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Laurent Charpin, Alain Ehrlacher

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A computational linear elastic fracture mechanics-based model for alkali-silica reaction

L. Charpin*, A. Ehrlacher

Université Paris Est, UR Navier, École des Ponts ParisTech, 6-8 av Blaise Pascal, Cité Descartes, Champs-sur-Marne, 77455 Marne-la-Vallée Cedex 2, France

*Corresponding author: laurent.charpin@enpc.fr

Abstract This article presents a fracture mechanics model for Alkali-Silica Reaction. The model deals with the case of a concrete made up of dense aggregates submitted to chemical attack. The chemistry and diffusion (of ions and gel) are not modelled. The focus is put on the mechanical consequences of the progressive replacement of the outer layer of the aggregate by a less dense gel. A schematic cracking pattern is assumed: a ring-shaped crack appears in the cement paste surrounding the spherical aggregate depending on the pressure build-up. The onset of cracking is determined using an incremental energy criterion. The stored elastic energy and deformation of a given configuration are determined assuming that each aggregate behaves as if it was embedded in an infinite cement paste matrix. The calculations are performed by Finite Element Analysis. We note a very different behaviour of aggregates of different sizes. Adding the contributions of different aggregate sizes leads to an estimation of the global free expansion of a concrete of given aggregate size distribution. A rate of attack is identified that leads to recover the usual sigmoid ASR expansion curve.

1. Introduction

The alkali-silica reaction (ASR) has been discovered in the USA by Stanton (Stanton 1940). It can be very detrimental to the affected buildings. Three conditions are required: high water content, high alkali concentration and reactive aggregates. It is visible through superficial cracking and expansion. Resistance to traction is also affected. The ASR gels first fill the available porous space, and then tend to create microcracks which are thought to play an important role concerning expansion and its anisotropy under loading.

First, we explain briefly why we propose a new fracture model for ASR and its differences with existing ones. Then follow the description of the considered ele-

mentary volume and the computation of the energies used in the energy fracture criterion presented right after. The simple rule used to sum the contributions of different elementary volumes to macroscopic expansion comes next. Later, we explain which parameters influence the results of the model, focusing on aggregate size and the properties of the ASR gel. Finally, we discuss the potential of our model for reproducing experimental expansion curves.

2. Restrictions of the model proposed in this article

In this first attempt to understand the behaviour of an aggregate submitted to an attack, we only study a simplified mechanical problem related to ASR. Our goal is to understand the role of cracking of the cement paste in the swelling of concretes submitted to ASR. Therefore, we restrict our model to the simplest elements leading to the appearance of a crack in the cement paste under gel pressure. We want to understand how the size of aggregates influence cracking and hence, ASR expansion. The model follows many ideas of Bažant's mechanical model for ASR (Bažant et al. 2000). In this model a schematic 14 days attack is considered, corresponding to the accelerated expansion test ASTM C 1260. The decrease of the concrete's resistance and its expansions due to fracture of the cement paste between a periodical glass aggregate pattern are estimated thanks to Linear Elastic Fracture Mechanics. Let us explain the main differences here. First, in our model, no assumption is made about the periodicity of the aggregates in the cement paste. Instead, each aggregate is assumed to be embedded in infinite cement paste. Second, the basis for crack propagation is a Finite Element Analysis (FEA), instead of an interpolation between analytically known stress intensity factors. On this point, our approach is close to that of Xiao (Xiao et al. 1999) where the authors study, through FEA, the evolution of stress intensity factors for ring cracks surrounding inclusions when varying various parameters, except that we work directly on energies. We also compute the volume available to the gel by FEA which makes it simpler than what is done for example in (Bažant et al. 2000) where it is deduced from the cracked medium's compliance which is obtained by integration (with respect to the crack size) of the stress intensity factor. Then, our determination of average deformations far from the reaction sites is quite simple. Finally we make no assumptions about the compressibility of the ASR products relatively to the cement paste and we briefly discuss its importance (like in (Lemarchand et al. 2005)).

