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# ACTA MECHANICA SOLIDA SINICA

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## A Special Issue for the 8th International Conference on Fundamentals of Fracture

Guest Editors: Tongyi Zhang, Biao Wang, Xiqiao Feng

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## PREFACE

This special issue contains 16 papers selected from the presentations at the 8th International Conference on Fundamentals of Fracture (ICFF VIII), which was successfully held during 3-7 January 2008 at the Clear Water Bay and Nansha Campuses, Hong Kong University of Science & Technology. ICFF are the series of international conferences on fundamentals of fracture with the highest academic reputation. ICFF VIII is the successor of the previous seven held at NBS, Gaithersburg (USA, 1983), Gatlinburg (USA, 1985), Irsee (Germany, 1989), Urabandai (Japan, 1993), NIST, Gaithersburg (USA, 1997), Cirencester (UK, 2001), and Nancy (France, 2005). This is the first time that ICFF was held in China. ICFF VIII provided an international forum for presentations and discussions of the latest scientific and technological development in fundamentals of fracture. The general theme of ICFF VIII covered all aspects of fracture at a fundamental level, including contributions from those working in the disciplines of continuum mechanics, physics, chemistry, bioscience, nanoscience, metallurgy, ceramics, polymer science, etc. Researchers from 18 countries/regions including many internationally eminent scientists participated in this academic event. 188 papers were presented, covering the following areas: Fracture, creep, and fatigue at the atomic, mesoscopic, and macroscopic scales; Fracture, creep, and fatigue of engineering materials; Fracture, creep, and fatigue of smart materials; Fracture, creep, and fatigue of biomaterial; Environment effects; Fracture, creep, and fatigue under mechanical, thermal, electrical, and/or magnetic loading; Reliability and failure analysis of electronic devices and electronic packaging; and Dynamic fractures.

We wish to thank all the authors and speakers who contributed papers and presentations to ICFF VIII. We are considerably grateful to the members of the International Advisory Committee and the Local Organizing Committee for their efforts in making ICFF VIII a success. ICFF VIII was financially and morally supported by various sponsors, including Hong Kong University of Science & Technology, the Sun Yat-Sen (Zhongshan) University, Hong Kong Polytechnic University, K.C. Wong Education Foundation, Hong Kong Research Grants Council, National Science Foundation of U.S.A., the Croucher Foundation, National Natural Science Foundation of China (NSFC), Chinese Society of Theoretical and Applied Mechanics (CSTAM), Hysitron Inc., Far East and Oceanic Fracture Society (FEOFS), and Hong Kong Society of Theoretical and Applied Mechanics (HKSTAM). In particular, we would like to thank the Editor-in-Chief, Professor Quanshui Zheng, Professor Yuantai Hu, and Professor Qin Qian, for their encouragement and support throughout the course of ICFF VIII and for kindly providing a space in the Journal for this special issue. Their support has made the job of editing the issue an enjoyable and rewarding experience.

> Guest Editors: Tongyi Zhang Biao Wang Xiqiao Feng

# EQUIVALENT MODEL OF EXPANSION OF CEMENT MORTAR UNDER SULPHATE EROSION \*\*

Jue Zhu<sup>1</sup> Minqiang Jiang<sup>2</sup> Jiankang Chen<sup>1 $\star$ </sup>

<sup>1</sup>(Mechanics and Materials Science Research Center, Ningbo University, Ningbo 315211, China) <sup>2</sup>(State Key Laboratory of Nonlinear Mechanics (LNM), Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China)

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**ABSTRACT** The expansion property of cement mortar under the attack of sulfate ions is studied by experimental and theoretical methods. First, cement mortars are fabricated with the ratio of water to cement of 0.4, 0.6, and 0.8. Secondly, the expansion of specimen immerged in sulphate solution is measured at different times. Thirdly, a theoretical model of expansion of cement mortar under sulphate erosion is suggested by virtue of represent volume element method. In this model, the damage evolution due to the interaction between delayed ettringite and cement mortar is taken into account. Finally, the numerical calculation is performed. The numerical and experimental results indicate that the model perfectly describes the expansion of the cement mortar.

