MODELING AND SIMULATION OF CONCRETE DETERIORATION SUBJECTED TO EXTERNAL SULFATE ATTACK

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Abstract
In order to estimate theoretically the deterioration of concrete under sulfate attack, a chemo-
mechanical model is proposed to simulate the response of concrete exposed to external sulfate
solutions. The nonsteady diffusion equation of sulfate ion, in which chemical reactions
depleting sulfate ion concentration in the concrete are considered during diffusion, is
presented firstly. Based on the chemical reactions between sulfate and aluminates, the
expansion strain due to the growth of the reaction product resulting in the damage and the
failure of concrete is calculated. And then, a simplifed mechanical model describing the
changes of the expansion strain and stress in concrete due to the product growing is proposed,
and Drucker-Prager criterion is used to evaluate the yield failure of concrete caused by
expansion stress. Finally, numerical simulation is used to analyze the concrete deterioration
under sulfate solution, and results show that the model can predict the responses of concrete
with the diffusion time, such as sulfate ion concentration distribution, expansion strain and
stress, and yield failure process of concrete due to the chemical product growing.

1. INTRODUCTION
Sulfate attack is a chemical reaction between sulfate ions and some constituents of the
hydrated cement paste [1]. Concrete deterioration under sulfate attack may occur in two
different forms, cracking and spalling caused by concrete expansion or loss of strength and
mass [2]. In order to evaluate theoretically the deterioration of concrete under sulfate attack,
Marchand et al. [3] developed the numerical model STADIUM to predict the diffusion of ions
in unsaturated porous media, and the model considers chemical interaction of various ions
with the cement hydrated products and the effects of chemically induced microstructural
alterations on the diffusion properties of the material subjected to external sulfate attack.
Gospodinov et al. [4] proposed a mathematical model associated with sulfate ion diffusion
into cement composite considering the influence of the microcapillary filling and subsequent
liquid pressure due to chemical reaction products. Atkinson et al. [5] propose a model for
concrete damage that the rate of spalling can be expressed as a function of the elastic and
fracture properties of concrete, the intrinsic sulfate diffusion coefficient, the external sulfate concentration and the concentration of ettringite. Tixier and Mobasher [6] proposed a mathematical model for simulating the responses of cement-based materials subjected to sulfate attack, and the model may be utilized to predict expansion of a matrix phase, generation of internal stresses, evolution of damage.

This paper presents a chemo-mechanical model and analysis associated with sulfate ion diffusion, chemical reaction and concrete yield failure for simulating the responses of concrete exposed to external sulfate solutions.

2. MODEL

2.1 1-D diffusion equation

When the concrete specimen is subjected to the sulfate attack under the ambient ion concentrate $c_0$, the ion transfer processes are described as 1-D nonsteady diffusion in Figure 1. We assume that the concrete is an isotropic porous material, and its porosity is unchanged without sulfate attack, and the diffusion coefficients of the sulfate ion are identical in the section along the $x$ direction, as well as the molar concentration of the sulfate ion diffusing from the sulfate solution $F$ to the interior $I$ in the specimen. Therefore, based on Fick's second law, the diffusion equation is expressed as

$$\frac{\partial c}{\partial t} = \frac{1}{\partial x} D \frac{\partial^2 c}{\partial x^2} - \frac{1}{D} \frac{\partial c_d}{\partial t}$$

(1)

where $c = c(x, t)$ refers to the sulfate ion concentration, $x$ and $t$ represent the section position and the time respectively, and $c_d$ is the dissipated sulfate ion concentration due to chemical reactions. Depending on the dynamical equation of chemical reaction, there is [7]

$$\frac{\partial c_d}{\partial t} = -k \cdot c_{C3A}^0 \cdot f(c, t) \cdot c \cdot e^{-\frac{1}{3}t_{cr}}$$

(2)

where $k$ is the reaction constant of the sulfate ion, $c_{C3A}^0$ is the $C_3A$ initial concentration in the cement and $f(c, t)$ is determined by [7]

$$f(c, t) = 1 - h_a \cdot e^{-\frac{1}{2} \beta h_a + \beta h_a \cdot e^{\frac{1}{3}t_{cr}}}$$

(3)

where $\beta$ refers to the gypsum content in the cement, $h_a$ is the hydration degree of the cement, which can be approximately determined by [8]

$$h_a = 1 - 0.5 \cdot e^{1 + 1.67\tau} - 0.29\tau^{0.48}$$

(4)

$\tau$ is the cement hydrated time.

