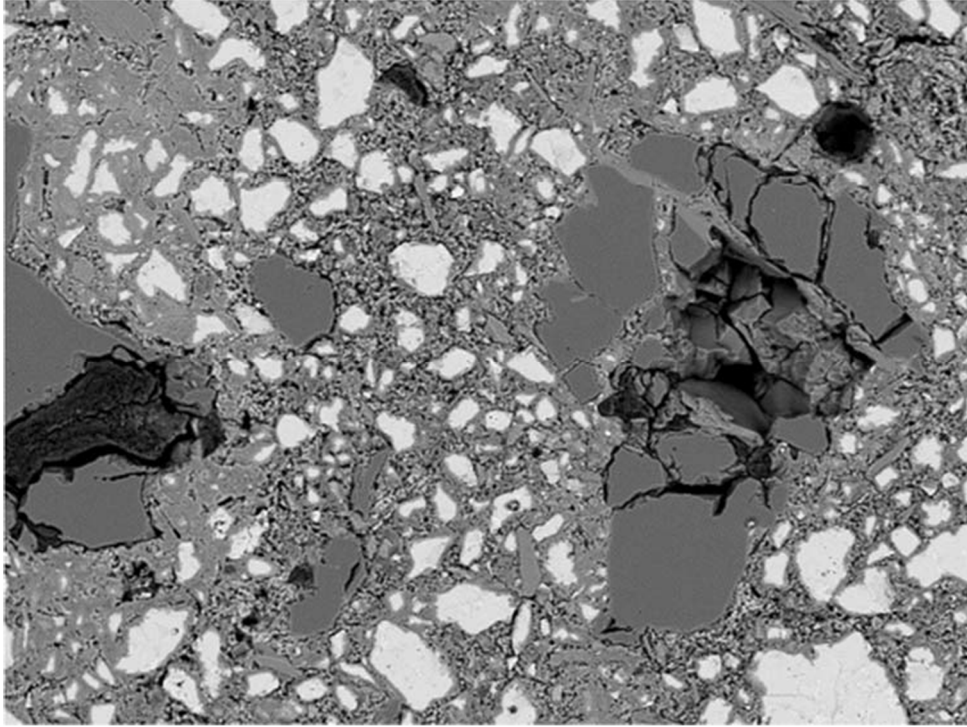




Study of ASR at LMC



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1 Overall strategy and experimental work

1.1 Background

When the research started at LMC, the phenomenological understanding of the ASR was built upon the experiments by notably Larive. These experiments strongly suggested that the expansion had an initiation period, an acceleration, and eventually the expansion reached a plateau upon the exhaustion of the reactive materials. The preferred form to represent this development was a symmetric 'S' curve, where the time to the maximum rate of expansion is the same as the time required for the reaction to finish.

The standard experimental assessment of the reactivity was a multi-stage screening. The first stage, designed to be extremely aggressive, was the MICROBAR test, where 1x1x4 micro-mortar samples are cured for 24h at 127 °C and 1.3 bar in 1.6M sodium hydroxide solutions. An aggregate that tests negative in this test is then assumed innocuous. A second set of tests, inspired by the ASTM are the accelerated mortar bar tests, at 1M and 80°C for 28 days. Finally, the test that is assumed closest to field performance is the concrete prism test at 38°C at 100% relative humidity for 1 year. These tests of decreasing severity and increasing representativeness were at the time thought to mostly produce false positives, and thus to be safe.

1.2 Hypothesis of Ben Haha thesis

Based on this background, the aim of the thesis of Ben Haha was to quantify the evolution of the reaction at a microstructural level and to link this to the macroscopic expansion. The hypothesis was that if a quantitative relationship could be established between the degree of reaction measured microscopically and the state of expansion relative to the 'S' curve: microscopic examinations could determine the state of the reaction in a samples from the field and indicate how the macroscopic expansion would progress and when it would stop. However, it was later found that the 'S' curve is mainly an artefact of laboratory testing. For the relative small size of specimens, the alkalis quickly leach out and then the expansion stops. This point will be returned to later.

Samples were made with three aggregates thought to be reactive, stored at 3 temperatures and with three levels of alkali addition. A protocol was developed to quantify the degree of reaction as the area of cracks and voids in aggregates, relative to the total area of aggregates. (Note: for representative flat sections the measured area fraction is direct an unbiased estimate of the volume fraction).

This protocol is described in the paper:

Ben Haha, M., Gallucci, E., Guidoum, A, Scrivener, K.L.

Relation of expansion due to alkali silica reaction to the degree of reaction measured by SEM image analysis. Cement and Concrete Research, 37 (8): 1206-1214, 2007

And illustrated in Figure 1. In order to obtain representative measurement many images must be measured for each specimen, but the process of image acquisition can be automated. In the figure, the aggregates have a fairly homogeneous mineralogy and so grey level, this is not always the case. Subsequently the image analysis protocol was improved as described below. It is now used routinely in LMC.

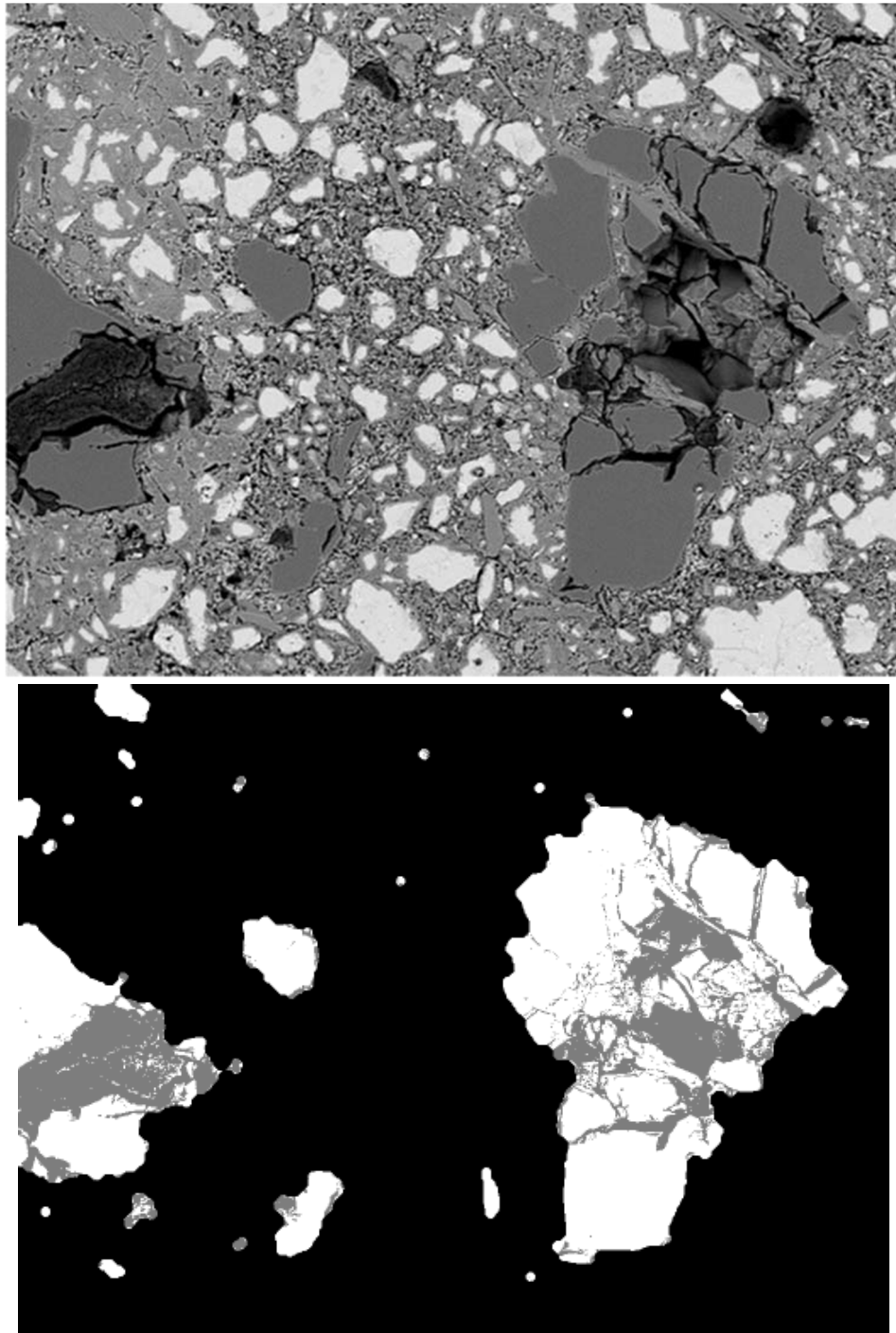


Figure 1. Image analysis determination of degree of reaction. On the polished section of the concrete first the areas of aggregates are identified (white) then the areas of cracks and void within these measured (grey)

