

MODELLING THE ALKALI-AGGREGATE REACTION WITHIN A PROBABILISTIC FRAMEWORK

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ABSTRACT

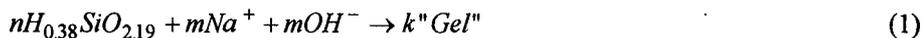
The main goals of this alkali-aggregate reaction study concern the comprehension of the elementary phenomena, calculation of the pessimal concentration in reactive components and the confinement effect in order to derive mechanical solutions aiming to slow down the reactions or their effects.

In this purpose, random gradients in alkalis concentration, ion substitution and gel growth are considered. The governing equations are expressed within the probabilistic framework in order to describe the initial concentrations in chemical components, position and granularity of the reactive sites as well as the porosity of concrete. The relationship between the volumic expansions (due to the gel pressure) and the physico-chemical phenomena (formation and growth of gels) is expressed through linear fracture mechanics concepts. Numerical calculations are run and compared to experimental results.

Keywords : Chemistry, Fracture mechanics, Numerical calculations, Probabilistic approach

INTRODUCTION

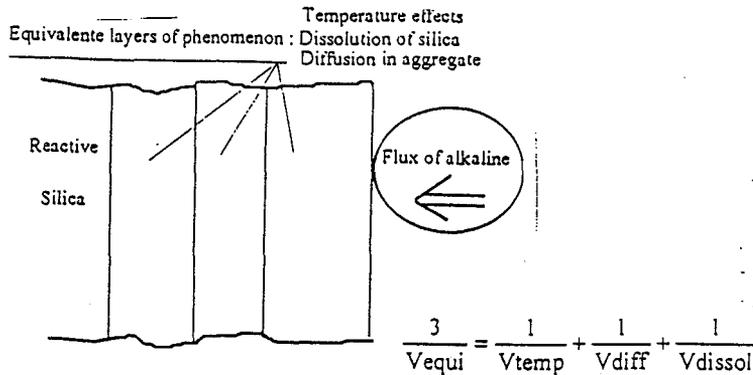
Reactional mechanisms of Alkali Silica Reaction have been studied by Dent Glasser (Dent Glasser & Kataoka 1981). The processus can be decomposed in two phases, the first one implies an attack of the silanol groups by hydroxyl ions and the second one an attack of the siloxane groups. This step leads to the destruction of the mineral structure and the creation of a silico-alkaline gel. This gel can absorb water, swells and creates pressure. This pressure can induce cracks in surrounding concrete. As proposed by Dent-Glasser and Kataoka (Dent-Glasser & Kataoka 1981), it is always possible to modelize this type of reaction as follows :



MODELLING OF CHEMICAL PHENOMENA

The kinetics of reaction depends on the rate of dissolution of the reactive silica, temperature and rate of alkaline ions diffusion in the solution. It is therefore necessary to define a pseudo-diffusivity equivalent at the periphery of a reactive aggregate (fig 1).

The volume and size of reactive silica particles are two important parameters used to describe the specific surface.



V_{equi} is the equivalent volume of reactive silica particle, and the others terms are equivalent layer of phenomenon linked to temperature, dissolution of silica and diffusion in the aggregate

Fig 1 : Definition of the equivalent pseudo-diffusivity

ASR involves the consumption of OH^- , Na^+ and K^+ at the level of reactive sites. These reactive sites are aggregates which contain more or less reactive silica, and consequently these reactive particles have a random distribution in the material. We assume that the quantity and granulometry of the reactive silica are known. The hydroxyle and alkali ions consumption induces local reduction of concentration, and so appearance of concentration gradients. Without boundary conditions, it is only these gradients which pilot alkaline flow in concrete. The classical Fick's law can be applied and gives :

$$\phi_M = -D \cdot \text{grad}(C)_M \quad (2)$$

where C (mol/m^3) is the ion concentration at point M , D (m^2/s) is the diffusivity and ϕ_M ($\text{mol}/\text{m}^2/\text{s}$) is the flow.

Nevertheless the distribution of ions due to the gradients of ionic concentration between a point and the rest of the matrix, the Fick's law has to be integrated. It is necessary to take into account the random character strongly marked of the geometrical position of reactive sites. The chemical reaction can happen in an elementary volume called ERCV, elementary representative chemical volume. The alkalis available for this reaction are localized in an equivalent volume EV (average volume of alkaline ressources by ERCV). By making the hypothesis of an uniform distribution in alkaline concentration on a constant radius around the ERCV, it is possible to integrate the Fick's law (Moranville-Regourd 1996).