$D$ is the diffusion coefficient of the sulfate ion in concrete determined by [7]

$$D = \varphi(x, t) D_s$$

(5)
where $\varphi(x, t)$ refers to the concrete porosity related to the position $x$ and the time $t$, and $D_s$ is the diffusion coefficient corresponding to the electrolyte solution, which is the pore solution in concrete, there is [7]

$$D_s = \frac{RT}{z^2F^2} \frac{\hat{\Lambda}}{\epsilon^2} \frac{z^2 e^2}{16 \pi \epsilon_o \kappa RT (1 + \kappa a)}$$  \hspace{1cm} (6)

$$\kappa = zF \sqrt{\frac{2c}{\epsilon_o \epsilon_o RT}}$$  \hspace{1cm} (7)

$$\Lambda_m = \Lambda_m^0 - \frac{z^2 e F^2}{3 \pi} \sqrt{\frac{1}{\epsilon_o \epsilon_o RT \epsilon_o \epsilon_o \epsilon_o} + \frac{(\sqrt{2} - 1)z}{4 \epsilon_o \epsilon_o RT} \cdot \Lambda_m^0 \sqrt{c} + \frac{(2 - \sqrt{2})z^2 e F^2}{12 \pi \eta \epsilon_o \epsilon_o RT} \cdot \sqrt{\frac{1}{\epsilon_o \epsilon_o RT} \cdot \epsilon_o \epsilon_o \epsilon_o \epsilon_o \epsilon_o}$$  \hspace{1cm} (8)

In Equations (6)~(8), $T$ is the temperature, the other parameters are shown in Table 1.

**Table 1: Natural and constants related to sulfate ion and solvent at $T = 298K$ [7]**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
<th>Quantity</th>
<th>Value</th>
<th>Unit</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R$</td>
<td>8.31451</td>
<td>J/Kmol</td>
<td>Universal gas constant</td>
<td>$z$</td>
<td></td>
<td>Ionic valency</td>
</tr>
<tr>
<td>$F$</td>
<td>9.64853×10⁴</td>
<td>C/mol</td>
<td>Faraday constant</td>
<td>$a$</td>
<td>2.58×10⁻¹⁰</td>
<td>m Ionic radius</td>
</tr>
<tr>
<td>$k$</td>
<td>1.38066×10⁻²³</td>
<td>Sm²/mol</td>
<td>Bolzmann constant</td>
<td>$\Lambda_m^0$</td>
<td>8.000×10⁻³</td>
<td>Sm²/mol Conductivity</td>
</tr>
<tr>
<td>$e$</td>
<td>1.60218×10⁻¹⁹</td>
<td>C</td>
<td>Elementary charge</td>
<td>$\eta_0$</td>
<td>8.91×10⁻⁴</td>
<td>Kg/ms Viscosity</td>
</tr>
<tr>
<td>$\epsilon_0$</td>
<td>8.85419×10⁻¹²</td>
<td>C²/Jm</td>
<td>Vacuum electric permittivity $\epsilon_r$</td>
<td>78.54</td>
<td></td>
<td>Relative permittivity</td>
</tr>
</tbody>
</table>