1.3 Relation between microscopic degree of reaction and expansion

The key finding of the Ben Haha thesis was the existence of a unique relation between the microscopic degree of reaction measured by image analysis and the macroscopic expansion, shown in Figure 2. This was the first time the microscopic aspects of the reaction had been quantitatively



linked to the expansion. It also suggested that the link between this reaction and the expansion was mechanical, as indicated by the role of the PSD in the differing expansion between mortars and concretes.

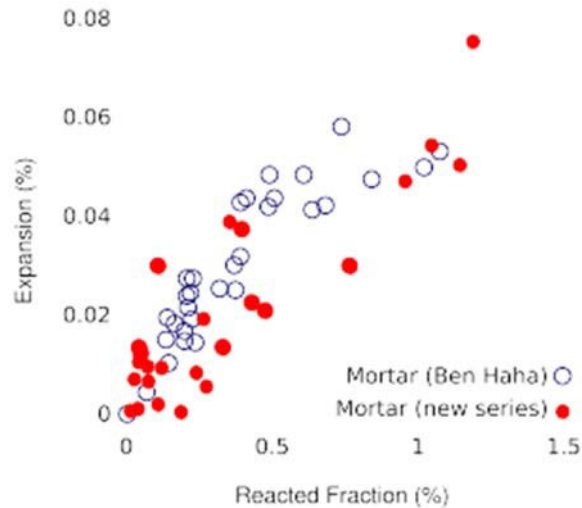


Figure 2. Relation between the microscopic degree of reaction measured by image analysis and the macroscopic expansion from the theses of Ben Haha and Dunant.

1.4 Other important results of Ben Haha thesis

The other important results of the Ben Haha thesis were:

- Effect of temperature: Follows an Arrhenius (exponential) relationship, with an activation energy of about 40 kJ/mol (similar to values reported in the literature). This is illustrated in Figure 3. For example, an expansion of 1 mm/m (0.1%) takes around 1.5 years at 38°C, but 27 years at 10°C.

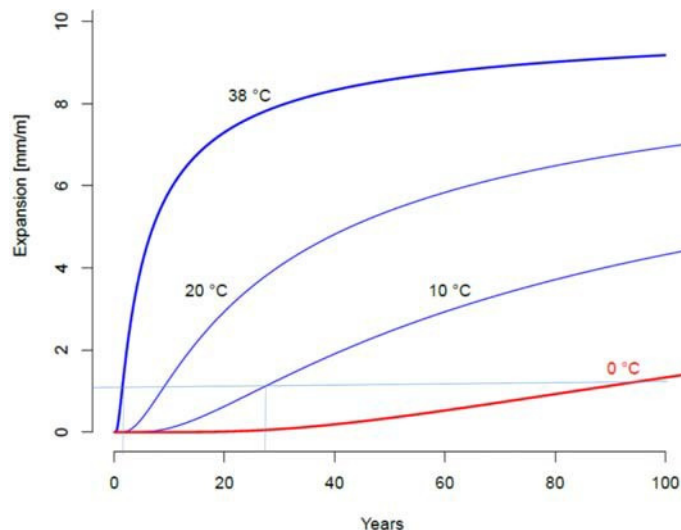


Figure 3. Expansion curve at 38°C transformed with activation energy of 40 kJ/mol to 20°C and 10°C.

- Relation between expansion and mechanical properties: Tensile strength degrades more than compressive strength. Again similar to results in the literature.



1.5 Dunant Thesis

The aim of the thesis of Cyrille Dunant was to build on the key finding of the Ben Haha thesis. To elucidate mechanisms linking microscopic reaction / damage and macroscopic expansion by the development of a numerical model. The model, which was further developed in the thesis of Giorla is described in Part II of this document.

Experimental studies were made, with the aim of being able to go from small specimens tested in the laboratory to real concretes in field structures:

- The effect of uniaxial loading on expansion, (discussed together with the triaxial test made by Giorla).
- The effect of aggregate size and distribution on expansion.

Furthermore improved protocols for curing specimens to avoid leaching and for measuring the degree of reaction by image analysis protocol were developed

1.5.1 Updated curing protocol

It is very difficult to control the relative humidity close to 100%, for this reason there considerable scatter in the results of Larive. For this reason in the thesis of Ben Haha the samples were immersed in water. However if the samples are immersed in tap water, as in the thesis of Ben Haha, leaching of alkalis occurs

To control for leaching sodium hydroxide was added to the cure water at concentrations close to that of pore solution. As the alkalinity of the surrounding solution is the same as the internal pore solutions, leaching is minimised. Subsequently, the protocol has been refined to measure the pore solution of samples at 28 days and to formulate the immersing solution to match this. The impact of the immersion solution is illustrated below, from a later study at LMC. This highlights the fact that, when leaching is avoided, the reaction does not stop, but is still continuing after 2 years.

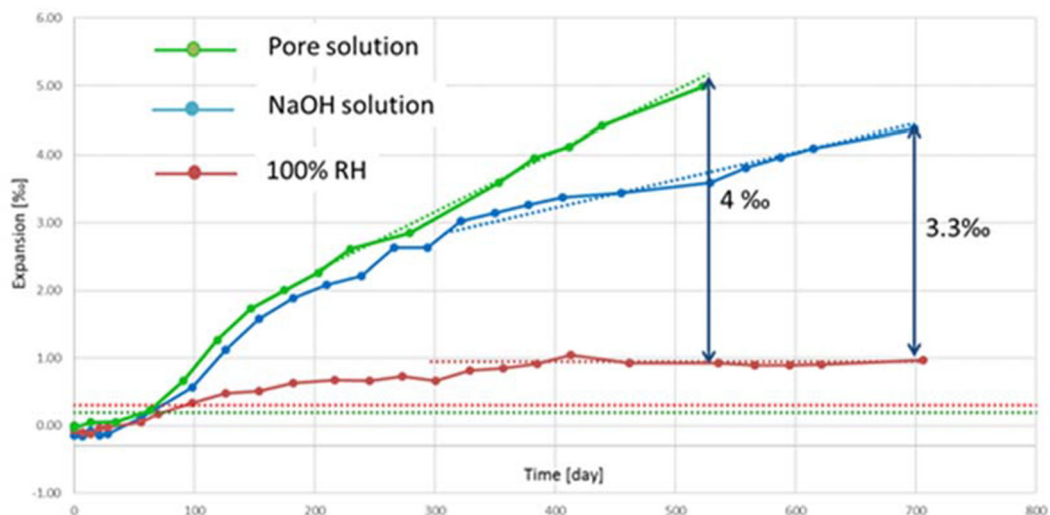


Figure 4. Expansion of samples in different storage solutions. This study was done at 60°C to further accelerate the reaction. Studies in the work of Dunant and Giorla were done at 38°C

If samples are put immediately at the high temperature of 38°C used to accelerate the reaction, this will affect the hydration of the concrete. To avoid these effects the protocol also required that specimens are stored for 28 days in a fog room before their cure in sodium hydroxide solution was started.