KEY WORDS size effect, microvoids, expansion, sodium sulfate attack

### I. INTRODUCTION

The expansion and damage evolution take place in concrete due to the sulphate erosion in the ocean environment. After diffusing in concrete, sulphate ions will be combined with the hydrate solution in microvoids to form ettringite crystals<sup>[1-6]</sup>. Such an ettringite is called as the delayed ettringite. At the contact of the delayed ettringite with the surface of the voids, the expansion of concrete will occur due to the growth of the voids and the nucleation of micro-cracks. It is well known that the damage evolution will affect the durability of concrete materials and structures, because of this, it is necessary to investigate the expansion and damage evolution for improving the durability of concrete structures.

Usually, the expansion and damage evolution take place in cement mortar or at the interface between the cement mortar and aggregates<sup>[3]</sup>. Hence, the expansion of cement mortar under sulphate erosion is investigated in this paper. Firstly, specimens of cement mortar are fabricated with different ratios of water to cement. Then the specimens are put into sulphate solution with different concentration. Secondly, the expansion of specimen immerged in sulphate solution is measured at different times. Thirdly, a theoretical model of expansion of cement mortar under sulphate erosion is suggested by virtue of volume element method. In this model, the cement mortar is considered as a porous material, the damage evolution due to the interaction between the delayed ettringite and cement mortar is taken

 <sup>\*</sup> Corresponding author. Phone: +86-574-87600075; Fax: +86-574-87608358; Email address: chenjiankang@nbu.edu.cn, zhujue@nbu.edu.cn (for Jue Zhu).

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into account. Finally, the numerical calculation is performed. The numerical and experimental results indicate that the model perfectly describes the expansion of the cement mortar.

### **II. EXPERIMENTAL APPROACH**

Specimens of Portland cement mortars of  $40 \times 40 \times 160$  mm are prepared as shown in Fig.1. The water-to-cement ratios of the specimen are taken as 0.4, 0.6, and 0.8. The maximum aggregate size of specimen is 0.2 mm, and it is much smaller than the dimension of the tested specimen. In order to measure more exactly the expansion behavior under the attack of sulphate radical ions, two small spherical metal balls are put into the ends of the specimen.

The erosion solution is chosen as the solution of sodium sulphate. In order to accelerate the expansion and damage evolution, the concentration of the solution is selected as 3.00 mass% and 8.00 mass% sodium (namely,  $\text{SO}_4^{2-}$  concentration is 20,250 and 54,000 ppm, respectively). Pure water is also selected as a solution (controlled solution) for comparison.

After the common initial curing time, the original length of specimens is measured by micrometer, and then stored in three different solutions (shown in Fig.2.). The total immergence time is 472 days. During the immergence period, the length of the specimen is measured at different immergence times. Experiment results indicate that the length of the specimen under sulphate erosion may increase. The expansion strain of the specimen is obtained by the length change divided by the original length of the specimen. The experimental results are plotted in Figs.3 $\sim$ 5.

The expansion mechanism is the interaction between the delayed ettringite crystal and the cement mortar matrix. After the diffusing in cement mortar, sulphate radical ions will be combined with the hydrate solution in the voids of cement mortar, which leads to the nucleation and growth of ettringite. Figure 6 shows the SEM photo of the delayed ettringite. When the ettringite contacts the surface of voids, it will apply internal pressure to the surface of voids. Under the internal pressure, the specimen will expand.

It can be seen from the experimental results that the expansion strain of the cement mortar increases with the increasing concentration of sulphate solution. If the concentration of solution is 0 ppm, namely, pure water, there is almost no expansion for the specimen. We also note that there exists a characteristic



Fig. 1. Specimen of cement mortar with the w/c = 0.6.



Fig. 3. Expansion strain of the specimen with w/c = 0.4.



Fig. 2. Specimens immerged in sulphate solution.



Fig. 4. Expansion strain of the specimen with w/c = 0.6.



Fig. 5. Expansion strain of the specimen with w/c = 0.8.



Fig. 6. SEM photo of delayed ettringite crystal.

time  $t_0$ , when the immergence time t is less than  $t_0$ , the expansion can hardly occur. If, however, t is equal to or greater than  $t_0$ , the expansion will take place. The characteristic time is affected by the concentration of sulphate solution and the value of w/c.

## III. EXPANSION MODEL OF CEMENT MORTAR UNDER SULPHATE EROSION

The cement mortar can be considered as a porous material (shown in Fig.7). The effect of the delayed ettringite is replaced by an internal pressure P. In order to propose a simple theoretical model of expansion, the method of represent volume element (RVE) with damage evolution is adopted (shown in Fig.8).



