EXPERIMENTAL AND NUMERICAL STUDY OF ALKALI-SILICA REACTION UNDER MULTI-AXIAL LOAD

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Abstract

The ASR-induced expansion in structures is notably affected by the load applied on the material. The effect of load on the expansion and degradation mechanism is still an open question. On one hand this study aims at observing the effect of multi-axial load on the ASR-induced expansions, notably how it is transferred to less-constrained directions. On an other hand a numerical model is provided in order to get a better understanding of the underlying phenomena at the microstructure level. **Keywords**: effect of load, simulation, transfer of expansion

1 INTRODUCTION

The Alkali-Silica Reaction (ASR) is a deleterious reaction which causes expansion and internal damage to some concrete structures exposed to water. This phenomenon reduces the service life of the affected structures. It is therefore important to be able to predict the effects of the reaction and their evolution.

Since its discovery in the 1940 [1], ASR has been extensively studied. It is a complex phenomenon which is influenced by various parameters. First, the presence of amorphous phases in the aggregates and abundant moisture are needed for the reaction to occur. Then, the reaction rate is driven by the alkaline concentration of the cement pore solution and the temperature. The mechanical impact of ASR is controlled by the mix design, in particular the particle size distribution and the reactive aggregate size, and the load applied to the concrete.

The ASR is a chemical process which has mechanical consequences [2-5]. Both phenomena can be studied and modelled separately. The temperature, the alkaline concentrations, the concrete permeability and other physical parameters play a role in the chemical process, while the mechanical part is dominated by the complex microstructure of the concrete, and the formation of crack patterns, and the mechanical boundary conditions.

The expansion observed at the structural level is notably caused by the opening of cracks in the concrete. They form a network which can be observed as map cracking on the surface of the affected structures, but before map cracking can be observed, micro-cracks will have opened at the micro-structure level. These cracks tend to naturally orient themselves with the load applied to the concrete [2]. ASR displays a strong anisotropic behaviour [6], which could be explained by preferential orientations of the cracks.

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One way of differentiating reactive aggregates is slowly-reacting aggregates and fast-reacting aggregates [7]. The first type usually contains small pockets of reactive material in an unreactive matrix, so silica gel is produced and entrapped in the aggregates. The second type may react from the surface, leading to the gel forming "reaction rims". Most aggregates found in structures in the field are of the slow-reactive type (as these were harder to diagnose as reactive when the structures were build several decades ago). These different reaction types have different influences on the micromechanics of ASR, notably giving difference in the crack pattern they exhibit.

ASR studies often focus on the expansion as the sole manifestation of ASR, yet the service life of structures can be reduced by the redistribution of stresses in the structure, which impair the serviceability or lead to dangers of failure. From one concrete formulation to another, cracking can occur at different times, or for different values of expansion. This is why a study of the mechanical effects of ASR must track both expansion and damage.

Internal damage is usually difficult to measure, and mechanical testing does not provide information on its distribution in the microstructure. However, micromechanical modelling can provide insights on the crack and damage propagation. Such models require validation against experimental results.

The current study aims at expanding the current state of knowledge on the effect of multiaxial load. Several experiments have been conducted on the effect of uniaxial load [2, 5, 8]. These have shown that the expansion is reduced in the direction of the load, or even negated if the load is high enough. However, the expansion is transferred to the lateral directions in a non-linear way. The volumetric expansion is not a simple function of the load (see Figure 1). The underlying phenomena are still not well understood, and might reside in a modification of the microstructural impacts of ASR.

The transfer of expansion effect has also been highlighted by the multi-axial study of Multon [6]. Steel rings were used in this experiment to restrain the concrete in the radial direction. As the rings provide passive restraint only, the lateral load is driven by the ASR-imposed expansion, and the stiffness of the ring. The reaction was monitored by measuring the external displacements of the steel rings, and showed a strong anisotropic effect, suggesting another phenomenon in addition to elastic isotropic expansion. The main hypothesis of this study is that the transfer of expansion under load is related to an anisotropy of the damage in the microstructure.