1.5.2 Updated image analysis protocol

The image analysis algorithm was improved so it could reliably assess aggregates with very different morphologies when observed under BSE. The new algorithm, devised by Dunant, is now used routinely for ASR expertise at LMC. However, the protocol for the preparation of the sections was improved to be able to correctly measure the damage in highly damaged samples.

In the initial protocol, used by Ben Haha and Dunant, the samples were cut, put under vacuum until they reached 0.1 mbar, and then coated with epoxy. The samples were subsequently polished. However, this method produces artefacts when the aggregates are heavily damaged.

The current protocol uses a double impregnation: the first under high pressure, and the second under vacuum, as before. The first impregnation helps stabilise the samples and avoids “pop-outs” which increase artificially the damage measure.

The detailed protocols for expansion and image analysis are given in the appendix.

1.6 Giorla Thesis

The main objective of the Giorla thesis was to develop triaxial cells, which could apply loading conditions more representative of those found in the field. In addition, creep was introduced into the numerical model as described in part 2

1.6.1 Expansion under load

To reproduce the expansion under conditions more representative of those found in dams, expansion measurements were performed in load cells. During Dunant’s thesis the load was applied uniaxially. Giorla developed triaxial cells where the samples could be stored in alkaline solutions under triaxial load.

Uni-axial cells

The numerical model of ASR as well as the microscopic observations strongly suggested that the degradation was due to the formation of small cracks in the microstructure. This implies that the degradation of mechanical properties, strength and stiffness can be highly anisotropic.

More importantly, it indicates that models which calculate a redistribution of the expansion or degradation as though it were a conserved quantity (like the volume of water balloon being pushed in one direction) are necessarily wrong for the purpose of extrapolation. They can be calibrated, of course, but they have little predictive value.

To formulate an engineering model, however, a more detailed understanding of the interactions between damage, load and creep is necessary. Therefore, a first experimental campaign was done during Dunant’s thesis. In this campaign, the expansion of samples under uni-axial load was recorded by embedded sensors, Figure 5.

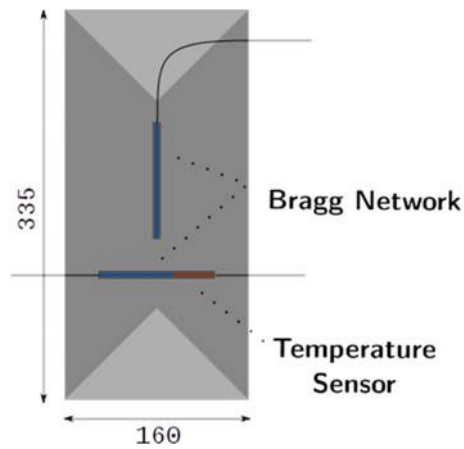


Figure 5. Diagram of the layout of the embedded sensors.

The samples were prepared according to the protocol outlined above, and cured in sodium hydroxide solutions in room maintained at 38°C. The samples were loaded longitudinally at 0, 5, 10 and 15 MPa.



Figure 6. Set up for tests under uniaxial compression. The Perspex jackets allow the samples to be maintained immersed in sodium hydroxide solution to avoid leaching

The results, confirmed previous reports of the expansion being suppressed in the direction of the load. A load of approximately 10 MPa suffices to eliminate almost all longitudinal expansion.

More interestingly, the results indicated a strong non-linear, non-monotonic relationship between the expansion and the load. This relationship confirmed earlier results from other laboratories, notably in France which had been interpreted differently

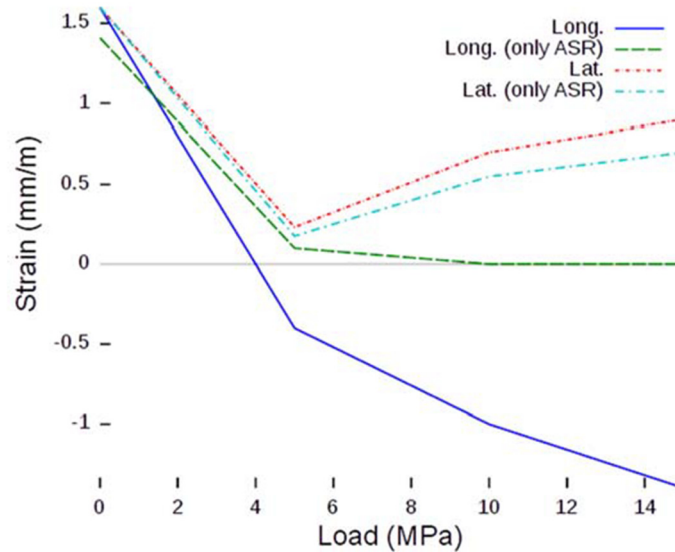


Figure 7. Effect of loading on longitudinal expansion

In the light of the micro-structural damage explanation of the ASR, the strongly non-linear relationship is explained by the competition of confinement under load and orientation of micro-cracks.

Tri-axial cells

Following the first campaign, it was decided to test the expansion under more realistic loading conditions. In a dam, the stress state is tri-axial, with the restraints from the wall, the water pressure and the gravity. There is almost no experimental data in the literature for samples undergoing ASR in triaxial stress states.

During' Giorla's thesis, triaxial cells, modelled after smaller soil mechanics ones were developed. The aim was to have the following characteristic properties:

- be capable of applying anisotropic loads;
- be of a dimension such that standard concrete cylinders could be tested;
- allow embedded sensors to give continuous measurements;
- allow a cure in simulated pore solutions.

These characteristics posed significant challenges, as the simulated pore solution is a very aggressive environment which had already caused the early failure of some embedded sensors during the Dunant thesis. Nonetheless, a design (Figure 8) was developed which satisfied all criteria.

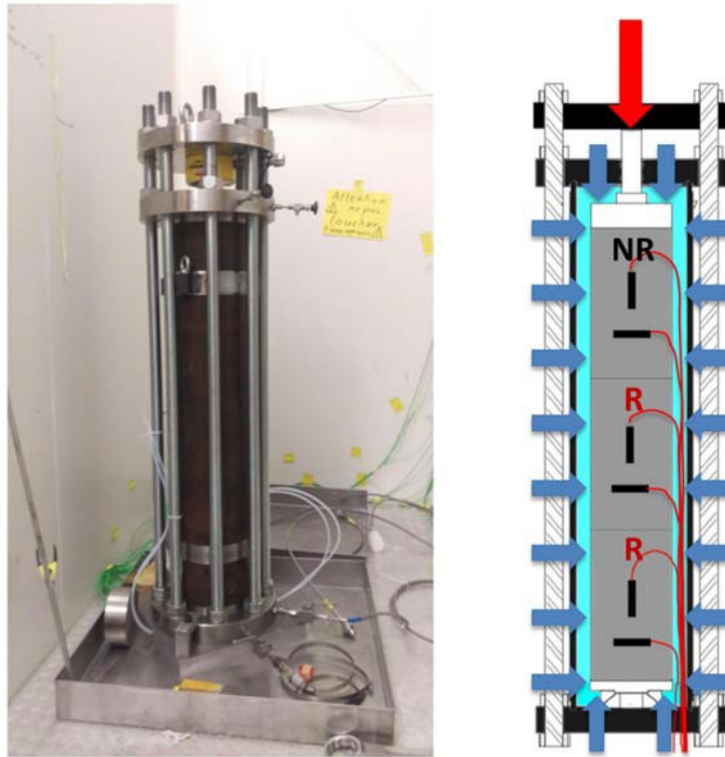
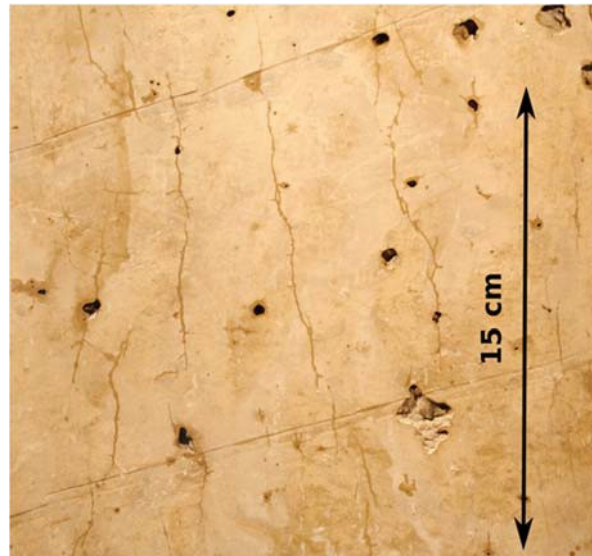


Figure 8. Tri axial cells and internal set up of reactive (R) and non-reactive (NR) cores with fibre optic sensors.