Combining Equations (1), (2) and (5), there may be obtained

$$\frac{\partial c}{\partial t} = D_s \frac{\partial^2 \varphi}{\partial x^2} + D_s \cdot \varphi \cdot \frac{\partial^2 c}{\partial x^2} - k c_0^0 \cdot f(c, t) \cdot c \cdot e^{\frac{1}{3} r t}$$  \hspace{1cm} (9)

For Equation (9), the initial and boundary conditions respectively are

$$c(x, 0) = 0, \quad \frac{\partial c}{\partial x} \in (0, L)$$  \hspace{1cm} (10)

$$c(0, t) = \varphi_0 c_0$$  \hspace{1cm} (11)

where $c_0$ is the sulfate concentration in the solution, and $\varphi_0$ is the initial concrete porosity.

**2.2 Simplified chemo-mechanical model**

Based on the mechanism of the sulfate aggression on the cement composites [1], the deterioration of concrete is caused by the potential volumetric expansions associated with the chemical reactions between penetrating sulfate ion and the hydrated calcium aluminates. The
volumetric expansion results in the expansion stress in concrete. In this paper, it is assumed that the volumetric expansion is evaluated by the formation of ettringite from the combination of the calcium aluminates with the gypsum produced by the reaction between the sulfate and the calcium hydroxide, whose reactions may be expressed by

\[
\begin{align*}
\text{CH} + 2\text{SO}_4^{2-} &\rightarrow \text{C\text{S}H}_2 + 2\text{OH}^- \quad (12) \\
\text{C}_4\text{A} &\rightarrow 3\text{C\text{S}H}_2 + 14\text{H} \rightarrow \text{C}_6\text{A\text{S}}_3\text{H}_{32} + \text{CH} \quad (13) \\
\text{C}_4\text{A}\text{S\text{H}}_{12} + 2\text{C\text{S}H}_2 + 16\text{H} \rightarrow \text{C}_6\text{A\text{S}}_3\text{H}_{32} \quad (14) \\
\text{C}_3\text{A} + 3\text{C\text{S}H}_2 + 26\text{H} \rightarrow \text{C}_6\text{A\text{S}}_3\text{H}_{32} \quad (15)
\end{align*}
\]

According to Equations (13)-(15), the volumetric change \( v_{\text{CaI}} \) caused by the formation of ettringite is calculated by the following formula [6]

\[
v_{\text{CaI}} = \frac{(m_{v-\text{ETT}})^{-1}}{(m_{v-\text{CaI}})^{-1} + \gamma_i/m_{v-\text{ETT}}} - 1 
\]

where \( \text{Ca}_i \) are the hydrated calcium aluminate, and \( \text{Ca}_1, \text{Ca}_2 \) and \( \text{Ca}_3 \) refer to \( \text{C}_4\text{A}\text{H}_{13}, \text{C}_4\text{A}\text{S\text{H}}_{12} \) and \( \text{C}_3\text{A} \) respectively. \( \gamma_i \) is the reaction coefficients, \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) are equal to 3, 2, 3 respectively. \( m_{v-\text{ETT}} \), \( m_{v-\text{ETT}} \), \( m_{v-\text{CaI}} \) represent the molar volume of ettringite, gypsum, hydrated calcium aluminates respectively; \( m_v = d/M \), \( d \), \( M \) and \( m_v \) are the density, molar mass, and molar volume of given compound, \( d \) and \( m_v \) are given in Table 2 [9].

<table>
<thead>
<tr>
<th>Compound</th>
<th>Chemistry notation</th>
<th>( d ) (g/cm³)</th>
<th>( m_v ) (kmol/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tricalcium aluminate</td>
<td>( \text{C}_3\text{A} )</td>
<td>3.04</td>
<td>11.2</td>
</tr>
<tr>
<td>Monosulfate</td>
<td>( \text{C}<em>4\text{A}\text{S\text{H}}</em>{12} )</td>
<td>1.95</td>
<td>3.20</td>
</tr>
<tr>
<td>Tetracaluminate hydrate</td>
<td>( \text{C}<em>4\text{A}\text{H}</em>{13} )</td>
<td>2.02</td>
<td>3.60</td>
</tr>
<tr>
<td>Gypsum</td>
<td>( \text{C\text{S}H}_2 )</td>
<td>2.32</td>
<td>13.50</td>
</tr>
<tr>
<td>Ettringite</td>
<td>( \text{C}_6\text{A\text{S}}<em>3\text{H}</em>{32} )</td>
<td>1.75</td>
<td>1.40</td>
</tr>
</tbody>
</table>