Our goal in this article is to build a reliable method to create and propagate cracks that we'll be able to use under external loadings to study the anisotropy of expansion, later on. We plan to use this methodology to finally be able to extract macroscopic information about the anisotropy of swelling and decrease of material properties that can be used in structure-size FEA.

3. Description of the behaviour of an elementary volume

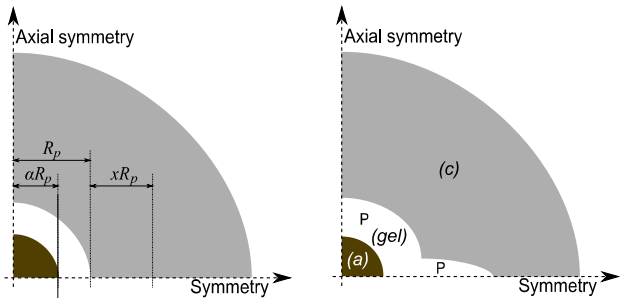

Fig. 1. Undeformed and deformed configurations. *(a)*: remaining aggregate. *(c)*: cement paste.

Our elementary volume is a single spherical aggregate of radius R_p surrounded by an infinite cement paste which is free at infinity (Fig. 1). Hence, the interaction between aggregates is neglected. The attack of the aggregate is represented by replacing the aggregate by a gel from the outside to the inside. The relative attack depth is called $\alpha \in [0;1]$, that is at a given time, an aggregate of radius $(1-\alpha)R_p$ remains. The aggregate is supposed to easily separate from the cement paste due to the mechanical weakness of the interface transition zone (ITZ) surrounding it. The aggregate and cement paste are considered linear isotropic elastic of properties (E_a, ν_a) and (E_c, ν_c). The gel bulk modulus is K_{gel}. Under zero pressure, the volume of gel replacing a given volume of aggregate is δ times bigger. Hence, the undeformed gel volume at a given attack degree writes $V_0(\alpha) = \frac{4}{3}\pi\delta R_p^3\left[1-(1-\alpha)^3\right]$. Let us stress that δ could be an effective value of the ratio of the gel volume to the aggregate volume accounting for physical phenomena such as the invasion of a part of the porous space by the gel (particularly the ITZ, of bigger porosity). It would then depend on the gel pressure and the aggregate size. To keep our model simple, we consider it as a constant.
We study the cracking of the cement paste under the increasing pressure created by gel accumulation around the aggregate. Quantities relative to the gel, the aggregates, and the cement paste, respectively have the indexes *gel*, *a*, and *c*.

4. Expression of gel pressure and elastic energies

The cracks we are considering are ring cracks developing in a symmetry plane of the spherical cavity (See Fig. 1). Therefore, we do not take the influence of

neighbouring aggregates on crack propagation into account. A crack around a cavity of radius R_p is characterized by its relative size x defined as the difference of the crack's outer and inner radii, divided by R_p.

The gel pressure first has to be computed. The compressed gel volume writes:

$$V(\alpha, x) = V_0(\alpha)\left(1 - P(\alpha, x)/K_{gel}\right) \tag{1}$$

where $P(\alpha, x)$ is the homogeneous gel pressure where as for $V(\alpha, x)$, we only keep explicit the dependence in the degree of attack α and the relative crack size x which are the two variables describing the evolution of our elementary volume. To find the gel pressure, this gel volume has to be compared to the volume left available by the deformation of the solid components. When a crack exists, no closed form solution is available. Hence, we resort to FEA to compute the variation of volume available to the gel, at given crack size, due to the deformation of the cement paste. Dimensional analysis leads us to write this quantity $\Delta V_c(\alpha, x) = \frac{4}{3}\pi\left(R_p^3 P(\alpha, x)/E_c\right)\Delta v(x)$ where $\Delta v(x)$ is dimensionless. Hence, the volume accessible to the gel writes:

$$V(\alpha, x) \approx \frac{4\pi}{3} R_p^3 \left[\left(1 + \frac{P(\alpha, x)}{E_c}\Delta v(x)\right) - (1-\alpha)^3\left(1 - 3P(\alpha, x)\frac{1-2\nu_a}{E_a}\right)\right] \tag{2}$$