The main observations, from the first experimental campaign, just completed are:

- Isotropic pressure load does not cause creep: the samples only exhibited creep from external loads applied through the mean of a piston
- If the applied pressure is 10 MPa or above, the expansion and damage from samples is accelerated. Notably, the expansions are double or treble the baseline unloaded case.
- Although the rate of expansion reduced after 11 months, the expansion did not plateau, rather it seemed to settle to a long-term constant rate
- When expansions are below 0.4 millistrains there is low variability between nominally similar samples. Beyond this threshold, a large dispersion of the results is observed. We interpret this as being the point where the samples start to have an important amount of cracks and damage.

Microscopic observations indicate that the direction of the cracks at the scale of a microscopic observation (a composite image of around a centimeter) are governed by the concrete microstructure (as expected, cracks mostly propagate in the ITZ). The macroscopic results, however, indicate that the percolation of the cracks is affected by the direction of the load. The coarser cracks are aligned to the direction of stress, Figure 9.



$$P_{\text{NaOH}} = 10 \text{ MPa} \text{ and } \sigma_a = 6 \text{ MPa}$$

Figure 9. Macroscopic orientation of cracks due to loading

2 The ASR model

2.1 Phenomenological aspects

Modelling ASR, for the purpose of monitoring structures, defines both the reliability constraints and the outputs of the model. ASR is first degradation at the microstructural level: cracks in aggregates and paste, gel pockets. Second, ASR induces degradation of mechanical properties at the macro-scale. The link between these two aspects is found in the phenomenological links between expansion and reaction and expansion and loss of stiffness. Confidence in a model comes from being able to verify both the practical outputs: degradation and expansion, as well as the underlying physical causes: the initiation and propagation of cracks in the microstructure.

2.1.1 Micro-cracking morphology

The cracks induced by the ASR initiate inside the aggregates, from so called 'gel pockets', which are localised areas of reactive silica, which react to form ASR gel. They then form a crack network connecting the gel pockets. As the reaction develops, the cracks percolate to the paste, and eventually join the aggregates. This description is consistent with the observation of many so-called slowly-reacting aggregates, which is typical in Switzerland. The literature also describes different cracking morphologies: more reacting aggregates form fewer cracks inside aggregates, and more in the paste. Also, more reactive aggregates may react more homogeneously and preferentially on the surface. Many models in the literature are based on the idea of "reaction rims" around the aggregates and do not reflect the reality of the typical mineralogy of a Swiss reactive aggregate. Most previous models are based on two erroneous assumptions: an assumption that the ASR reaction occurs only at the surface of the aggregates and an assumption that expansion occurs when the gel fills all the porosity in the cement paste. The relative amount of cracks in the paste and aggregates is critical for the resulting mechanical properties. First, the stiffness is affected differently by paste being weakened or the aggregates



being weakened. A crack in the paste lowers approximately twice as much the stiffness of the material as the same crack located in an aggregate.

But the relative amount of cracking in aggregate in paste is mechanically important also in terms of changing the creeping properties of the concrete. There is no easy analytical solution to that problem, however, and numerical modelling is necessary. The works of Giorla indicate that the cracking in the aggregate may increase the apparent visco-elastic properties of the concrete. This is easily understood: in a first approximation, softer aggregates redistribute more load to the paste, which therefore will creep more. A more complete model further indicates that damaged paste creeps more than sound paste.

A further complication, is the percolation of cracks. Cracks propagate according to the stress field around them. They tend to go towards areas of high tensile stress, and, linked to that, towards softer materials. Conversely, cracks tend to propagate away from compression and hard inclusions. The way cracks interact together is not so easily described. They tend to rejoin, but not merge. For a crack to join another, they must have the right configuration. In general, simulating the percolation of a dense network of cracks is a difficult problem. In the case of ASR it is critical as it defines the effective softening of the paste and aggregates.

These links show that reproducing the morphology of the microstructural degradation is critical to the prediction of macroscopic properties.

2.1.2 Macroscopic observation

Much of the earlier work on ASR tried to link the expansion to the macroscopic behaviour of the material. This approach is based on the idea that there is a simple stress-strain relationship which can explain the ASR behaviour.

The free expansion behaviour of concrete and mortar samples suggested that there existed such a relationship: the loss of stiffness followed an S-shaped curve in time, as did the expansion in the experiments of Larive. Further, it seemed that restraining the sample along an axis did not change the volumetric expansion. Unfortunately, these results are likely incorrect: when leaching is avoided there is no final plateau and no S-shape curve. Rather, the expansion continues indefinitely. The volumetric expansion is not conserved when restraining the samples. Regarding the effect of constraint, different aggregates have different behaviour, but all of them exhibit first a lowering of the volumetric expansion as the restraint increases, then a rise, Figure 10. This trend is particularly obvious in the experiments performed at LMC (Dunant 2009), but this may be due to the specific aggregate used: Illsee.

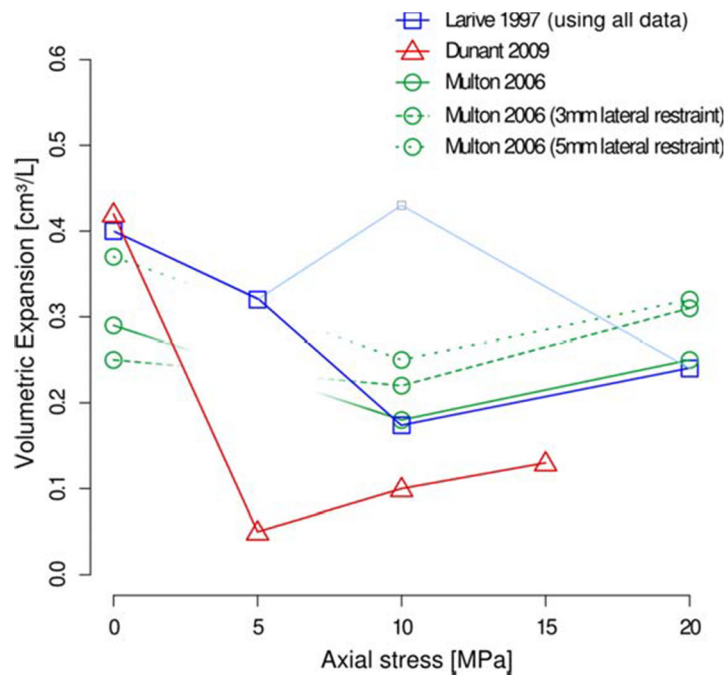


Figure 10. Variation of volumetric expansion with uniaxial load

All this points to a complex relationship between the formation of the gel, the expansion and the loss of stiffness. Such a complex relationship raises significant modelling challenges.

Modelling the ASR at the microstructural level is necessary, due to the complex phenomenology but in turn is difficult due to the complex nature of concrete.

2.2 Representing the microstructure: the mesher and XFEM

Aggregates

Concrete and mortars are frequently represented as two distinct, separable scales. However, there is no clear separation of scale between concrete and mortar. This is not crucial when modelling the elastic properties of the materials, but cannot easily be done when cracking occurs: modelling crack propagation across mortar is easy enough, but modelling the initiation of cracks inside the mortar aggregates, let alone their percolation in paste, phenomena which are critical to the ASR process is not possible. Therefore, the model representing the microstructure must explicitly represent the aggregates, down to the smallest size possible. Therefore a mesher capable of producing a good enough representation of a concrete microstructure with aggregate sizes spanning two orders of magnitude was a hard requirement.