This hypothesis can be confirmed or dismissed by the use of mechanical modelling. ASR models are usually based on chemically imposed expansion, equivalent to thermal deformation. Micromechanical models usually consider a single aggregate and its neighbourhood [3, 9], or use a poro-mechanical approach [10, 11]. Simulations of the full microstructure account for the interactions between the aggregates, and require extensive use of Finite Elements [5, 12, 13].

The current study aims at completing the set of multi-axial experiments. These experiments will be used to validate the Extended Finite Elements Methods (XFEM) framework AMIE, developed in [5, 13] to investigate the micromechanical consequences of ASR.

2 MATERIALS AND METHODS

A setup in which both the vertical and the radial loads can be controlled can be derived from the tri-axial cells used in soils and rocks mechanics. The evolution of the internal damage can be monitored both by simulation, and by use of SEM image analysis.

2.1 Experimental setup

Tri-axial cells consist in a sealed chamber in which a sample is subject to a fluid pressure. A vertical creep frame controls the vertical load, while the fluid pressure controls the radial load. Each cell can be operated with a unique pair of vertical and radial loads. Multiple cells can be used to test conditions going from uniaxial to isotropic loads.

Several samples can be stored in the cell. Having one non-reactive sample can provide the elastic and viscoelastic strains. Having two reactive samples is useful for the repetition of the results, or if one of the sensors were to fail. Unloaded samples can be cast and stored in the same conditions to monitor the free expansion.

The reactive aggregates come from the Swiss Alps, and are identified as slow-reacting aggregates, exhibiting small pockets of silica gel within their volume. They are the same aggregates as the ones used in [5]. The particle size distribution follows a Bolomey distribution, as prescribed in [14], with a maximum diameter of 16 mm. This maximum diameter is imposed by the length of the sensors (7 cm). The sample will be stored in sealed conditions, with an initial concentration alkali in the mix water of 250 mmol/L.

The reaction will be monitored by fibre-optic strain sensors cast directly in the concrete. The sensors will be placed in two orthogonal directions to provide the vertical and the radial strains. However, the connection of the fibre-optic wires from the cell is a technical challenge: the seal must hold for the full duration of the experiment, and the wires must be resistant to the aggressive conditions (high alkaline concentration, temperature, pressure).

2.2 Estimation of the internal damage

Expansion is not the only manifestation of ASR. The silica gel causes damage in the microstructure and this internal damage is a key point in the study of ASR under load. The crack propagation in each of the three spatial directions are not independent from one another, and may cause the strong non-linearity reported when expansion occurs under load. Therefore, the experiments should be designed to characterize the internal damage and the crack network.

Several methods to measure the internal damage exist, based on SEM image analysis [15, 16]. These are destructive methods as pieces of the sample must be extracted and polished to produce the SEM images. Therefore this method cannot be used on the samples that are stored in the cell. It can still be used on unloaded samples stored in the same conditions (temperature, alkali concentration, and sealing), and at the end of the experiment.

Even if the damage at the microstructure level cannot be measured, it is still possible to measure with the tri-axial cell the loss of elastic modulus. This can be done by increasing (or reducing) the load for a short period of time, and by measuring the strain response. The additional load should be low enough to stay in the elastic regime. The duration of the test should be short enough to a) ensure that the chemical reaction does not advance significantly and b) minimize any viscoelastic effect.

This mechanical test can provide the mechanical properties in the material in both the axial and the radial directions. This is important given the fact that anisotropy of the expansion may be related to an anisotropy in damage. However, the overall damage is dominated by the damage at the microstructure level, which cannot be directly observed for the practical reasons stated above. Numerical simulations can be used to estimate the internal damage, and confirm the relation between the degree of reaction and the expansion.

2.3 XFEM modelling

The XFEM framework AMIE was developed in [5] to study the mechanical effects of ASR. The use of FEM is dictated by the fact that the model should conform to the microstructure. It is reasonable to assume that at this level, cement paste can be modelled as a homogeneous material. XFEM is needed to represent the gel zones (either reaction rims or gel pockets) without meshing them explicitly: the gel forms in tiny zones compared to the size of the aggregates, and meshing them would be too expensive from a computational perspective.

