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DURABILITY OF CONCRETE: THE CROSSROAD BETWEEN CHEMISTRY AND MECHANICS

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ABSTRACT

The evaluation of the durability of concrete in severe environments is a real challenge for civil engineers. In order to simulate the behaviour and evolution of the cement paste with time, designers need sophisticated models coupling chemistry, physics, and mechanics. Chemistry and physics give the evolution of the material submitted to different attacks such as the alkali-aggregate reaction. Mechanics gives the behaviour of the material in terms of stress and strain. It is a complex problem because it exists on different scales in the material, i.e., the microstructural level for the diffusion of chemical species, the macrostructural level for cracks and damage. On the other hand, the heterogeneity of the material provides another problem and implies the use of probabilities. Based on some examples, different models and results are given to show the interest of such an approach. © *1997 Elsevier Science Ltd*

Introduction

Up to now, concrete has been studied mainly by two different communities. Chemists and physicists have considered the mechanisms of cement hydration, development of microstructure, evolution of matrices, and interfaces with aggregates under chemical attack. Mechanical researchers have modelled the behavior of concrete elements under service loads. However, the prediction of the service life of concrete structures under environmental loading implies the examination of the material and structure at local and global levels by experts of different fields.

The durability of concrete is a function of the nature and evolution of its basic components with the exposure conditions of the structure (1). A global approach had already been purposed (2,3). The last one is called holistic model (4), which implies a multiscale approach. An application to alkali-aggregate reaction (AAR) mechanical-induced effects is presented in this paper.

Modelling Alkali-Aggregate Reactions

Strain and stresses induced by AAR with resulting deflection cracking, spalling, erosion, and stainning (Fig. 1) are a real problem for civil engineers. Designers need mathematical models

FIG. 1.
Structure deteriorated by ASR (macroscopic level).

evaluating the residual mechanical capacity of deteriorated structures such as dams and bridges. In fact, the chemical reaction takes place at a microscopical level, i.e., local formation of an alkali silica gel (Fig. 2). Therefore, it is important to be able to go backward and foward from the microscopic level to the macroscopic level.

Microscopic Level

The mechanism of the alkali-silica reaction (ASR) was published by Dent-Glasser and Katoaka (5): diffusion of alkaline ions from the pore solution to the reactive solid sites, dissolution of silica, and formation of a gel able to swell. The global kinetics of chemical reactions has been evaluated through the amount of alkalis consumed in a function of time (6). The apparent diffusion of OH^- ions (7), silica dissolved in function of time (8). A probabilistic approach (9) considers a random distribution of reactive sites in the material and local gradients of ionic concentrations. The chemical reaction happens in an elementary volume called elementary representative chemical volume (ERCV). The alkalis available for

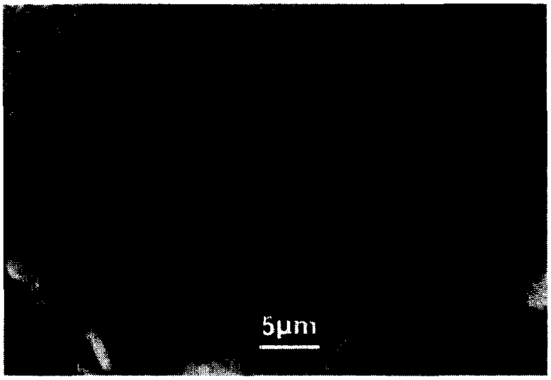


FIG. 2.
ASR product (microscopic level).

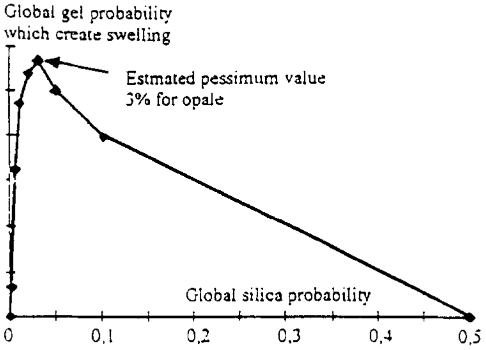


FIG. 3.
Global probability of efficient gel vs. global probability of reactive silica at a given time (9).

this reaction are localised in an equivalent volume (EV). Considering a uniform distribution of alkalis in a layer around the ERCV, it is possible to integrate Fick's diffusion law. As the medium is always alkaline, the probability of the presence of OH^- ions is taken equal to 1. The gel formation is effective if all elements (reactive silica and alkaline ions) are present in the ERCV, expressed as:

$$\Pr ob(I_{\text{gel}} = 1) = \Pr ob\{(I_{\text{Na}^+} = 1) \cap (I_{\text{sir}} = 1)\} \tag{1}$$

As soon as the gel is formed it is going to absorb water, swell, and flow in the connected porosity of the surrounding cement paste (5). The swelling of a concrete element is effective if the volume of gel is greater than the connected porosity, which corresponds to the global probability of efficient gel.