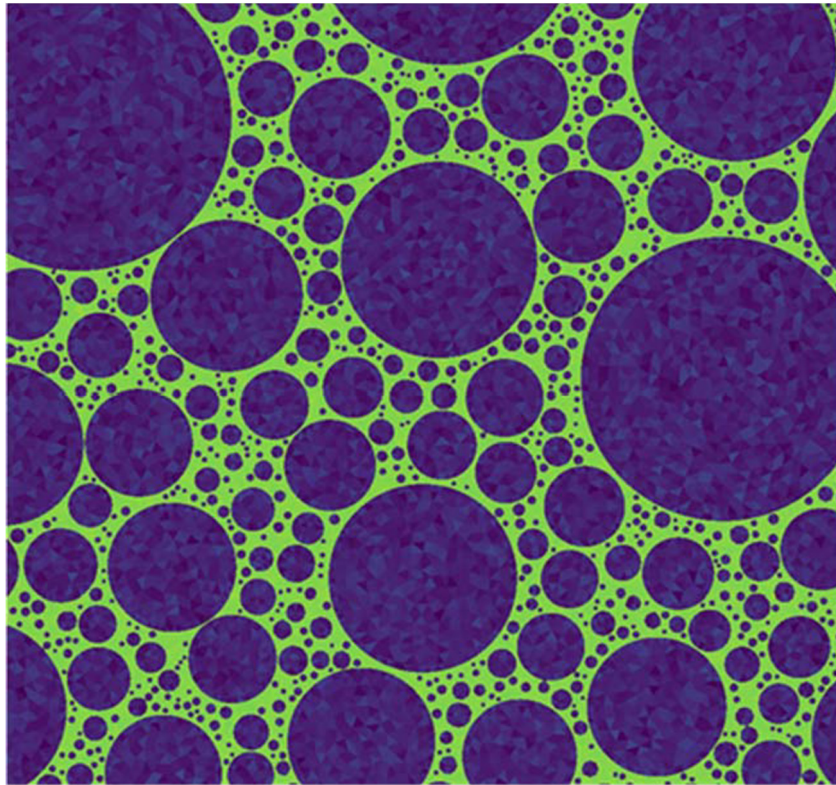


Figure 11. Representation of concrete

The shapes chosen for the aggregates are simple circles. Although the geometrical engine of the LMC code allows for realistic aggregate shapes, these are not useful in the modelling of ASR. As the cracks initiate inside the aggregates, the stress concentration effects due to aggregate shapes are not very significant. Anisotropy of the reaction can be easily modelled using ellipses with a bias in their orientation.

An in-house mesher was developed which was robust enough to handle the highly intricate geometries generated to represent the ASR. Importantly the mesher should be able to generate meshes automatically with a high degree of robustness. Recent developments have seen the availability of commercial meshers which can mesh concrete microstructures, but controlling mesh density, a crucial aspect of the damage calculations is still not generally satisfactory.

Gel

A key aspect of ASR is the growth of gel pockets. It is not practical or effective to represent such fine features in a mesh. Further, the growth of the gel pockets implies moving interfaces. The gel pockets are represented using extended finite elements in the LMC code. Such finite elements are used to represent the effects of interfaces or discontinuities without explicit meshing. A new development at the time of the implementation, they required special developments to be used effectively in the case of ASR.

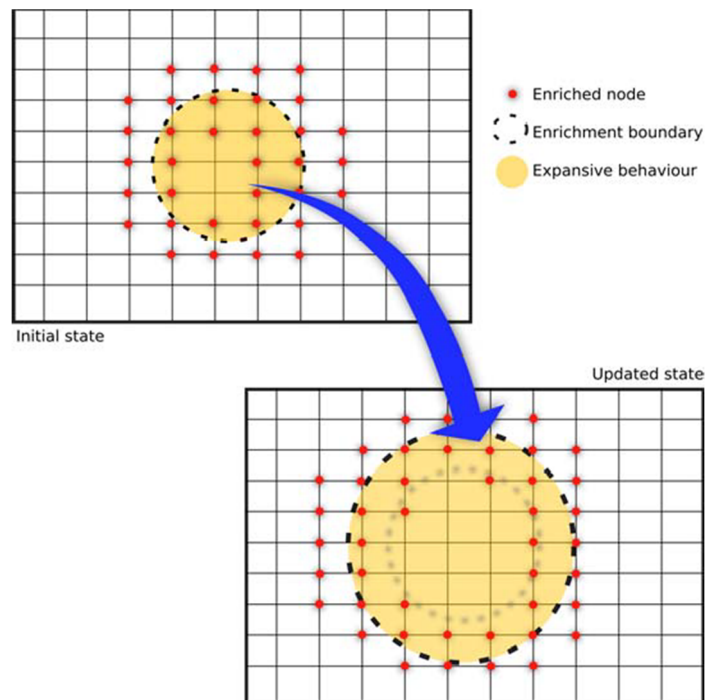


Figure 12. Representation of gel pockets in XFEM

A high-performance of the extended finite element method requires integration with the mesher. As the elements represent surfaces which are not explicitly meshed, these interfaces must be located within existing elements. In usual mesher implementations, finding which elements lie at a particular geometrical locus is a computationally expensive operation. In the LMC code, this operation is helped by the particular data-structure which stores the mesh information, making it considerably faster. This integration of the mesher with XFEM within a single code architecture is, to our knowledge, still state-of-the-art 10 years later.

XFEM were originally considered to model the cracks induced by ASR. However, physics-based crack initiation and merging using XFEM is not a solved question. Indeed it is currently still an open research question. Nonetheless, the generic capabilities of the simulation platform we developed allowed us to explore this option. In the end a damage model, rather than an explicit representation of each crack was found to be a more practical solution.

Further developments during the Giorla thesis introduced a creep model to the paste. In this case, it is not possible to simply grow the elements stepwise. Rather, the XFEM were extended to smoothly expand with time. This allows for a realistic loading case on the microstructure, which is crucial for simulating ASR damage in a visco-elastic model of concrete.

2.3 Material models: paste and aggregates

Microstructural modelling of ASR is a non-linear problem. The initiation and propagation of damage in the aggregates and paste must be computed. Due to the very high density of cracking in ASR, this is numerically difficult. This section describes the models developed for paste and aggregates as well as the numerical tools implemented to run the simulations.

2.3.1 Material properties of the phases

Elastic properties

The elastic properties of both the aggregates and paste can easily be measured in the laboratory



and can be verified by comparing with the literature. The overall behaviour of the composite, aggregates and paste can be further compared with non-destructive measures. The overall behaviour of the sound concrete results only from the average modulus and Poisson ratio of the aggregates and paste as well as from the shape of the aggregates. The shape can easily be assumed to be spherical, but the behaviour must take into account variability, for the purpose of computing damage.

Variability

Both aggregates and cement paste are intrinsically variable materials: although they have well-defined average properties in terms of their moduli and strengths, many of their properties from the point of view of modelling damage stem from their variability: weak zones at which damage can easily initiate, stronger ones which prevent the straight propagation of cracks.

To model this intrinsic variability, each element in the mesh has a slightly different behaviour: different strength, different modulus. A simple Weibull distribution is used to generate the values around the average. This distribution is also helpful to spread the location of damage initiation.

Brittleness

There are no satisfactory models for the behaviour of paste or aggregate fracture which have been published, therefore the approach chosen was the simplest which could phenomenologically reproduce experimental observations.

The aggregate and paste behaviour are assumed to be elastic-brittle. When the Tresca equivalent stress in the materials reaches a critical level, the materials are softened by 10%. This process is repeated until softening reaches 70% at which point the material is deemed broken and the stiffness is reduced to 0. This very simple behaviour is a good phenomenological representation of the degradation process of heterogeneous materials. The degradation of materials is linked with the dissipation of energy. This energy is necessary to form the surfaces of micro-cracks. The size of the softening steps and the limit at which fracture occurs can be adjusted to have the material dissipate realistic amounts of energy.