Where in the term concerning the compression of the aggregate, the assumption $P(\alpha, x) \ll E_a$ has been used to keep the expression linear in the pressure. Thanks to this approximation, equating expressions (1) and (2) yields a linear expression of the pressure which can hence be easily written as:

$$P(\alpha, x) \approx \frac{(\delta - 1)\left[1 - (1-\alpha)^3\right]}{\dfrac{\delta\left[1-(1-\alpha)^3\right]}{K_{gel}} + \dfrac{\Delta v(x)}{E_c} + 3(1-\alpha)^3\dfrac{1-2\nu_a}{E_a}} \tag{3}$$

The elastic energies of all components are needed. For the aggregate and the gel, their expressions are in closed form. For the gel it writes:

$$E_{gel}^{el}(\alpha, x) = \frac{2\pi}{3}\delta R_p^3\left[1 - (1-\alpha)^3\right]\frac{P^2(\alpha, x)}{K_{gel}} \tag{4}$$

While concerning the aggregate:

$$E_a^{el}(\alpha, x) = 2\pi R_p^3 (1-\alpha)^3 \frac{1-2\nu_a}{E_a} P^2(\alpha, x) \tag{5}$$

Regarding the cement paste, dimensional analysis leads us to write it under the following form:

$$E_c^{el}(\alpha, x) = 2\pi R_p^3 \frac{P^2(\alpha, x)}{E_c} e(x) \tag{6}$$

Where $e(x)$ is dimensionless. Now let us stress the fact that the equality of the work done by the pressure in the variation of volume of the cavity and the stored elastic energy leads to:

$$\Delta v(x) = 3e(x) \tag{7}$$

Thanks to this, the determination of $e(x)$ by FEA (see Fig. 2 Left) gives us access to the stored elastic energies and the pressure (Eqs. (3-7)), for any Young's moduli of the cement paste and the aggregate and bulk modulus of the gel (but at fixed Poisson's ratios since e in fact also depends on ν_c).

The closed form solution for the uncracked situation gives us the uncracked value of the dimensionless energy: $e(0) = (1+\nu_c)/2$.

5. Thermodynamic study of crack initiation and propagation

We decided to create the cracks from scratch, avoiding the question of the initial crack size. When there is enough energy stored in the system to create a crack of given surface, it can happen. We consider this necessary condition as sufficient and therefore, we use the equality of released energy and dissipated energy as a crack initiation criterion.

The dissipated energy during crack growth is defined as:

$$E^{diss}(x) = G_c \pi R_p^2 \left[(1+x)^2 - 1\right] \tag{8}$$

Which is the product of the surface of the crack by a material parameter G_c (surface fracture energy). This energy is to be compared to the energy released during the creation of a crack of size x which we define as:

$$E^{rel}(\alpha, x) = E_{total}^{el}(\alpha, 0) - E_{total}^{el}(\alpha, x) \tag{9}$$

Where, taking advantage of equations (4), (5), and (6):

$$E_{total}^{el}(\alpha, x) = 2\pi R_p^3 \left[\frac{\delta\left[1-(1-\alpha)\right]^3}{3K_{gel}} + (1-\alpha)^3 \frac{1-2\nu_a}{E_a} + e(x) \right] P^2(\alpha, x) \tag{10}$$

Then, as can be seen on Fig. 2. Right, while the loading parameter α increases, the inequality $E^{rel}(\alpha, x) \geq E^{diss}(x)$ is more and more likely to be verified for a given relative crack size x . When this inequality is first verified, the two energies as functions of the relative crack size are also tangent.