As the medium is always alkaline, the probability of the presence of OH⁻ ions is taken equal to 1. The formation of gel is possible only if all elements (reactive silica, alkaline ions) are present in the ERCV, expressed as :

$$\text{Prob}(I_{gel} = 1) = \text{Prob}\{(I_{Na^+} = 1) \cap (I_{sr} = 1)\} \quad (3)$$

I_{sr} is the indicator of probability of presence of reactive silica

As soon as the gel is formed it is going to absorb water, to swell (Dent-Glasser and Kataoka 1981) and to flow in the connected porosity of the surrounding cement paste. The swelling of a concrete element will be possible only if the volume of gel is upper than the connected porosity. It corresponds to the global probability of efficient gel.

The curve of global probability of efficient gel versus the global probability of reactive silica at a given time (fig 2) shows that there exists pessimal zones (Burlion, Sellier, Bournazel 1995). in which the efficient gel is maximal. A reactive aggregate has therefore lesser effects if it is present in great quantities in the concrete.

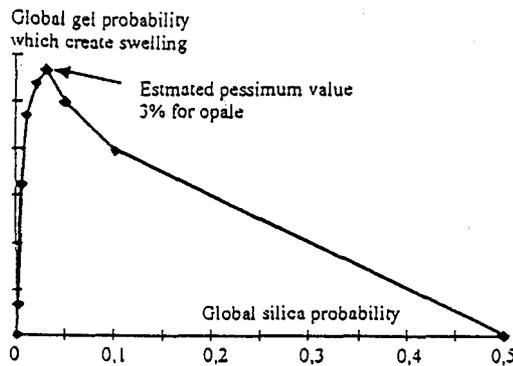


Fig 2 : Variation of quantity of efficient gel versus the percentage in reactive silica (Burlion et al 1995)

MODELLING OF EXPANSION INDUCED BY ASR

The observations under scanning electron microscopy show that the gel can filled up the connected porosity around the reactive aggregate (Moranville-Regourd 1989). Sometimes a pressure appears and it is able, in some cases, to create and propagate a crack. This results in an important degradation of concrete and a large swelling.

Estimation of the volume of gel created and induced pressure

In the previous paragraph we have calculated the probability of presence of gel conditioned by the presence of reactive silica. The gel created is able to absorb in volume 200 to 400% water of its weight in a saturated atmosphere (Davies and Oberholster 1988). With this it is possible to deduce the mass of gel formed around a

reactive aggregate, and with an approximation on its density, we can deduce the volume of gel created.

The gel can fill up the connected porosity, the capillary pressure of this gel considered as a fluid follows the Laplace's law :

$$P_c = \frac{2\sigma \cos \theta}{r_p} \quad (4)$$

P_c : capillary pressure, r_p : pore radius, $2\sigma \cos \theta$: capillary characteristic of the gel (superficial tension)

This relation is used for the well known Hg porosimetry, we use it here to calculate the pressure in the gel, the porosity distribution of the cement paste is supposed to be a lognormal curve.

If we note P_g the gel pressure, E_g 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 noted P_c . Assuming that the gel pressure is equal to the capillary pressure, the compatibility between the occupied volume, the quantity of gel and pressure is given by

$$P_g = \frac{E_g}{3} \left[1 - \frac{V_{vo}}{V_{gel}} \phi \left(\frac{-\ln(2\sigma \cos(\theta) / P_c) - \bar{\ln} r_p}{\ln r_p} \right) \right] \quad (5)$$

V_{vo} : pore volume connected to the reactive site, V_{gel} : gel volume at atmospheric pressure, ϕ : Gaussian distribution function, $\bar{\ln} r_p$ and $\ln r_p$ the average and standard deviation of the lognormal distribution of porosity

Definition of the volume of voids connected to the reactive site

Before cracking, the connected voids are those localized in volume surrounding the reactive site and defined by a critical length l_c (fig 3). This critical length is equal to the maximal length reached by a fluid under infinite pressure. l_c is a function of the connectivity of the porous network (Buil and Ollivier 1993)

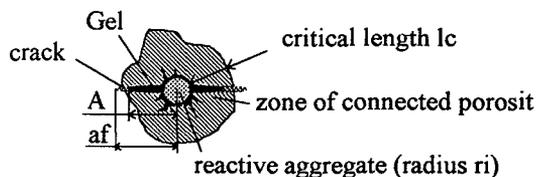
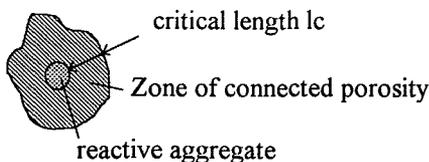


Fig 3 : Volume of concrete including connected voids to a reactive aggregate

Fig 4 : Partial filling in a crack and connected porosity by the ASR gel

One assumes that a crack propagates in mode I (Capra, Bournazel & Moranville - Regourd 1996) a local modelling of the crack can be realized using linear fracture mechanics (François, Pineau & Zaoui 1993). This hypothesis permit to calculate the widening and the volume of the crack and crack opening, noted $H(r)$ (Sellier, Bournazel, Mébarki 1995 and Moranville-Regourd 1996).