Visco-elastic behaviour

The creep of concrete is an important parameter in the long-term modelling of structure. The creep comes exclusively from the cement paste. Although there are many published experiments for concrete, the behaviour of pure paste is less well described. Nonetheless, using the microstructural model from LMC, it was relatively easy to back-calculate the creep properties of cement paste.

This was done using a Maxwell chain approximation.

2.3.2 Computing damage: a new algorithm

Computing damage in the case of ASR cannot be done using simple Newton-Raphson schemes. This is for two reasons. The first is that the chosen mechanical behaviour which has good empirical behaviour is not continuous, and therefore is not easily solved using fixed point methods. The second is that Newton-Raphson schemes are stable and correct under two critical assumptions:

1. The number of elements affected is small. This in practice is achieved by having a small load step. As the load step is governed in the case of ASR by the growth of the gel pockets, small steps are difficult to achieve.
2. The damage is not strongly localised. In general, Newton schemes cannot capture the peak of the stress-strain curve. In practice, this is usually solved using small loading steps, but



importantly, the common case of numerical simulations has a single crack growing, meaning that even though the peak is not well captured, the small loss in precision this implies is acceptable.

The second assumption is not theoretically satisfied in general, but it is generally assumed that the results are nonetheless valid. Work performed by Giorla indicates that the effects of not capturing well enough the localisation may be more dramatic than is usually assumed. In the case of ASR both assumptions are violated. The number of elements affected by a small increase in the gel pocket radius can be very large. Therefore, the error introduced by over-damaging can be very large. The second assumption is further violated at every damage step in every element: due to the behaviour formulation, there are in principle several peaks to capture.

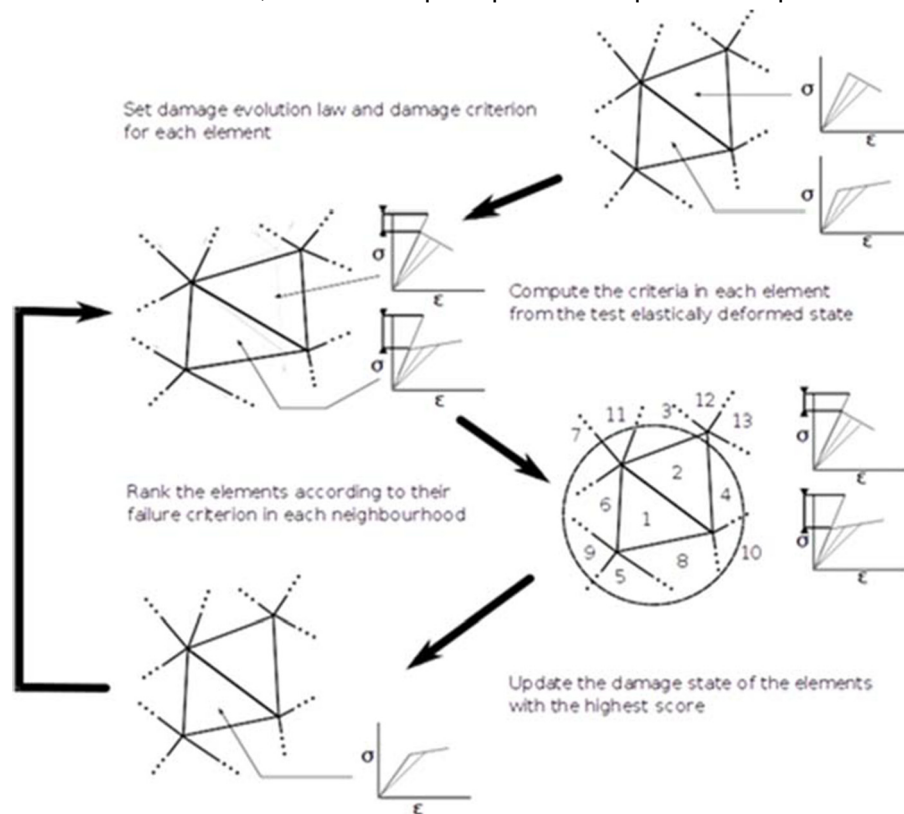


Figure 13. Schematic of new damage algorithm developed

Due to the limitations of Newton-Raphson, a completely new approach had to be introduced. The critical aspect of this new development is that the problem solved is the dual of the NR. In Newton Raphson, the algorithm finds the behaviour which is compatible with the new boundary conditions by adjusting the damage variable in each element. In the new algorithm, the objective is to find the boundary conditions which are compatible with a damage increase. The location of the damage increase is determined by ranking the elements according to their failure criterion.

This new damage algorithm is appropriate for the simulation of ASR as it is always stable and always captures the peaks of the behaviour. This allows the simulation to reach very high damage levels. Using this algorithm, it is possible to distinguish between numerical limits to the model (simulations become unstable because of the approximation) and physical limits (simulations fail because there exist no valid solution).

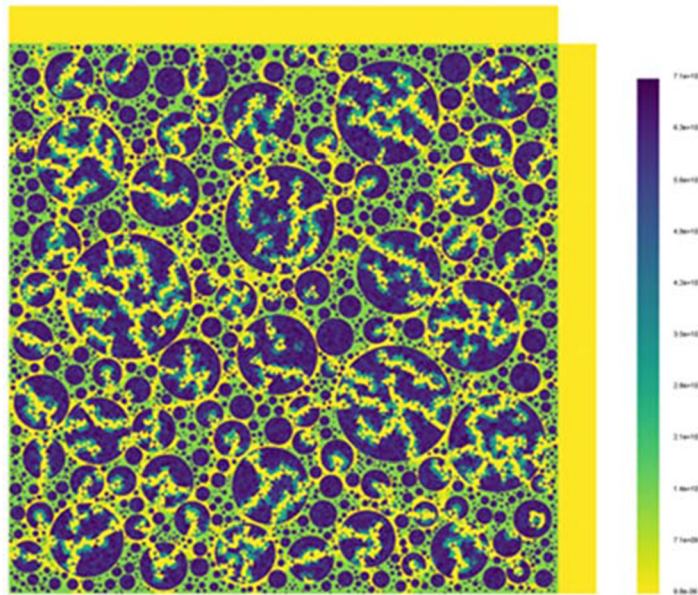


Figure 14. Example of complex damage (cracking pattern) possible in LMC code

2.3.3 Non-local damage approximation

An energetically correct approximation of damage requires either careful calibration to the mesh, or a non-local approximation. The non-local damage method was introduced to represent the fracture process zone in metals. However, it can also be used to represent a degradation process occurring in a material which has an underlying, unrepresented microstructure.

This is the case notably of cement paste: although the Weibull distribution accounts for some of the heterogeneity, it cannot account for the propagation of cracks around hard anhydrous grains or pores. Therefore, a non-local representation of damage, where the damage is not located on a single element band but rather “smeared” over a distance characteristic of the underlying microstructure, is a more accurate representation of reality.

Non-local damage has other important numerical benefits. First, it is mesh independent, this, although the mesh density is not uniform, the energy dissipation is not affected by this heterogeneity. Further, mesh independent means that cracks do not follow the orientation of elements, a bias frequently observed in simulations using local damage. Second, the stability of crack growth depends only on the set behaviour. In local damage simulation, artificial brittleness can be introduced. Finally, branching and merging of cracks are more physically accurate. Local representations tend to initiate more cracks than is realistic, and these have a much stronger tendency to branch.

2.3.4 Computing creep: space-time finite elements

Modelling creeping materials is commonly done using iterative finite difference schemes. Such schemes work well if the damage and creep problems can be decoupled. They do not allow for the simultaneous solving of these two phenomena. This is not possible in the case of ASR, as the rate at which cracks grow is commensurate to the speed at which creep relaxation occurs. Therefore, new numerical developments were required, notably a new finite element representation in space and time.