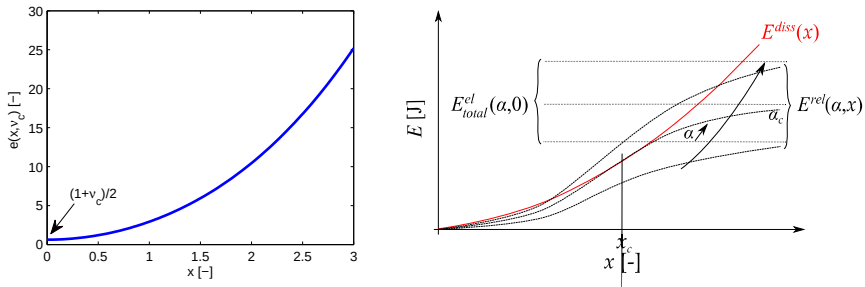

Fig. 2. Left: Dimensionless stored elastic energy, determined by FEA for different crack sizes x. Right: Schematic representation of the dissipated and released energies as functions of the relative crack size x while increasing the attack degree α

Therefore, for a given aggregate size and set of material constants, the initially uncracked system instantaneously jumps to a first crack of size x_c, created at the attack degree α_c which verifies:

$$\begin{cases} E^{rel}\left(\alpha_c\left(R_p\right), x_c\left(R_p\right)\right) = E^{diss}\left(x_c\left(R_p\right)\right) \\ \dfrac{\partial E^{rel}}{\partial x}\left(\alpha_c\left(R_p\right), x_c\left(R_p\right)\right) = \dfrac{dE^{diss}}{dx}\left(x_c\left(R_p\right)\right) \end{cases} \tag{11}$$

Then, the propagation of the crack follows the energy rate equation (Eq. 12) which gives the relative crack size corresponding to each attack degree $x\left(\alpha\right)$.

$$\frac{\partial E^{rel}}{\partial x}\left(\alpha, x\right) = \frac{dE^{diss}}{dx}\left(x\right) \tag{12}$$

Now, starting from the knowledge of the volume fraction of each aggregate size at the macroscopic level and that of the pressure and the crack size for each aggregate size at the microscopic level, we need to define a macroscopic deformation.

6. Macroscopic deformation

This part explains our method to compute macroscopic deformations starting from the crack volume obtained for each aggregate size from crack propagation under gel pressure as explained above. First we consider one aggregate in infinite cement paste and a domain Ω including the aggregate. Its current state is described by the couple $\left(x, P\left(\alpha, x\right)\right)$. Let us consider $\underline{\underline{U}} = \int_{\partial\Omega} \left(\underline{u} \otimes \underline{n}\right)^s dS$ where $\underline{u}$ is the displacement field, $\underline{n}$ the outward normal to Ω, and s is used to take the symmetric part of the tensor. Takana-Mori's theorem (Tanaka and Mori 1972) states that

if Ω is a sphere, $\underline{\underline{U}}$ does not depend on its size and position as long as it includes the cavity.

Suppose there is only one aggregate size R_p representing a volume fraction f throughout the concrete. Then the sphere Ω has to be chosen such that $f = \frac{4}{3}\pi R_p^3 \big/ |\Omega|$ to make sure that the volume fraction of the aggregate in the domain used to compute the average deformation due to the attack is equal to the volume fraction in the concrete considered. Finally we define the macroscopic deformation $\underline{\underline{E}} = |\Omega|^{-1} \underline{\underline{U}} = \left[f \big/ \left(\frac{4}{3}\pi R_p^3 \right) \right] \underline{\underline{U}}$.

We now need to take into account the aggregate size distribution. To each aggregate size $R_{p,i}$ corresponds a volume fraction f_i in the concrete. Each aggregate class contributes to the macroscopic deformation through a partial average deformation defined as $\underline{\underline{E}}_i = \left[f_i \big/ \left(\frac{4}{3}\pi R_{p,i}^3 \right) \right] \underline{\underline{U}}_i$ where $\underline{\underline{U}}_i$ is computed relatively to the aggregate of size $R_{p,i}$, a crack of size x_i, and a pressure $P_i = P\left(\alpha_i, x_i\right)$. The macroscopic deformation is then defined as $\underline{\underline{E}} = \sum_{\substack{aggregate \\ size\ i}} \underline{\underline{E}}_i$.