According to Equation (16) and Table 2, the volumetric change \( v_{\text{CaI}} \) from \( \text{C}_4\text{A}\text{H}_{13}, \text{C}_4\text{A}\text{S\text{H}}_{12} \) and \( \text{C}_3\text{A} \) to \( \text{C}_6\text{A\text{S}}_3\text{H}_{32} \) are 0.48, 0.55 and 1.31 [9]. To calculate expansion stress in concrete, the volumetric change \( v_{\text{CaI}} \) is converted into the volumetric strain \( \varepsilon_{\text{v}} \). If not considering the capillary porosity in concrete, there is

\[
\varepsilon_{\text{v}} = \frac{V}{V_{\text{CaI}}} 
\]

where \( V \) is total molar volume including all compounds; \( V_{\text{CaI}} \) represents the molar volume of the reacted calcium aluminates, which is calculated based on the amount of the dissipated gypsum in Equations (13)~(15).

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Based on Equation (17), applying the averaging scheme for three reactants in the cement in Table 2, the total volumetric strain $\varepsilon_v$ of concrete is obtained from the amount of the reacted calcium aluminates and the corresponding volumetric changes

$$
\varepsilon_v = \frac{3}{i=1} \varepsilon_v^i = \frac{3}{i=1} \bar{V}_{C_{Al}} \frac{V}{V}
$$

(18)

Due to existed porosity in concrete, the volumetric strain and the expansion stress begin to occur until the porosity is full of the products. Therefore, the reduction of the volumetric strain $\varepsilon_v$ in Equation (18) caused by dissipating ettringite for filling the porosity should be considered [6]

$$
\varepsilon_{VR} = \varepsilon_v - \phi
$$

(19)

where $\varepsilon_{VR}$ refers to the real concrete volumetric strain; $\phi$, the capillary porosity being filled with ettringite crystals. Considering the inhomogeneity in the process of the crystal filling, $\phi$ is the discount of total capillary porosity $\Phi$ in concrete

$$
\phi = f \Phi
$$

(20)

where $f$ is the volumetric fraction of capillary porosity being filled with ettringite crystal, and $\Phi$ is total capillary porosity in concrete, determined by [9]

$$
\Phi = \begin{cases}
\frac{w}{c} - 0.39 h_{\alpha}, & \frac{w}{c} > 0.39 h_{\alpha} \\
\frac{w}{c} + 0.32, & 0 \leq \frac{w}{c} \leq 0.39 h_{\alpha} \\
0, & \frac{w}{c} < 0.39 h_{\alpha}
\end{cases}
$$

(21)

where $w/c$ is the water-cement ratio; $f_c$, the volumetric fraction of the cement in concrete.

The average expansion strain $\bar{\varepsilon}$ in concrete is obtained by the real volumetric strain $\varepsilon_{VR}$

$$
\bar{\varepsilon} = \frac{\varepsilon_{VR}}{3}
$$

(22)

2.3 Concrete constitutive law

As the expansion strain is formed in concrete, the expansion stress is caused in the specimen. A simplified uniaxial concrete constitutive law is used to represent the stress-strain responses [10], and described as follows:

$$
\sigma = \begin{cases}
1.2 \frac{\varepsilon f_i}{\varepsilon_y}, & \varepsilon \leq \varepsilon_y \\
0.312 f_p^2 \varepsilon_{y_p}^{1/2} - 1.0 \frac{\varepsilon f_i}{\varepsilon_y} + \varepsilon, & \varepsilon \geq \varepsilon_y
\end{cases}
$$

(23)
where \( f_r \) and \( \varepsilon_{up} \) are the ultimate stress and the corresponding strain, which are the peak stress and the corresponding strain in the stress-strain curve.