Fig. 7. Deformation of voids under internal pressure P.



Fig. 8. Represent volume element considering microcrack.

The constitutive relation of the cement mortar matrix is approximately assumed to be linear viscoelastic, and it may be expressed as  $in^{[7]}$ 

$$\boldsymbol{\sigma}(t) = \int_0^t \boldsymbol{L}(t-\tau) : \dot{\boldsymbol{\varepsilon}}(\tau) \,\mathrm{d}\tau, \qquad \boldsymbol{\varepsilon}(t) = \int_0^t \boldsymbol{J}(t-\tau) : \dot{\boldsymbol{\sigma}}(\tau) \,\mathrm{d}\tau \tag{1}$$

where L(t) and J(t) are the fourth order relaxation modulus and creep compliance, respectively. By means of separation of variables<sup>[7]</sup>, the stress and strain may be expressed as the product of time-dependent and spatial-dependent functions as follows:

 $\boldsymbol{\sigma}\left(\boldsymbol{x},t\right) = \hat{\boldsymbol{\sigma}}\left(\boldsymbol{x}\right)f\left(t\right), \qquad \boldsymbol{\varepsilon}\left(\boldsymbol{x},t\right) = \hat{\boldsymbol{\varepsilon}}\left(\boldsymbol{x}\right)g\left(t\right)$ (2)

Assume that  $\boldsymbol{L}(t)$  and  $\boldsymbol{J}(t)$  can also be expressed as in<sup>[8,9]</sup>

$$\boldsymbol{L}(t) = \boldsymbol{L}l(t), \qquad \boldsymbol{J}(t) = \boldsymbol{J}j(t)$$
(3)

where

$$\hat{\boldsymbol{L}} = \boldsymbol{L}(0), \qquad \hat{\boldsymbol{J}} = \boldsymbol{J}(0) \tag{4}$$

and l(t) and j(t) are functions of time, and l(0) = j(0) = 1.

From Eqs.(1)-(3) we obtain

$$f(t) = \int_0^t l(t-\tau) \dot{g}(\tau) d\tau, \qquad g(t) = \int_0^t j(t-\tau) \dot{l}(\tau) d\tau$$
(5)

The relation between increments of stress and strain can be obtained as the followings:

$$\Delta \boldsymbol{\sigma} = \boldsymbol{\Lambda} \left( t \right) : \Delta \boldsymbol{\varepsilon} \left( t \right) \tag{6}$$

where

$$\boldsymbol{\Lambda}(t) = \psi(t) \boldsymbol{L}(0), \qquad \psi(t) = 1 + \frac{1}{\dot{g}(t)} \int_0^t \dot{l}(t-\tau) \dot{g}(\tau) \,\mathrm{d}\tau$$
(7)

Equation (6) indicates that the relation between the increments of stress and strain may be described by a 'linear elastic' relation with a variable fourth order tangential modulus,  $\Lambda(t)$ .

Based on Eq.(6), the increment of displacement of the outside boundary of RVE is obtained  $as^{[10]}$ 

$$\Delta u = \frac{\Delta P}{E_0 \psi(t) (b^3 - a^3)} \left[ (1 - 2\nu) a^3 r + \frac{1 + \nu}{2r^2} a^3 b^3 \right]$$
(8)

Therefore, the increment volume strain of entire RVE can be obtained by

$$\Delta \varepsilon_{kk} = \frac{3\Delta u}{b} = \frac{9\Delta P f_v \left(1 - \nu\right)}{2E_0 \psi \left(t\right) \left(1 - f_v\right)} \tag{9}$$

where  $f_v = a^3/b^3$  is the volume fraction of voids as well as in cement mortar. Since the damage evolution takes place when the cement mortar is under the internal pressure, hence,  $f_v$  includes two parts, one is the initial volume fraction of voids before the action of internal pressure, the other is the damage, namely,

$$f_v = f_{v0} + D\left(t\right) \tag{10}$$

where D(t) is the equivalent volume fraction due to the damage evolution. Substituting Eq.(10) into Eq.(9) yields

$$\Delta \varepsilon_{kk} = \frac{9\Delta P \left[ f_{v0} + D(t) \right] (1 - \nu)}{2E(t) \left[ 1 - f_{v0} - D(t) \right]}$$
(11)

Assume that the internal pressure is directly proportional to the immergence time, t,

$$\Delta P = P_0 \Delta t \tag{12}$$

Also, we assume that the damage evolution is directly proportional to the internal pressure,

$$D\left(t\right) = Ct\tag{13}$$

where C is the speed of the damage evolution.