A corollary of Takana-Mori's theorem (Tanaka and Mori 1972) for which we will give our own proof in a later paper relates the volumetric part of $\underline{\underline{U}}_i$ to the dimensionless stored elastic energy in the cement paste surrounding the considered aggregate (defined in Eq. 6 and related to the volume variation of the cavity through Eq. 7, and computed by FEA) through the expression:

$$tr\underline{\underline{U}}_i = \frac{R_{p,i}^3 P(\alpha_i, x_i)}{E_c} \frac{4\pi}{3} \frac{1+\nu_c}{1-\nu_c} \left[1 - 2\nu_c + e(x_i) \right] \tag{14}$$

Eqs. 13 and 14 finally give us access to the macroscopic volumetric deformation:

$$tr\underline{\underline{E}} = \sum_{\substack{aggregate \\ size\ i}} f_i \frac{P(\alpha_i, x_i)}{E_c} \frac{1+\nu_c}{1-\nu_c} \left[1 - 2\nu_c + e(x_i) \right] \tag{15}$$

7. Numerical results: effect of aggregate size

In this section, we investigate the behaviour of our model when we vary some of its parameters. Setting the best known parameters to: $E_c = 20GPa$, $E_g = 60GPa$, $\nu_c = \nu_a = 0.25$, $G_c = 40J.m^{-2}$ following (Wittmann 2002)

and the less known parameters to $K_{gel} = 1GPa$ and $\delta = 1.03$, we study the effect of the aggregate size looking at 5 aggregate sizes ranging from $40\mu m$ to $6mm$. These values of the parameters K_{gel} and δ as well as the aggregate size distribution have been chosen to underline the different behaviour of different aggregates. Higher values of those parameters would lead all aggregates to crack the cement paste at low α. Lower values could lead to no cracking at all. We plot the relative crack size, the gel pressure (Fig. 3.), and the volumetric average deformation (Fig. 4.) as functions of the proportion of the aggregate already changed into gel $1-(1-\alpha)^3$. The results relative to the biggest aggregate size are the dashed curves. We can see that bigger aggregates crack their surrounding cement paste at a lower pressure level, producing initially shorter cracks, and that the bigger the aggregate, the bigger the expansion at full attack.

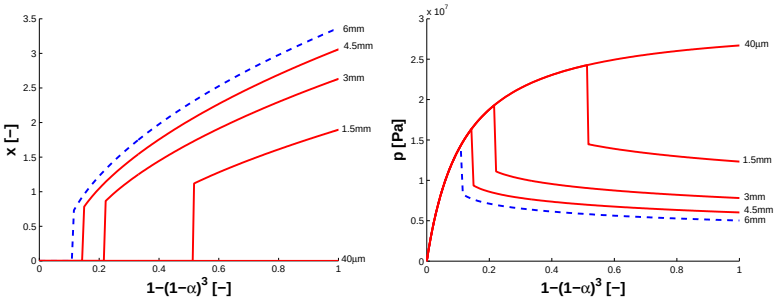

Fig. 3. Evolution of the relative crack size x and the gel pressure for different aggregate sizes.

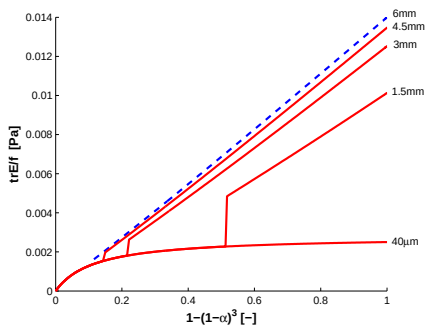

Fig. 4. Evolution of the average volumetric expansion.