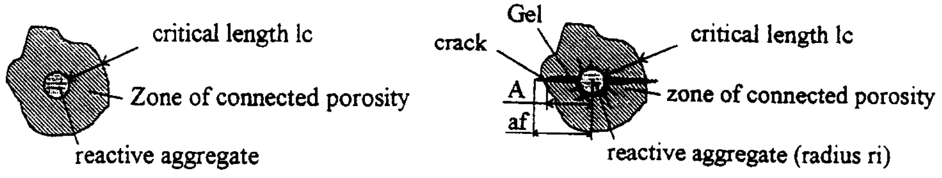
The curve of global probability of efficient gel vs. the global probability of reactive silica at a given time (Fig. 3) shows that there exists pessimal zones in which the efficient gel is maximal. A reactive aggregate therefore has lesser effects if it is present in great quantities in the concrete.

The gel is able to absorb in volume 200 to 400% water of its weight in a saturated atmosphere (10). It is thus possible to deduce the mass and volume of gel formed around a reactive aggregate. The gel can fill up the connected porosity. The capillary pressure of this gel considered as a fluid follows the Laplace's law:

$$Pc = \frac{2\sigma \cos \theta}{r_{\text{p}}} \tag{2}$$

If we note Pg the gel pressure and Eg the Young's modulus of the gel, it is possible to evaluate the probability for the gel pressure to be lower than a given capillary pressure, Pc. Assuming that the gel pressure is equal to the capillary pressure, the compatibility between the occupied volume, quantity of gel, and pressure is given by:

$$Pg = \frac{Eg}{3}\left[1 - \frac{Vvo}{Vgel}\,\phi\left(\frac{-\ln\left(\dfrac{2\sigma \cos \phi}{Pc}\right) - \overline{\ln rp}}{\overline{\overline{\ln rp}}}\right)\right] \tag{3}$$



(a) (b)

FIG. 4.
(*a*) Volume of concrete including connected voids to a reactive aggregate. (*b*) Partial filling in a crack and connected porosity by ASR gel.

Before cracking, the connected voids are those localized in a volume surrounding the reactive site and defined by a critical length, *lc* (Fig. 4). This critical length is equal to the maximal length reached by a fluid under infinite pressure. This length is a function of the connectivity of the porous network (11).

Cracks are assumed to propagate in mode I. Therefore, a local modelling of the crack can be realized using linear fracture mechanics. This hypothesis allows the calculation of the volume of the crack and crack opening, noted *H(r)* (12). The stress intensity factor takes into account the pressure in the gel, the confinement effect of a concrete piece, and the mechanical size effect of a concrete block. After Capra et al. (12), the confinement stress can be considered as anisotropic. It is possible to calculate the volume of gel filling the crack (Eq. 4) and the pressure in the ASR gel (Eq. 5) as follows:

$$Vgf = \frac{K_1(k+1)}{\mu\sqrt{2\pi}}\left[\frac{2}{3}af\left(r\max^{3/2} - r\min^{3/2}\right) - \frac{2}{5}\left(r\max^{5/2} - r\min^{5/2}\right)\right] \tag{4}$$

with $r\min = af - A$ and $r\max = af - ri$;

$$Pg = \frac{Eg}{3}\left[1 - \frac{Vvo}{Vgel}\left[\phi\left(\frac{-\ln\left(\frac{2\sigma\cos\phi}{Pc}\right) - \overline{\ln rp}}{\overline{\overline{\ln rp}}}\right) + \frac{Vgf}{Vvo}\right]\right] \tag{5}$$

The linear fracture mechanics calculate the crack propagation and swelling due to the opening of cracks induced by ASR.