It is interesting to note that the stress intensity factor permits to take into account the pressure in the gel, the confinement effect of a concrete piece and the mechanical size effect of a concrete block. Capra et al (Capra, Bournazel, Moranville - Regourd 1996) also show that the confinement stress has not to be isotropic but it can be considered as anisotropic.

It is now possible to calculate the volume of gel filling the crack (6) the pressure in the ASR gel (7) as follows :

$$V_{gf} = \frac{K1(k+1)}{\mu\sqrt{2\pi}} \left[\frac{2}{3} af \cdot (r \max^{3/2} - r \min^{3/2}) - \frac{2}{5} (r \max^{5/2} - r \min^{5/2}) \right] \quad (6)$$

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

$$P_g = \frac{Eg}{3} \left[1 - \frac{V_{v0}}{V_{gel}} \left[\phi \left(\frac{-\ln(2 \cdot \sigma \cdot \cos(\theta) / Pg) - \bar{\ln} rp}{\bar{\ln} rp} \right) + \frac{V_{gf}}{V_{v0}} \right] \right] \quad (7)$$

Crack propagation criterion of ASR cracks

The classical criterion of crack propagation (François, Pineau & Zaoui 1993) is used. For a crack linear propagation in mode I, it is possible to calculate G (energy restitution rate (Capra, Bournazel, Moranville-Regourd 1996).

Estimation of induced swelling

Swelling are due to opening of cracks induced by ASR. The swelling can be directly identified to the volume created by widening of cracks as follows :

$$\varepsilon_{i(i=1,3)_g} = \frac{1}{3} tr(\varepsilon_g) \approx \frac{1}{3} \frac{vf}{ve} \quad (8)$$

with ε_g : unidirectional swelling, (ε_g) : isotropic strain tensor due to the gel, vf : the volume of the initiated crack and ve : elementary volume of concrete

APPLICATION

Simulation of Diamond's experience

This model has been applied to an experimental study made by Diamond, Barneyback and Struble (Diamond, Barneyback and Struble 1981). Figure 5 permits to compare experimental data, and swelling and alkalis used versus time, obtained by numerical simulation

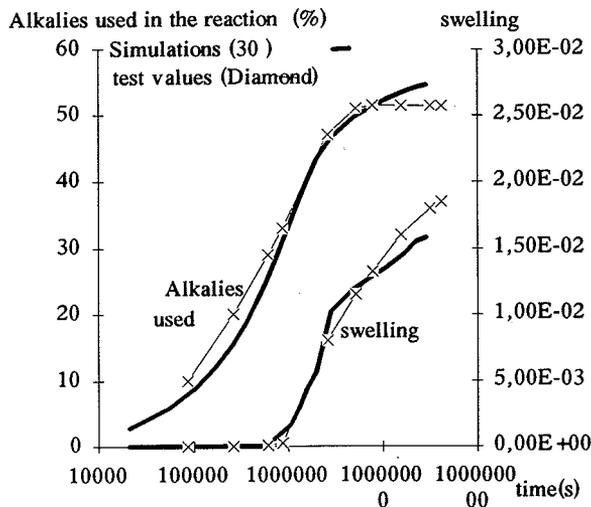


Fig 5 : Simulated and experimental evolution of swelling and alkalis used versus time

The results show a good adequation between experimental values and numerical simulations. It is possible to interpret this results in an other way (fig 6).

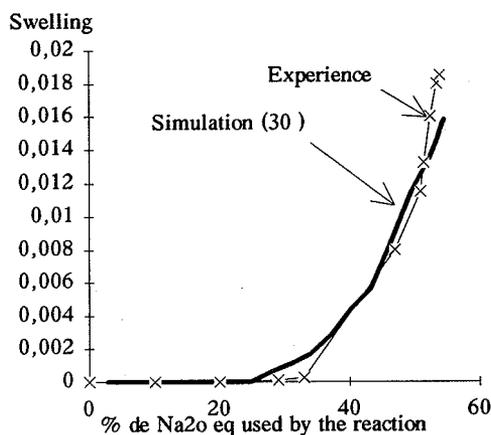


Fig 6 : Experimental and simulated evolution of swelling versus time

As already shown by Chatterji and Christensen 1990 and Diamond, Barneyback and Struble 1981, the simulations show an induction period. As an example, around 30% of alkalis produce a gel which is non efficient regarding the swelling. It is interesting to note that the maximal quantity of available alkalis is around 55%. This value is recommended in most of national codes (French recommendations 1990 and 1992)

Pessimun content

As shown by Hobbs (Hobbs 1988), in some cases ASR presents a pessimun content. The model proposed has been used to simulate this pessimun content. For that, swelling

has been calculated for various reactive silica contents. The results are presented on figure 7.