Fig. 4. shows that once a crack has appeared around the aggregate, the expansion is roughly proportional to the amount of aggregate turned into gel, but it is not the case at all for uncracked aggregates.

8. Numerical results: fit to an experimental expansion curve

We must keep in mind that usual ASR expansion curves have a sigmoid shape characterized by a latency time, a characteristic time and an asymptotic expansion value. We can wonder if our model can be used to fit such an expansion curve, even if it would not mean that the model is predictive in any way. We use an expansion test found in Riche's PhD thesis (Riche 2003). In this test on $7*7*28cm$ prismatic samples, high alkalinity cement is used. The reactive aggregate is flint ranging from $5mm$ to $20mm$, for a total volume fraction of around 22.5%, while a volume fraction of 45% is occupied by a limestone non-reactive aggregate (notice that the reactive aggregates are quite big, so according to Fig. 3. they all crack early and the expansion is roughly linear with the attacked proportion of aggregate). We have two choices to explain the end of expansion: scarcity of aggregates, or scarcity of chemical products to attack the aggregates. Even if the formulation has a very high equivalent alkali content (around $5kg/m^3$), it is unlikely that it is sufficient to attack $500kg/m^3$ of reactive aggregates. Hence, we assume that here the expansion stops even if some aggregates are left. Following Bažant (Bažant et al. 2000), we assume that at a given time, the attack depth is the same for all aggregate sizes. We then identify a function $r(t)$ which links the attack depth to the physical time through $\alpha(R_p,t)=r(t)/R_p$. Thanks to this deformation of the time scale, we obtain a realistic but artificial expansion profile (Fig. 5.). The values used here are $K_{gel}=1GPa$ and $\delta=1.05$. These values were chosen to achieve a sufficient asymptotic deformation.

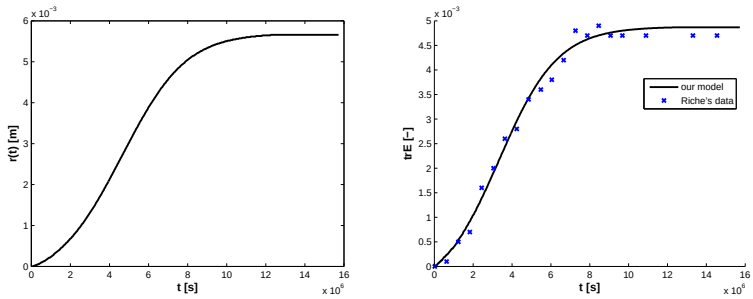

Fig. 5. Optimized volumetric expansion profile.

More physics is needed to explain the shape of this curve. To explain why expansion starts slowly, at least two options. The first is that diffusion of the chemical species attacking the aggregate take time. The second one is that the gel created in the beginning of the reaction does not contribute to cracking but fills the porosity

of concrete. These two points will be studied as next steps of our research, starting with a study of the rheological properties of synthetic gels.

9. Conclusion

A model for Alkali-reaction was proposed. It is a strictly mechanical model, partly inspired by that of Bažant (Bažant et al. 2000). Aggregates are supposed to behave as if they were embedded in an infinite cement paste. The chemical attack is modelled by progressively replacing each aggregate by a less dense gel. The subsequent pressure increase leads to cracking of the surrounding cement paste. The initiation and propagation of the crack are governed by energy balance only. An interesting behaviour is observed. Aggregates of different sizes have a different impact on the overall expansion. First of all, even fully attacked, smaller aggregates are shown not to lead to any cracking of the cement paste. The pressure reached for these aggregates is important, but according to our energy criterion the cement paste can take such pressures when there is no (or a very small) initial crack, because the elastic energy stored in the cement paste around a small aggregate is not sufficient to provide the energy needed to create a crack. Finally we apply the model to try to reproduce the expansion obtained in an experiment lead on a concrete specimen by Riche (Riche 2003) and manage to identify the attack rate, which is one of the inputs of our models, to reproduce the usual sigmoid expansion curve.

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