This model has been applied to an experimental study done by Diamond et al. (6). Figure 5 compares swelling and alkalies used versus time as either experimental data or data obtained by numerical simulation. There is a good adequation between experimental values and numerical simulations. These results can also be interpreted in another way (Fig 6).

As already shown by Diamond et al. (6), Furusawa et al. (7), and Chatterji and Christensen (13), the simulations show an induction period. As an example, around 30% of alkalies produce a gel that is nonexpansive. Swelling and cracking are in fact due to the later consumption of alkalis, between 25 and 45%. The maximal quantity of available alkalies is around 55% of the total alkalis in concrete. This value is recommended in most of national codes.

After Hobbs (14), in some cases ASR expansion presents a pessimun content. The model

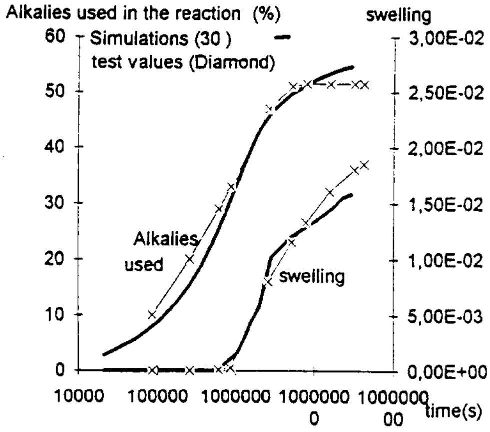


FIG. 5.
Simulated and experimental evolution of swelling and alkalis used vs. time.

proposed has been used to simulate this pessimun content. For that, swelling has been calculated for various reactive silica contents. The results are presented in Figure 7 which shows that if the reactive silica content is low, the swelling is proportionnal to the introduced silica content. In fact, each reactive aggregate receives enough alkalies to produce enough ASR gel to initiate and propagate cracks. If the reactive silica content is high, each reactive site can get a reduced quantity of alkalies. Some reactive sites cannot have enough alkalies to produce an efficient quantity of ASR gel, resulting in cracks and consequently swelling.

Macroscopic Level

The first model presented is complete but difficult to be used in industrial cases. It is thus necessary to propose a more global model that takes into account mechanical effects induced by ASR. From a phenomenological point of view, the principal parameters of chemical

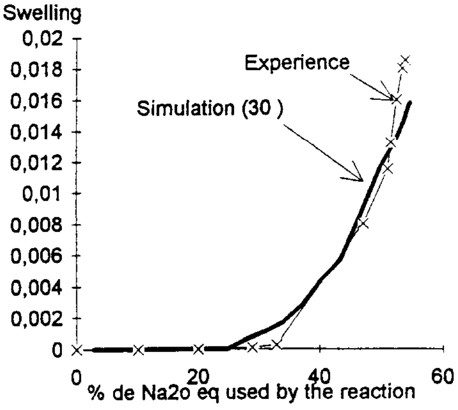


FIG. 6.
Experimental and simulated evolution of swelling vs. time.

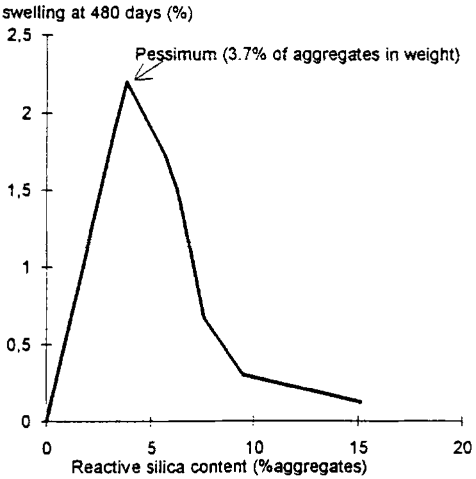


FIG. 7.
Pessimun content obtained by numerical simulations.

reactions are the potential of reactivity (A), temperature (T), and relative humidity (H). Furthermore, from a structural point of view, the function of the stress (σ) is far from being explained. Therefore, we can express the AAR free expansion by:

$$\varepsilon^{aar} = \varepsilon^{aar}(A, T, H, \sigma) \qquad (6)$$

This formulation leads to a homogeneous formulation and a probabilistic approach must be introduced. Using a random distribution of reactive sites, the first results obtained (15) have shown interesting achievements. Unfortunately, such an approach needs a large number of simulations, with different random distribution. In the case of site structure, this will be unrealistic due to the cost of calculation. Therefore, it is possible to have a new approach including probabilistic considerations but easier to use. Based on the experimental work by Diamond et al. (6), we supposed that the relation between expansion (ε^{aar}) and alkalies reacted (A) is bilinear. We can write:

$$\text{for } A < A_0 \quad \varepsilon^{aar} = 0 \qquad (7)$$

and

$$\text{for } A > A_0 \quad \varepsilon^{aar} = \frac{\varepsilon_0}{A_0}(A - A_0) \qquad (8)$$

where ε_0 and A_0 are defined in Figure 8.