Substituting Eqs.(12) and (13) into Eq.(11), then integrating Eq.(11), we obtain

$$\varepsilon_{kk} = \int_0^t \frac{9P_0\left(f_{v0} + Ct\right)\left(1 - \nu\right)}{2E_0\psi\left(t\right)\left(1 - f_{v0} - Ct\right)} \mathrm{d}t \tag{14}$$

The expansion is isotropic, namely, the longitudinal strain,  $\varepsilon$  is one third of  $\varepsilon_{kk}$ ,

$$\varepsilon = \frac{1}{3}\varepsilon_{kk} = \int_0^t \frac{3P_0\left(f_{v0} + Ct\right)\left(1 - \nu\right)}{2E_0\psi\left(t\right)\left(1 - f_{v0} - Ct\right)} \mathrm{d}t \tag{15}$$

where  $P_0$  and C are parameters to be determined. It is obvious that  $P_0$  and C are all greater than zero,

$$P_0 > 0, \qquad C > 0$$
 (16)

If Maxwell model is adopted to describe the constitutive relation of the cement mortar, we obtain

$$l(t) = \exp\left(\frac{-t}{\theta}\right), \qquad j(t) = 1 + \frac{t}{\theta}$$
(17)

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It is easy to obtain

$$g(t) = \frac{t^2}{2\theta}, \qquad \dot{g}(t) = \frac{t}{\theta}$$
 (18)

and

$$\psi(t) = \frac{\theta}{t} \left( 1 - e^{-t/\theta} \right) \tag{19}$$

The related parameters are taken  $as^{[11]}$ 

$$f_{v0} = 0.1, \quad \nu = 0.16, \quad E_0 = 0.4 \text{ GPa}, \quad \theta = 47.8 \text{ d}$$
 (20)

Note the constraint condition.

From Eqs.(16)-(20) and Eq.(15), as well as the experimental results shown in Figs.3-5, the parameters  $P_0$  and C are obtained and listed in Table 1.

Table 1. Magnitude of $P_0$ and $C$			
Samples	$P_0$ (Pa)	C (1/d)	
$w/c = 0.4, 20,\!250 \text{ ppm}$	$2.47 \times 10^{4}$	$1.67 \times 10^{-4}$	
w/c = 0.4, 54,000  ppm	$2.18 \times 10^{2}$	$3.84 \times 10^{-1}$	
$w/c = 0.6, 20,\!250 \text{ ppm}$	$4.18 \times 10^4$	$1.14 \times 10^{-4}$	
$w/c = 0.6, 54{,}000 \text{ ppm}$	$5.07 \times 10^4$	$1.77 \times 10^{-3}$	
$w/c = 0.8, 20,\!250 \text{ ppm}$	$4.23\times 10^4$	$7.52 \times 10^{-6}$	
$w/c = 0.8,  54,\!000 \text{ ppm}$	$2.66 \times 10^4$	$1.30 \times 10^{-3}$	

The curves of theoretical model and experimental results are plotted in Figs.9-14. From the results, we can see that the theoretical model coincides with the experimental results.



Fig. 9. Expansion strain of the specimen with w/c = 0.4, sulphate concentration of 20,250 ppm.



Fig. 10. Expansion strain of the specimen with w/c = 0.4, sulphate concentration of 54,000 ppm.



Fig. 11. Expansion strain of the specimen with w/c=0.6, sulphate concentration of 20,250 ppm.

Fig. 12. Expansion strain of the specimen with w/c = 0.6, sulphate concentration of 54,000 ppm.



Fig. 13. Expansion strain of the specimen with w/c = 0.8, sulphate concentration of 20,250 ppm.



#### **IV. CONCLUSIONS**

Some new results are obtained in the present work:

- Expansion of cement mortar is caused by the internal pressure due to the delayed ettringite. The viscosity and the damage evolution are the dominate mechanisms for the expansion.
- Expansion strain depends not only on the concentration of the sulphate solution, but also on the ratio of water to cement.
- Expansion of the cement mortar strongly depends on the relaxation time of the cement mortar.
- A new theoretical model for describing the expansion of the cement mortar is suggested.

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Strain (%)