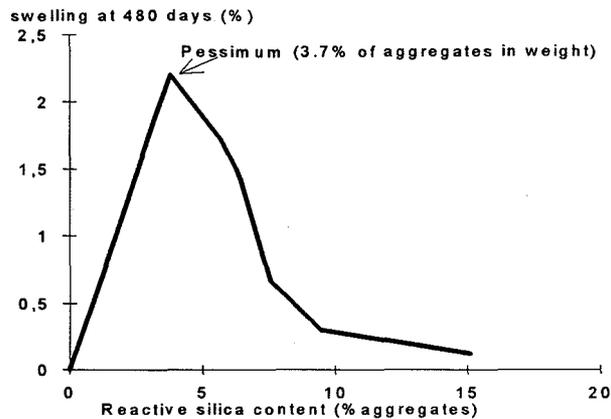


Fig 7 : Pessimum content obtained by numerical simulations

This figure shows that if the reactive silica content is low, the swelling is proportional to the introduced silica content. In fact, each reactive aggregate receive enough alkalis to produce enough ASR gel which initiates and propagates cracks. If the reactive silica content is high, each reactive site can have a reduced quantity of alkalis. In this case, some reactive sites can not have enough alkalis to produce an efficient quantity of ASR gel to create cracks and consequently swelling. The pessimum content appears as the result of a competition between swelling (proportional to reactive silica content) and the distribution of alkaline and reactive silica supplies in concrete.

CONCLUSIONS

This study have permitted to build a mathematical model of ASR induced effects. All basic phenomena, involving in ASR, have been modelised. In first chemical phenomena have been modelized based on Dent-Glasser's approach. This chemical model has been integrated in a probabilistic framework. The simulations obtained with the model proposed permit to obtain the local and global evolution of each chemical component involved in ASR. The mechanical induced effects are reproduced using the fracture mechanics theory.

The first numerical results show that there is a good adequation between experimental results published and computations. In this way, the pessimum content can be refounded easily.

References

Buil, M. and Ollivier, J.P. 1993 "Conception des Bétons : La Structure Poreuse" Chapitre III in *La durabilité des bétons*, presses de l'ENPC, 57 - 106

Burlion, N., Sellier, A. and Bournazel, J.P. 1995 "Pessimun Modeling of Alkali-Aggregate Reaction with Heterogeneities Description" ICASP 7, Lemaire, Favre & Mébarki eds, Balkema, 271 - 276

Capra, B., Bournazel, J.P., Moranville-Regourd, M. 1996 "A Mathematical Modelling to Describe the Effects of Alkali-Aggregate Reactions in Concrete Structure" 10th ICAARC, Melbourne, Australia

Chatterji, S., Christensen, P. 1990 "Studies of Alkali-Silica Reaction" Part 7, Modelling of Expansion" Cement and Concrete Research, Vol 20, n°2, 285-290

Davies, G., Oberholster, R.E. 1988 " Alkali-Silica Reaction Products and Their Development" Cement and Concrete Research, Vol 18, n°4, 621-635

Dent Glasser, L.S. & Kataoka, N. 1981 "The Chemistry of Alkali Aggregate Reaction" Proc. of 5th Int. Conf. on AAR, Cape Town, Paper S 252/23.

Diamond, S., Barneyback, R.S. and Struble, L.J 1981 "On the Physics and the Chemistry of Alkali-Silica Reaction". 5th ICAAR, Cape Town SA, S 252/22

François, D., Pineau, A. and Zaoui, A. 1993 "Comportement Mécanique des Matériaux : Viscoplasticité, Endommagement, Mécanique de la Rupture, Mécanique du Contact" Hermès ed, Paris

Hobbs, D.W. 1988 "Alkali Silica in Concrete" Thomas Tedford, London

Moranville - Regourd, M. 1989 "Product of Reaction and Petrographic Examination", 8th Int. Conf. on AAR, Kyoto, Japan, 445-456

Moranville - Regourd, M. 1996 "Modelling of Expansion Induced by ASR : New Approaches" 10th ICAARC, Melbourne, Australia

Sellier, A., Bournazel, J.P. and Mébarki, A. 1995 "Une Modélisation de la Réaction Alcali-Granulat Intégrant une Description des Phénomènes Aléatoires Locaux" Materials and Structures, RILEM, Vol 28, 373-383

"Les alcalis-réaction : Recommandations Mai 1990, FNB - FNTP - SNBATI" Annales de l'ITBTP, n°485, série matériaux 76, 42 pages. 1990.

"Granulats pour Bétons Hydrauliques : Guide pour L'Elaboration du Dossier Carrière" Recommandations provisoires pour la prévention des désordres dus à l'alcali-réaction, Note LCPC, Février 1992.