### 2.4 Drucker-Prager yield criterion

With the growing of the ettringite crystal under sulfate attack, the expansion strain and stress are gradually increasing, and distribute scalarly from the surface to the interior of the specimen. Consequently, concrete cracks caused by the expansion stress extend from the surface to the interior. To account for the crack extension when concrete is subjected to sulfate attack, Drucker-Prager yield criterion is used [11]. The yield function under uniaxial tension is

\[
f = \frac{3}{2} \left( \frac{\sigma}{\varepsilon} \right)^{\frac{2}{3}} - \kappa \alpha = 0 \tag{24}\]

### 2.5 Numerical methods

The concrete plate specimen, thickness \( L \), is immersed into the sulfate solution with the concentration \( c_o \), and the diffusion processes of the sulfate ion in the specimen are obtained by solving the nonsteady diffusion equation, formulated by Equation (9), together with the boundary conditions (10) and the initial condition (11). An implicit difference scheme is applied for solving numerically the formulated diffusion equation. Considering symmetrical diffusion of the sulfate ion from the two surfaces to the interior of the specimen, the diffusion equation is solved along a half of the specimen thickness \( L/2 \). The discretization scheme is that a half of the specimen thickness \( L/2 \) is divided into \( N \) parts with the proportional spacing and the increment \( \Delta x \). There are \( N+1 \) sections, that are perpendicular to the \( x \)-axis, and their coordinates are

\[
x_0 = 0 \ , \ x_1 = \Delta x \ , \ x_2 = 2\Delta x \ , \cdots \ , \ x_i = i\Delta x \ , \cdots \ , \ x_{N+1} = \frac{L}{2} \tag{25}\]

On the other hand, in the process of sulfate aggressing, the discretization step of time is selected as the increment \( \Delta t \). The sulfate ion aggressing history are described by the following time points

\[
t_0 = 0 \ , \ t_1 = \Delta t \ , \ t_2 = 2\Delta t \ , \cdots \ , \ t_j = j\Delta t \tag{26}\]

It is obtained that, the discrete solutions of the diffusion equations (9)-(11), the time-history changes of the sulfate ion concentration distribution in the specimen, are expressed by the following iterative equations [7]

\[
\{c_j\} = [B]^{-1} \left( \{c_{j-1}\} + \{F_j\} \right) \tag{27}
\]

\[
\{c_{0,j}\} = \begin{bmatrix} c_0 \\ 0 \\ 0 \\ 0 \\ \cdots \\ 0 \end{bmatrix}^T \tag{28}
\]

where \( c_j \) represents the sulfate ion concentration in every sections at the time \( t_j \); the matrix \([B]\) and \( \{F_j\} \) are determined by the following expressions
\[
\{ F_j \} = \mathcal{H} \mathcal{D}_{i,j} \varphi_{0,j} c_{i,j} \quad 0 \quad 0 \quad \cdots \quad 0 \quad rD_{(N-1,j)} \varphi_{(N-1,j)} c_{(N-1,j)} \frac{\Delta \varphi}{\Delta x^2} \quad r = \frac{\Delta t}{\Delta x^2} \quad (30)
\]

In Equations (29) and (30), \((x_{ij})\) denotes the variable at the section position \(x_i\) and the time \(t_j\), and \((x_{ij})\) represents the variable in every sections at the time \(t_j\).

3. RESULT AND DISCUSSION

Numerical results are given for the specimen that is kept in 2% water solution of sodium sulfate. The mineral compositions of the cement in the specimen are shown in Table 3. Proportions of concrete mixes design are presented in Table 4. One-dimension diffusion of sulfate ion and expansion damage of the specimen with thickness 40 mm are considered based on the above model and numerical methods. The related parameters are presented in Table 5.