Both the cement paste and the aggregates are modelled as a linear elastic fragile material. Their material properties can be measured, and are found in Table 1. In the simulations, the material properties for the paste and the aggregates follow a Weibull distribution to account for the material inhomogeneities.

The silica gel is modelled as a linear elastic material with imposed strain. The material properties of the gel are set to the values used by Dunant [5] to fit his experimental results (see Table 1). The gel is modelled as gel pockets as it corresponds to the experimental evidences for the aggregates used [17].

The entire aggregate particle size distribution (PSD) is modelled, but the simulations are done in 2 dimensions. The diameter of each aggregate is adjusted in order to convert the 3D distribution to a 2D distribution with an equivalent distance between the aggregates. This way, the neighbourhood properties of the microstructure and the interactions between the aggregates are preserved.

The rotational symmetry of the sample enables its representation by a vertical slice, the left side of it being the cylinder axis. The left side is blocked in the horizontal direction, while the bottom side is blocked in the vertical direction. The axial load is imposed on the top of the numerical sample, and the radial load on the right. A sketch of the microstructure, the sample geometry and the boundary conditions is portrayed in Figure 2.

This model gives the expansion and the damage as a function of the amount of gel produced, and not as a function of time. It means that a link is missing to compare the numerical results with the experiments.

3 DISCUSSION

The experiments and simulations are designed to provide information on both the internal damage and the expansion caused by ASR. The challenge comes from the interpretation of the expansion curves, and the correlation between the experiments and the simulations.

3.1 Image analysis

This correlation can be done using SEM image analysis. By using image segmentation [16, 17], Ben Haha identified a relation between what he designated as *reaction degree* and the measured expansion (see Figure 3). This relation was confirmed for other slow-reactive aggregates in [5]. This relation depends only on the aggregate content, and not on the aggregate reactivity, the temperature or the alkali concentration.

This relation supports the hypothesis that the mechanical consequences of the ASR are directly derived from the amount of gel formed, regardless of the rate of the chemical reaction.

In our case, we presume that different samples stored in the same chemical conditions, but at different loads, have the same rate of the chemical reaction. With this assumption we can measure the advancement of the reaction in only one system. The simplest way to do so is to store unloaded samples in the same chemical conditions as the loaded samples, and to measure the reaction degree in those

samples. The image analysis technique being a destructive method, we cannot afford to stop an experiment under load to measure its reaction degree.

This method has still some disadvantages. First, the segmentation algorithm does not distinguish between gel pockets and cracks. Therefore it gives the *degree of damage* instead of the *degree of reaction*. Second, the sample preparation (most notably the sawing and the polishing) can damage sometimes the aggregates, which leads to an overestimation of the degree of damage. As the reaction advances, this error becomes larger because the aggregates are more damaged by the ASR, then more sensitive to the sample preparation.

The additional degree of damage measured can easily be detected: it forms large black zones within the aggregates. These zones come from the fact that a fragment of aggregate was weakened by a surrounding crack, and removed during the sawing. A first approach consists in removing these zones.

However, the boundaries of these zones are likely to be cracks that should be included in the analysis. A more realistic approach consists of counting in the degree of reaction a layer of n pixels on the boundaries of these zones, where n is the average crack width found in the same aggregate (see Figure 4).

By using these correction methods, we can get the following values : lower limit of the degree of damage (without the additional damage), approximated limit of the degree of damage (with the boundaries of the additional damage), and finally upper limit of the additional damage (with the additional damage). Further, the data can be post-processed to obtain an estimation of the production of gel: it can be assumed that once the thin cracks are removed, the remainder is reacted aggregate.

This way, we can plot the expansion and the loss of elastic modulus (measured by mechanical testing) as a function of the damage in the aggregates, and therefore compare the results with the numerical simulations.

