effects; however, it significantly increases computational time. In this study, the resolution was limited to that of the SEM images, and no further refinement was performed due to computational constraints.

3.2 Microstructural Imaging and Digital Model Development

Modeling of microstructural degradation driven by sulfide diffusion from a pyrrhotite source is demonstrated in this section. After the sample was polished and carbon-coated, it was examined using SEM. Selected crack-free image was further processed and segmented into the main constituent phases, aggregate, mortar, voids, and pyrrhotite, as shown in Figure 3.2 (b). Appropriate elastic properties and predefined expansion strains were then assigned to the relevant phases. The resulting digital microstructure image generated from the developed model is presented in Figure 3.2 (c), with image dimensions of 1,000 by 1,000 pixels, representing 3 cm by 3 cm (30 μm/pixel).

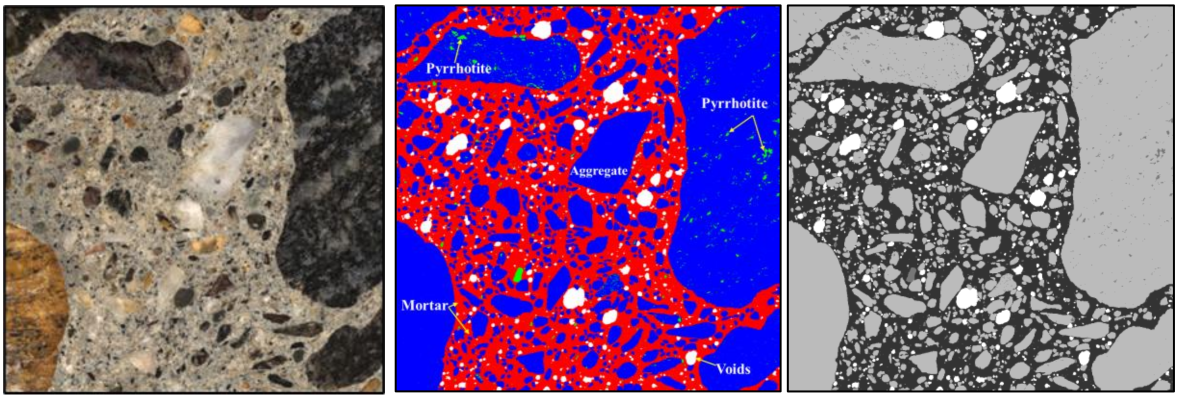


Figure 3.2: (a) Polished cross-section; (b) segmented SEM image (Blue: Aggregate, Red: Mortar, White: void, Green: Pyrrhotite); (c) digital microstructure

3.3 Crack Initiation and Propagation

Crack formation was examined. The expansive phases develop hoop tension around them, which drive cracks radially outward. Moreover, the results show that cracks initiate within the pyrrhotite-bearing phases and then extend toward other nearby pyrrhotite regions, where stresses are increased due to expansion. Cracks then propagate through the aggregates and continue into the surrounding mortar. The crack propagation after 30 and 80 iterations is shown in Figure 3.3.

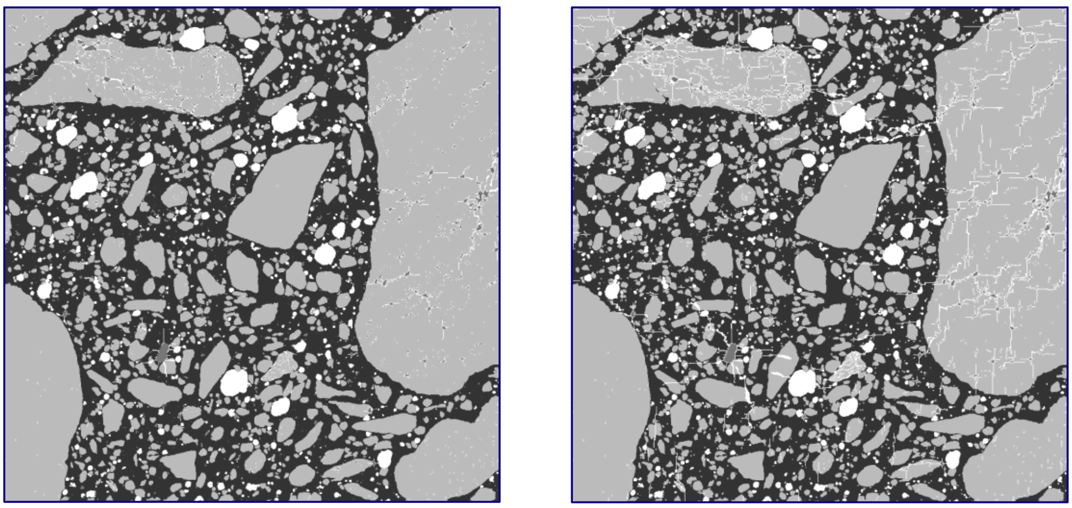


Figure 3.3: Crack formation after (a) 30 iterations and (b) 80 iterations

4. CONCLUSIONS

This work presented a finite element model designed to illustrate how cracks might develop when internal phases within cement-based materials expand due to pyrrhotite oxidation. A key advantage of the model is the ability to start from actual microstructural images, allowing the simulations to better reflect the real material. A sensitivity analysis was conducted and proper convergence criteria were selected. The model also provides estimates of how the elastic properties change as damage progresses, offering a way to evaluate the mechanical consequences of internal phase expansions in concrete materials. Future work will focus on extending the framework to capture internal sulfate attack, thereby allowing a more complete representation of sulfate driven deterioration.

5. ACKNOWLEDGMENT

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