**Table 3: Chemical compositions of raw materials**

<table>
<thead>
<tr>
<th>Composite</th>
<th>SiO&lt;sub&gt;2&lt;/sub&gt;</th>
<th>Al&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</th>
<th>CaO</th>
<th>MgO</th>
<th>SO&lt;sub&gt;3&lt;/sub&gt;</th>
<th>Fe&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Content w/%</td>
<td>20.60</td>
<td>5.03</td>
<td>65.06</td>
<td>0.55</td>
<td>2.24</td>
<td>4.38</td>
</tr>
</tbody>
</table>

**Table 4: Proportions of concrete mixes design**

<table>
<thead>
<tr>
<th>Cement kg/m&lt;sup&gt;3&lt;/sup&gt;</th>
<th>Water kg/m&lt;sup&gt;3&lt;/sup&gt;</th>
<th>Sand kg/m&lt;sup&gt;3&lt;/sup&gt;</th>
<th>Aggregate kg/m&lt;sup&gt;3&lt;/sup&gt;</th>
<th>Water-cement ratio w/c</th>
</tr>
</thead>
<tbody>
<tr>
<td>387</td>
<td>282</td>
<td>587</td>
<td>1091</td>
<td>0.48</td>
</tr>
</tbody>
</table>

**Table 5: Related calculation parameters in Model**

<table>
<thead>
<tr>
<th>Specimen thickness (L)</th>
<th>40 mm</th>
<th>Concrete ultimate stress (f_t)</th>
<th>1.42 Mpa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial C&lt;sub&gt;3&lt;/sub&gt;A content (c_{0_{3,4}})</td>
<td>6 or 673 mol/m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Concrete peak strain (\varepsilon_p)</td>
<td>0.00015</td>
</tr>
<tr>
<td>Initial gypsum content (\beta)</td>
<td>3%</td>
<td>Material parameter (\alpha)</td>
<td>0.211</td>
</tr>
<tr>
<td>Residual C&lt;sub&gt;3&lt;/sub&gt;A content hydrated</td>
<td>134.6 mol/m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Material parameter (\kappa)</td>
<td>1.004 Mpa</td>
</tr>
<tr>
<td>C&lt;sub&gt;4&lt;/sub&gt;AH&lt;sub&gt;13&lt;/sub&gt; content in hard cement</td>
<td>8.1 mol/m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Initial porosity (\varphi_0)</td>
<td>8%</td>
</tr>
<tr>
<td>C&lt;sub&gt;4&lt;/sub&gt;AH&lt;sub&gt;13&lt;/sub&gt;H&lt;sub&gt;12&lt;/sub&gt; content in hard cement</td>
<td>16.2 mol/m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Water-cement ratio w/c</td>
<td>0.48</td>
</tr>
<tr>
<td>Na&lt;sub&gt;2&lt;/sub&gt;SO&lt;sub&gt;4&lt;/sub&gt; solution concentration (c_0)</td>
<td>2% or 77 mol/m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Thickness interval (\Delta x)</td>
<td>0.5 mm</td>
</tr>
<tr>
<td>Capillary volumetric fraction (f)</td>
<td>40%</td>
<td>Time interval (\Delta t)</td>
<td>1 days</td>
</tr>
<tr>
<td>Chemical reaction constant (k)</td>
<td>3.05 × 10&lt;sup&gt;-8&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Cement volumetric fraction (f_c)</td>
<td>0.332</td>
</tr>
</tbody>
</table>
Figure 2 presents the concentration distribution of sulfate ion in the sections of the specimen with the diffusion time, considering the dissipated sulfate ion due to chemical reactions but neglecting capillary filling. Seen from the figure, under the constant solution concentration 2% immersed, the ion concentration in the specimen increases with the diffusion time, but the increasing rate of the ion concentration descend gradually from the surface to the interior of the specimen. In the same interval $\Delta t = 200$ days, the cumulation of the ion concentration increases companied with continual diffusion, and the farther from the surface of the specimen, there is more ion concentration cumulation, as illustrated in Figure 2(a). At the midpoint of the section in the specimen $x = 0.02m$, the sulfate ion concentration is close to zero before 2200 days, while after 2200 days, the ion concentration cumulation gradually increases, at $t_M = 3401$ days, the ion concentration $c(0.02m, t_M)$ is 5.07 mol/m$^3$.