A relation between A and time, representing the kinetics of chemical reaction, is then introduced. AAR is expected to follow a first order kinetic law described by:

$$\frac{dA}{dt} = k_0 e^{-\frac{Ea}{RT}}(1 - A) \qquad (9)$$

The moisture distribution, RH, in concrete is very important towards the reactions. Under approximatively 50%, there is enough water for the completion of reactions. Poole (16) has

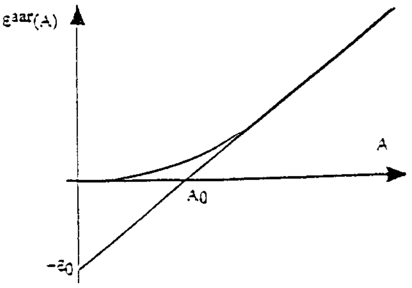


FIG. 8.
Determination of the parameters.

published a curve showing the evolution of the expansion versus the relative humidity (Fig. 9). This curve can be represented by a power function.

$$\frac{\varepsilon^{aar}}{\varepsilon_0} = H^m \qquad (10)$$

where H is the relative humidity and ε_0 the free expansion at $H = 100\%$.

Now, the most important point to be considered is the role of stress on the expansion. Shayan and Quick (17) have studied precast and prestressed concrete railway sleepers deteriorated by AAR. Although they were prestressed in the longitudinal direction, these structures were cracked parallel to the prestress. Therefore, we can see that an applied stress can reduce, by a structural effect, the expansion in this direction but not in the perpendicular one. Considering this, we tried to reproduce these observations using fracture mechanics. In order to model the expansion anisotropy, some hypotheses have been made. Cracks are considered to open only in mode I, and cracks interactions are not taken into account. The volume of gel created by AAR (Vg) is proportional to the free expansion. Therefore, this involves a state where structural expansions have started:

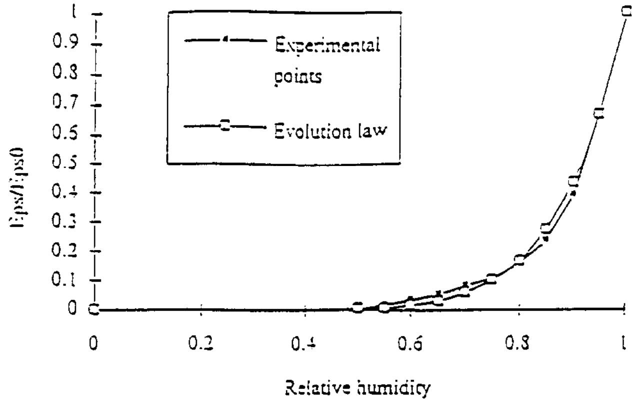


FIG. 9.
Evolution of expansion vs. relative humidity, comparison between experimental data and theoretical relation proposed.

$$g(t) = \alpha_1 \varepsilon_0^{aar}(t) \tag{11}$$

The local pressure (σ_{eq}) developed by the gel swelling is proportional to the volume of gel created: the greater the gel volume, the greater the pressure. According to the previous hypothesis, this leads to:

$$\sigma_{eq}(t) = \alpha_2 V g(t) = \beta \varepsilon_0^{aar}(t) \tag{12}$$

Therefore, we consider that the local pressure developed by ASR gel is proportional to the only global variable we can measure: the free expansion. Expansions will be created by crack openings, which is controlled by fracture mechanics. In a bidimensional case, the stress intensity factor (K_I) is a function of the two principal stresses and the pressure inside the crack. This leads to:

$$K_I = \sqrt{\pi a}\left(\beta \varepsilon_0^{aar}(t) + \sigma_1(t)\cos^2\theta + \sigma_2(t)\sin^2\theta\right) \tag{13}$$

