Modelling of chemo-damage in concrete due to sulfate corrosion

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1. Introduction

The sulfate corrosion of concrete is a process in which a series of chemical reactions between migrated sulfate ions and active concrete particles lead to the degradation of concrete structure [1]. The product of this reaction, a strongly expansive crystal – ettringite, exerts a pressure on the surrounding concrete walls, which leads to propagation of pre-existing microcracks. The ettringite may crystallize in two type of reactions: through-solution reaction and topochemical reaction. Despite long lasting discussion in specialized literature there's still no agreement between researchers which type of reaction leads to expansive ettringite creation. In this paper a micromechanical model is proposed of sulfate attack in concrete element with and without external load. The model involves coupled processes of nonsteady diffusion of sulfate ions (second Fick's law), expansion of ettringite inclusions calculated from micromechanical solutions and microcracking induced by this expansion. The difference between expansions calculated from the model assuming a topochemical reaction and the one with a through-solution reaction of the ettringite crystallization will be presented. The obtained solutions will be compared with the experimental data in order to find out which type of reaction leads to harmful ettringite crystallization.

2. Expansion of ettringite crystal

The crystallizing ettringite exerts pressure on the surrounding concrete walls. Depending on the form of the ettringite crystallizing reaction, the pressure will be calculated from chemical thermodynamics (through-solution reaction) Equation (1), or from micromechanics (topochemical reaction) Equation (2).

(1) $$p_{tsr} = \frac{RT}{\bar{v}_s} \ln \frac{c_e}{c_{e0}}$$ (2) $$p_{tch} = \frac{2}{9} \frac{E}{(\nu - 1)} \varepsilon_{kk}^{**}$$

where R is the universal gas constant, T is the temperature, $\bar{v}_s$ is the stoichiometric coefficient of ettringite, c_e and c_{e0} are actual and "in referred state" concentrations of ettringite, respectively, E is the Young's modulus, ν is the Poisson's ratio, ε_{kk}^{**} is the inclusion eigenstrain calculated using the equivalent inclusion method. When the external stress is applied, the stress caused crack propagation is calculated from

(3) $$\sigma_{ij}^0 + \sigma_{ij} = 2\mu\left(\varepsilon_{ij}^0 + S_{ijmn}\varepsilon_{mn}^{**} - \varepsilon_{ij}^{**}\right) + \lambda\delta_{ij}\left(\varepsilon_{kk}^0 + S_{kkmn}\varepsilon_{mn}^{**} - \varepsilon_{kk}^{**}\right),$$

where σ_{ij} is the stress field generated by the ettringite, σ_{ij}^0 is the external stress, S_{ijkl} is the Eshelby's tensor.

3. Damage induced by ettringite formation

Assuming that the growing spherical ettringite crystal generates a penny-shaped microcrack, the stress intensity factor at the crack perimeter was derived as [2]

(4) $$K_I = \frac{p}{\sqrt{\pi a}}\left(a - \sqrt{a^2 - r^2}\right),$$

where p is the pressure calculated from Equation (1) or (2) or (3) depending on type of reaction and on the applied external stress. Once the sulfate concentration was known from the solution of second Fick's law [2] and the microcrack radius from the Griffith criterion $K_I = K_{IC}$, it was possible to determine Walsh-Budiansky-O'Connell crack density parameter ω ($\omega = N<a^3>$; N-number of cracks per unit volume, a-crack radius) and, thus, the effective diffusivity and stiffness from the self-consistent model and percolation theory. The microscale model was then volume averaged to arrive at the macroscopic constitutive stress-strain relation.

4. Application

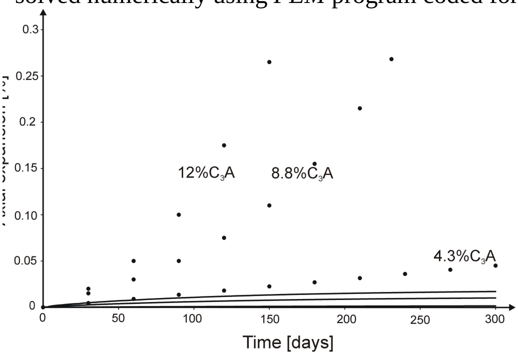
The proposed model was implemented numerically to compute the expansion of a slender mortar prism (ASTM C490) specimen immersed in sodium sulfate solution of concentration 0.352 mol/l. Calculations were carried out for ettringite formation in through-solution (Fig. 1) and topochemical (Fig 2) reaction and when specimen was under external compressive load. The axial strain due to plane diffusion in x, y directions in the region with low-to-moderate microcracking is:

(5) $$\varepsilon_z = \frac{\sigma_{33}^0}{E_{(x,y,t)}} + \frac{1}{E_{(x,y,t)} w_0} \int_0^1 \int_0^1 E_{(x,y,t)} f^I_{(x,y,t)} \varepsilon^{**}_{(x,y,t)} dxdy \qquad \text{for} \quad \omega < \omega_c$$

and for heavily damaged region:

(6) $$\varepsilon(\tilde{x}, \tilde{y}, \tilde{t}) = f^I \varepsilon^{**} \qquad \text{for} \quad \omega > \omega_c$$

where f^I is volume density of ettringite inclusions and σ_{33}^0 is the external load. The problem was solved numerically using *FEM* program coded for the present case.



'ig. 1. Expansion of mortar specimen (through-solution ɛaction). Solid lines - predictions of the present model, ircles - test data [3]

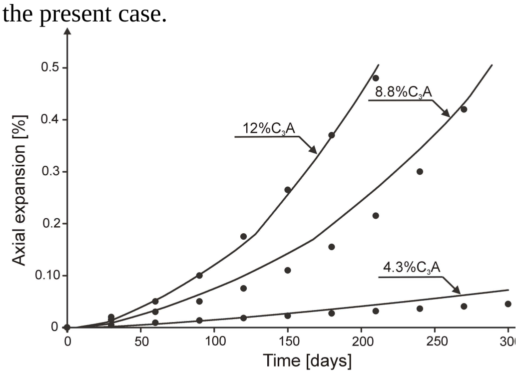


Fig. 2. Expansion of mortar specimen (topochemical reacti Solid lines - predictions of the present model, circles - data[3]

5. Conclusions

A micromechanical model has been proposed for the progressive damage in hardened concrete induced by the external sulfate attack. Expansions induced by two different types of ettringite formation have been studied. For the model with topochemcal reaction of ettringite formation (Fig. 2) a good agreement with experiment data has been obtained. This supports the view of a number of researchers that expansive ettringite crystallizes in a topochemical reaction. The influence of external load on microcracking, diffusion and axial expansion have also been considered.

6. References

[1] Skalny, J., Marchand, J., and Odler, I. (2002). *Sulfate Attack on Concrete*, Spon Press, London.
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[3] Ouyang, C., Nanni, A. and Chang, W.F. (1988). Internal and external sources of sulphate ions in portland cement mortar: two types of chemical attack, *Cement and Concrete Research*, **18**: 699-709.