![Figure 2: Concentration distribution of sulfate ion with diffusion time in the specimen](image)

Figure 3 gives the expansion strain distribution curves due to the ettringite growth. It is seen from the figure that, the change of the average expansion strain in the specimen with the diffusion time is similar to that of the dissipated hydrated calcium aluminates. But at the beginning of the sulfate ion diffusion, for example, before the time $t=200$ days, as the existed

![Figure 3: Changes of the average expansion strain caused by the chemical products](image)
Porosity in concrete need be filled with the ettringite, the expansion strain of the parts of the section positions in the specimen is equal to zero. The expansion strains in the specimen increase with the diffusion time. When the diffusion time $t_M = 3401$ days, the hydrate calcium aluminates have been depleted, and the expansion strain caused by the ettringite in the specimen reaches 0.0027, which is greater than the ultimate compression strain 0.002 under concrete restrained. Therefore, the concrete have been yield failure.

With the diffusion of the sulfate ion and the growth of the ettringite in the concrete, there cause the expansion stress in the specimen. Figure 4 describes the relations between the expansion stress due to the growth of the ettringite, the diffusion time and the section position. It is seen from the figure that, owing to the slow filling of the ettringite crystal, the expansion stress at any section positions along the thickness increases from zero to the peak stress $f_c = 1.42$ Mpa, and then decreases from the peak stress to the yield stress 1.27MPa where the yield stresses are 1.27MPa calculated by Drucker-Prage yield criterion Eq.(24) as a results of the concrete material yielding (See in Figure 4(b)). Figure 4(a) indicates that the peak stress point moves from the surface to the interior of the specimen with the increasing of the diffusion time, and the interior expansion stresses increase and the concrete work up to the yield along the $x$-direction. When the diffusion time $t_M = 3401$ days, the stress at any section positions in the specimen reaches 1.27MPa, and the stress-position curve becomes a horizontal line.

Figure 5 presents the change of the critical yield point in the specimen with the diffusion time, where the yield stresses are 1.27MPa, and shows that the movement rate of the yield point increase with the diffusion time. When the yield point moves from the surface to 0.007 m inwards, from 0.007 m to 0.14 m inwards, from

![Figure 4: Changes of the expansion stress caused by the chemical products](image1)

(a) Expansion stress changes with position          (b) Expansion stress changes with position and time

![Figure 5: Changes of the critical yield point with the diffusion time](image2)
0.14 m to 0.2 m inwards, there need 1220 days, 520 days, 140 days, respectively. For the critical yield point to arrive at the midpoint of the specimen $x = 0.02$ m, it takes $t = 1880$ days.

4. CONCLUSIONS
− Based on Fick’s second law, the nonsteady diffusion equation of the sulfate ion, in which the chemical reaction depleting the sulfate ion concentration in the concrete are considered during diffusion, are given.
− The finite difference method is applied to solve the diffusion equation and to simulate the diffusion process and concentration distribution of sulfate ion in the concrete.
− A simplified model describing the change of the expansion strain and stress in the concrete due to the growth of the ettringite resulting in concrete damage is proposed.
− Numerical simulation is used to analyze the concrete deterioration under the sulfate solution, and the results show that the model can predict the response of concrete with the diffusion time, such as sulfate concentration distribution, expansion strain and stress, yield failure of the concrete due to ettringite growing.

5. ACKNOWLEDGEMENTS
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6. REFERENCES