The crack propagation, which is related to the bulk deformation and thus the expansion, is controlled by a fracture mechanics statement: cracks propagate if the stress intensity factor is greater than the critical stress intensity factor. Given that $f(\theta,t)$ is the fraction of cracks that propagate at time t and $\varepsilon^{aar}(\theta,t)$ is the strain at time t in the direction θ, it is assumed that:

$$B(\theta,t) = \frac{\left(\dfrac{K_{Ic}}{(\beta\varepsilon_0^{aar}(t) + \sigma_1(t)\cos^2\theta + \sigma_2(t)\sin^2\theta)}\right) - \bar{\alpha}}{\bar{\bar{\alpha}}} \tag{14}$$

The initial cracking can be characterized by an image analysis (12). Then the expression in the principal directions is expressed by a projection of the contribution of $\varepsilon^{aar}(\theta,t)$ for each θ in the principal axes. This leads to the following expressions:

$$\varepsilon_1^{aar} = \frac{\int_0^{\frac{\pi}{2}} \varepsilon^{aar}(\theta,t)\cdot\cos\theta\cdot d\theta}{\int_0^{\frac{\pi}{2}} \cdot\cos\theta\cdot d\theta} \tag{15}$$

and

$$\varepsilon_2^{aar} = \frac{\int_0^{\frac{\pi}{2}} \varepsilon^{aar}(\theta,t)\cdot\sin\theta\cdot d\theta}{\int_0^{\frac{\pi}{2}} \cdot\sin\theta\cdot d\theta} \tag{16}$$

This work has been done for a two-dimensional problem, but it can easily be extended to a three-dimensional one, considering an ellipsoidal inclusion for crack and projection on the three axes. The evolution of the two principal strains, ε_1 and ε_2, in a unixial compression σ_1, is presented on Figure 10. There is a great reduction of the strain in the direction of the load,

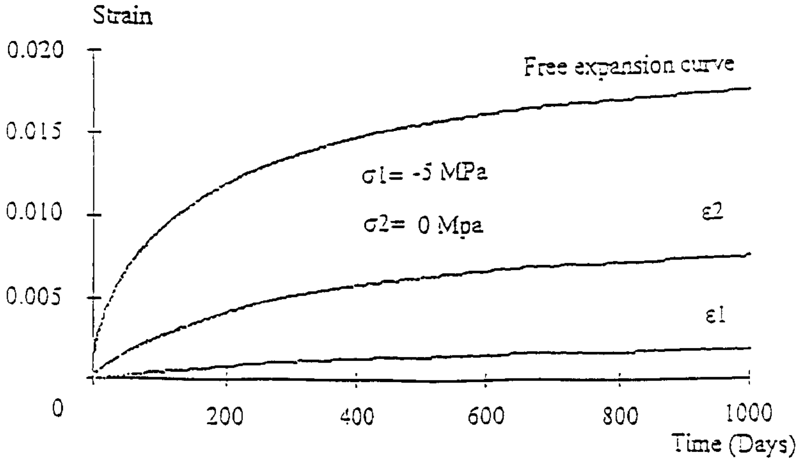


FIG. 10.
Evolution of the free expansion ε_1 and ε_2 in a uniaxial compression case vs. time.

but in the perpendicular one, the reduction is less important. This point is still open to discussion. New experimental results seem to show an important increasing of strains in perpendicular directions (18).

Conclusions

The ASR has been considered from two scales, microscopic and macroscopic levels. The first ASR model includes all basic phenomena. Chemical processes have been modelized based on Dent Glasser's approach. This chemical model has been integrated in a probabilistic framework. The mechanical induced effects are reproduced using the fracture mechanics. The first numerical results show that there is a good adequation between experimental results already published and computations. However these computations are heavy and costly.

The second model takes into account some phenomenological parameters of chemical reactions. Such an approach is able to be modelled thanks to simple and quick calculations of the anisotropy of the reaction. From a structural point of view, this anisotropy seems to be a very important parameter. However, simulations have to be validated by some experiment or in situ observations.

Nevertheless, modelling some hypotheses have been used in both in order to simplify the mathematical model. In a more global modelling, mechanical phenomena such as autogeneous shrinkage, creep, and relaxation must be linked to the chemical-induced effects. Although complex, it is necessary to set realistic simulations in the case of real structures. The role of the parameters of water molecules and calcium ions in the reaction processes must be determined more accurately by an important experimental work.

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