A simultaneous solving process is required, because both creep and damage relax stresses. Therefore, as the gel grows, the stress is increased in the microstructure, but not as fast as in the elastic case. The effective rate of stress increase depends on the rate of gel growth and on the



visco-elastic properties of the cement paste. Nevertheless, a critical stress may be reached at any point during this process which will initiate damage. The damage algorithm can be easily adapted provided the time at which this critical stress is known.

Using space-time finite elements, where displacements are approximated as functions of time and space, this is easily accomplished. The finite element approximation has a further benefit. It gives the displacement field at all times during a load step, meaning it is possible to initiate the damage *during* the load step. This is similar to the quasistatic case described above: this method captures exactly the peak load. But importantly, it also allows taking into account the creep relaxation at the same time.

The damage model, adapted to the space-time case allows distinction between stress dissipated by damage and stress dissipated by creep. The slow loading rates induced by ASR make it impossible to distinguish between these two cases. The simulations run with this updated algorithm are unique: they are, to our knowledge, the only truly coupled creep-damage simulations.

2.4 ASR model results

The model was run to help understand a number of experiments during the Dunant thesis. The LMC model was originally conceived as a tool to validate or invalidate our understanding of the physics and micromechanics of ASR. The model was not intended to be run to be able to make predictions on real structures. Rather, it was designed to be able to provide physics-based inputs to empirical models applicable at a larger scale.

There are few free parameters in the model: the mechanical properties of the gel described in the literature are becoming better defined, although it seems that there is no single gel, but rather a range of possible compositions. Therefore, the gel stiffness is assumed to be in the range of values reported in the literature, but can be adjusted depending on the aggregate. The PSD of the concrete is usually known. The mechanical properties of the paste and aggregates can be easily measured.

These parameters suffice to run the quasi-static version of the model, which relates the amount of gel produced to expansion and damage. Extrapolation requires a relation between the gel production and time. The rate at which gel grows depends on mineralogy, temperature and relative humidity. Laboratory experiments performed at multiple temperatures can give the activation energy.

The visco-elastic version of the model can take into account the effects of creep. This requires additional parameters: the visco-elastic properties of paste can be obtained from a creep experiment. The visco-elastic fracture properties of paste are much more difficult to measure, and a large part of the Giorla thesis was designed to establish sets of physically plausible parameters. An important breakthrough was to establish that the fracture criterion had to be stress-based. This finding has important repercussions in the wider field of concrete modelling: in the quasistatic case, stress or strain based criteria are indistinguishable. Visco-elastic modelling gave an answer to that question: stress, and not strain causes the fracture.

2.5 Free expansion

The first set of simulations tried to reproduce the free expansion experiments normally conducted in the lab. Free expansion experiments are used in many cases as a starting point to calibrate models. In the case of the LMC ASR model, they are used to validate the model as the parameters are all obtained from separate experiments or the literature.

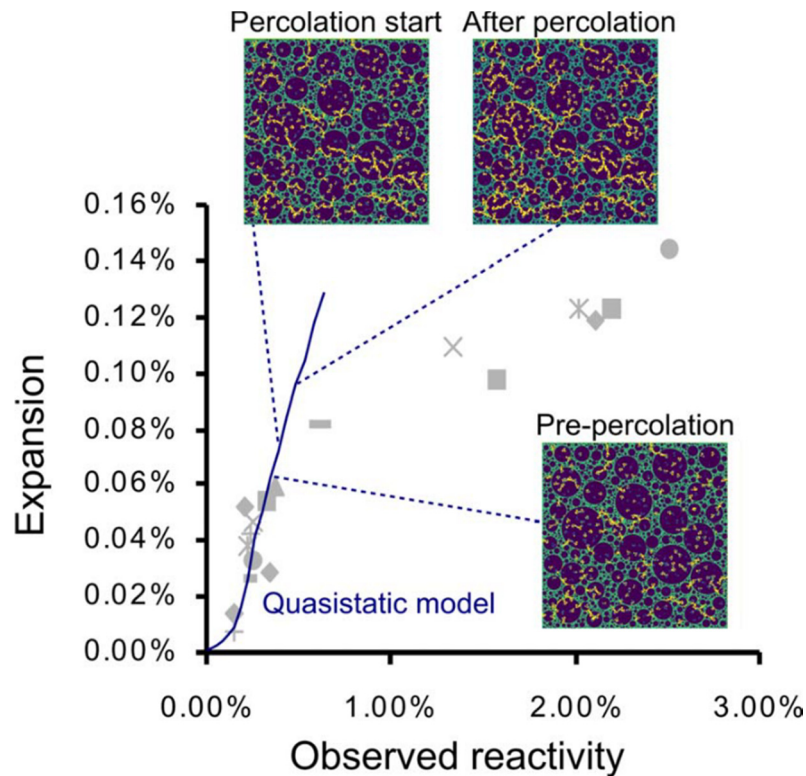


Figure 15. Evolution of damage in model

The only fit which needs to be performed, is to measure the reaction rate of the gel using image analysis. As the model is quasistatic, it does not depend on kinetics. Rather, it relates the amount of gel produced to degradation, expansion and load.

2.5.1 Expansion-reaction

The model, using the default parameters works very well in predicting the correlation between expansion and reaction as measured by image analysis up to approximately 0.6% of reaction. This corresponds to a very advanced state in practice, at which structures would not be considered safe. The quasistatic model stops following the experimental trend around 0.6% of reaction for two reasons. The first reason is that the measure of reaction by image analysis becomes less precise at this point due to the difficulty of keeping the aggregates intact: large holes in the aggregates, interpreted as reaction, are typically artefacts of sample preparation (see figure from Ben Haha for an illustration, Figure 16). The second reason is that this is also the point at which damage in the paste starts to percolate. Percolation of cracks in 2D has different consequences on the apparent strength of the sample than the percolation of cracks in 3D would.

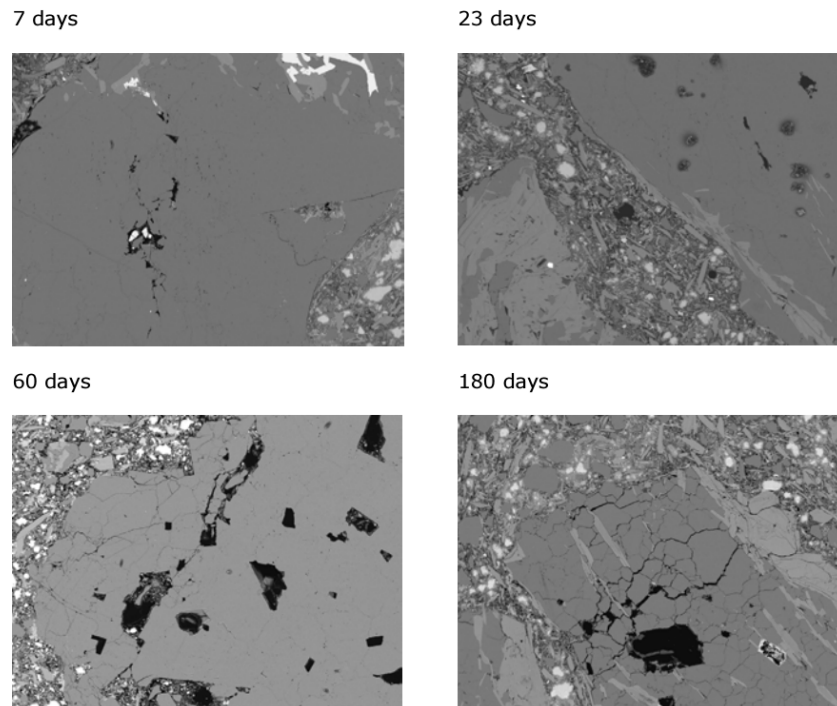


Figure 16. Damage in typical aggregates from thesis of Ben Haha

2.5.2 Loss of stiffness

To predict the long-term behaviour of dams affected by ASR, the evolution of the stiffness of concrete as well as the free expansion need to be considered. These two aspects are only loosely connected, as anisotropic loading of the concrete can affect the development of the damage.