3.2 Interpretation of the mechanical results

From a mechanical perspective, the main point of comparison between the experiments and the simulations is the average strains in the axial and radial directions. In order to exploit the results of this study in civil engineering structural codes, we need more information, like the expansive force applied to the concrete, or the loss in the internal energy. The goal is to provide a relation similar to Equation 1, in which both the internal damage + and the expansive force + depend on the stress state + and the advancement of the reaction. In Equation 1, + is the fourth-order identity tensor, and + the concrete stiffness tensor.

 $\sigma = \begin{bmatrix} I - D \end{bmatrix} C \varepsilon + \beta \quad (1)$

Note that the concept of expansive force is mathematically equivalent to a concept of an imposed deformation (similar to thermal expansion, for example), in which $\alpha = -[[I-D]C]^{-1}\beta$

Analysis of the overall damage

In order to identify the damage, it is enough to apply two different stresses 4 and 4 to the same microstructure (either real or simulated). If the difference between the two applied stresses is small enough not to damage any further the microstructure, then the damage can be calculated from the stress difference, see Equation 2.

$$\sigma_2 - \sigma_1 = [I - D]C[\varepsilon_2 - \varepsilon_1] \tag{2}$$

If we suppose that the damage is a diagonal tensor, then Equation 2 consists in a set of 3 equations (in 2 dimensions) with 3 unknown, which is then trivial to solve. Note that the simulation of the mechanical test can give proof that the test does not increase the damage.

Analysis of the expansive force

Once the overall damage is found, it is easy to use Equation 1 to find the expansive force which is the sole remaining unknown. From a numerical perspective, another way of calculating it is by imposing e^{-0} on the boundaries and by preventing the elements to damage themselves any further.

Numerical analysis

The imposed expansion and the overall damage are determined by the microstructure and the damage at the microstructure level. That's why Finite Elements methods at the microstructure need to be used to study the relation between the applied load, the expansive force and the damage.

AMIE has been validated on various free expansion experiments [5]. It can notably identify the difference in the damage caused by the slow- and the fast-reactive aggregates (see Figure 5). On the one hand the cracks in slow-reactive aggregates are first contained in the aggregates, and only propagate into the cement paste after a certain advancement of the reaction. On the other hand the cracks in the fast-reactive aggregates first develop in the paste around the aggregates, which are suddenly split in half after a certain advancement of the reaction.

However AMIE simulations have not yet been validated for ASR under load. One reason could be that the 2D simulations done so far cannot represent the three dimensional crack network produced by ASR under load, the 2D cracks connecting too quickly compared to the experiments. Another reason might be that the viscoelastic behaviour of the cement paste is not accounted for, as the visco-elasticity interacts with the damage propagation in concrete (see [18] for an ASR model including both damage and visco-elasticity). These two points are currently under development in the framework AMIE.

4 CONCLUSIONS

A multi-axial experiment is set to investigate the effect of applied load on ASR. The reaction is studied both from an expansion and from a damage perspective. As the link between the load, the expansion and the damage lies in the microstructure, numerical simulations are required. Validation of an XFEM tool at the microstructure level is required before upscaling the model to the structure level.

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Material	Aggregates	Cement paste	Silica gel
Young's modulus [GPa]	59	12	22
Poisson ratio [-]	0.3	0.3	0.28
Maximum tensile stress [MPa]	5.7	2.9	-
Maximum compressive stress [MPa]	45.6	23.2	-
Expansion coefficient [-]	-	-	0.5

Table 1: Mechanical properties of the materials for the XFEM simulations.



Figure 1 : volumetric expansion for 0, 5, 10 and 15 MPa vertical compressive loads. Figure from Dunant [5].



Figure 2: sketch of the simulated microstructure, with gel pockets embedded in aggregates, themselves embedded in cement paste. The vertical load and the lateral loads can be set independentely.



Figure 3: expansion as a function of the degree of reaction measured by image analysis. Figure from Ben Haha [16].



Figure 4: Top left: additional damage caused by rough sawing. Top right: original segmentation using the image analysis from [5, 16]. Bottom left: segmentation with removal of the sawing defects. Bottom right: segmentation with selection of the cracks around the sawing defects.



Figure 5: different crack pattern caused by gel pockets (left) and reaction rims (right).