The quasistatic model predicts too much damage in the paste, as noted above. Therefore, after the cracks have percolated in the paste, the stiffness keeps falling in the model, whereas real concrete is less affected by the ongoing reaction. The discrepancy between the model and the experiments prompted the start of the Giorla thesis.

Nonetheless the model predicts quite well the loss of stiffness before the cracks percolate, and therefore gives useful predictions in the range most relevant to massive concrete structures.

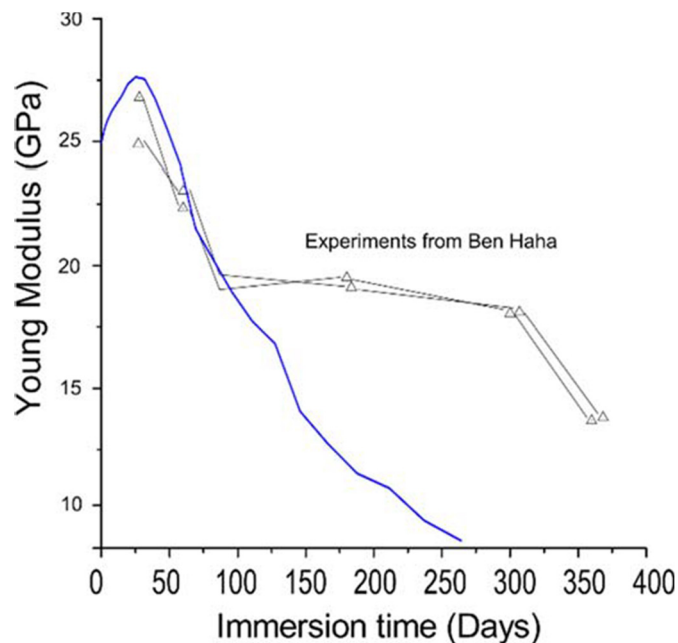


Figure 17. Low of stiffness, comparison of experiments with simulation (blue line). The model overestimates the loss of stiffness due to the absences of creep in this version.

2.6 Size effects – role of the PSD

2.6.1 Role of the Dmax

A key goal for the model was to guide the extrapolation from the laboratory to the field. It is impractical to cast concrete samples with the same PSD as dam concrete. The reaction would take too long and the samples would be too massive to easily manipulate. Therefore the model needed to account for the effect of PSD.

During the Dunant thesis, samples prepared with continuous PSD following the Bolomey curves prescribed by the Swiss norms were cast. The free expansion of these samples was modelled, and the increase in gel diameter was interpreted as time. The results showed a very good match between the simulations and the experiments.

Such simulations could be used to disprove certain hypotheses: in many models, it is assumed that the initial delay before the expansion is due to the time needed for the diffusion of the alkali ions to the reactive silica. The results from the simulation rather suggest that it is different fracture behaviour of different aggregate sizes which is the cause of longer or shorter “induction” periods.

Two physical process need to be considered in interpreting the expansion as a function of the PSD: the fracture behaviour of individual aggregates as a function of their size and the effect of the PSD on the propagation of cracks once they have reached the paste. Fully reactive PSD experiments are more appropriate to test the first of these aspects, whereas mixes of reactive and non-reactive aggregates can be used to test the second.

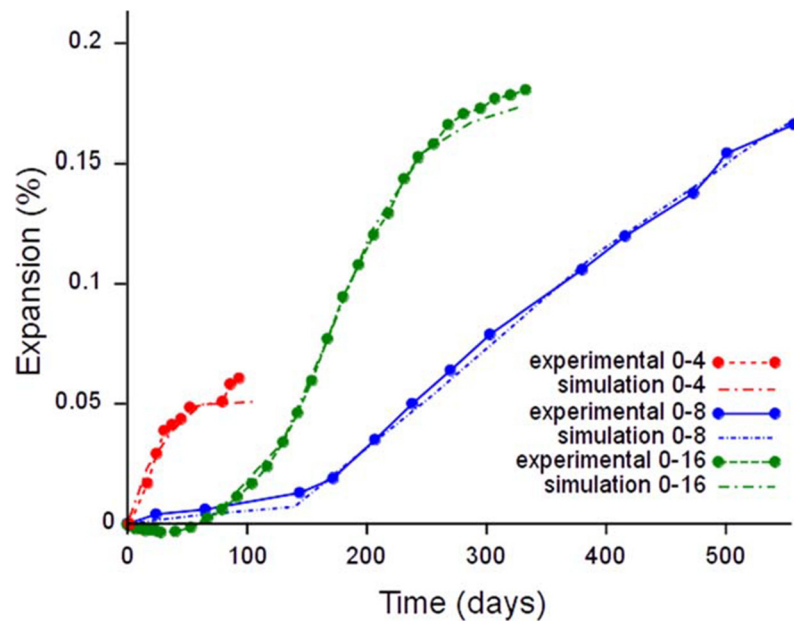


Figure 18. Experiments and simulation on effect of aggregate size

2.6.2 Role of individual fractions

To investigate the role of individual reactive fractions, samples with identical PSD were prepared using a mix of reactive and non-reactive aggregates. The results confirmed well-established observations: the potential for early expansion is larger for aggregates of size 2-4 mm. It provided an explanation for this observation: the cracking behaviour of aggregates depend on their size. The length of a critical crack which will split an aggregate is comparably smaller for aggregates of sizes around 2-4.

The model showed that the critical difference between aggregate sizes was not in fact their expansion potential, once the amount of reactive material is taken into account, but the kinetics of the formation of the critical crack network. This important finding indicates that the shape of the expansion curve is affected by the PSD, but the total amount of expansion only depends on the amount reactive material.

This finding is also useful to interpret experimental results: many testing protocols do not take into account the PSD of the reactive aggregates, rather they only specify the amount of sand and gravel. The findings from the model show that the results are then only comparable over the long term, and if no leaching occurs, which would limit the reaction.

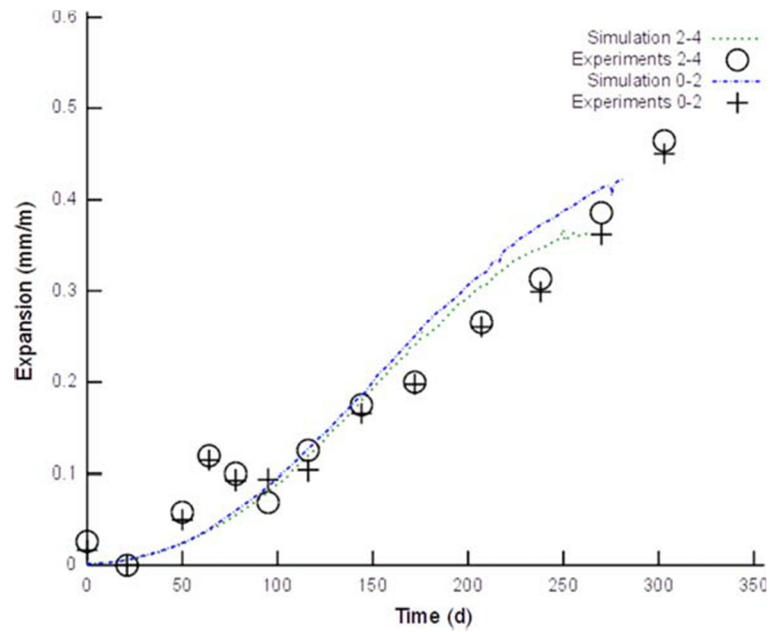


Figure 19. Simulation of different reactive aggregate fractions.

2.7 Effect of aggregate shape

Aggregate shape is frequently believed to affect the damage and expansion caused by the reaction. The micromechanical model was used to investigate the effect of shape on the damage patterns. Samples with ellipsoidal inclusions were generated with different aspect ratios and different bias in their orientations.

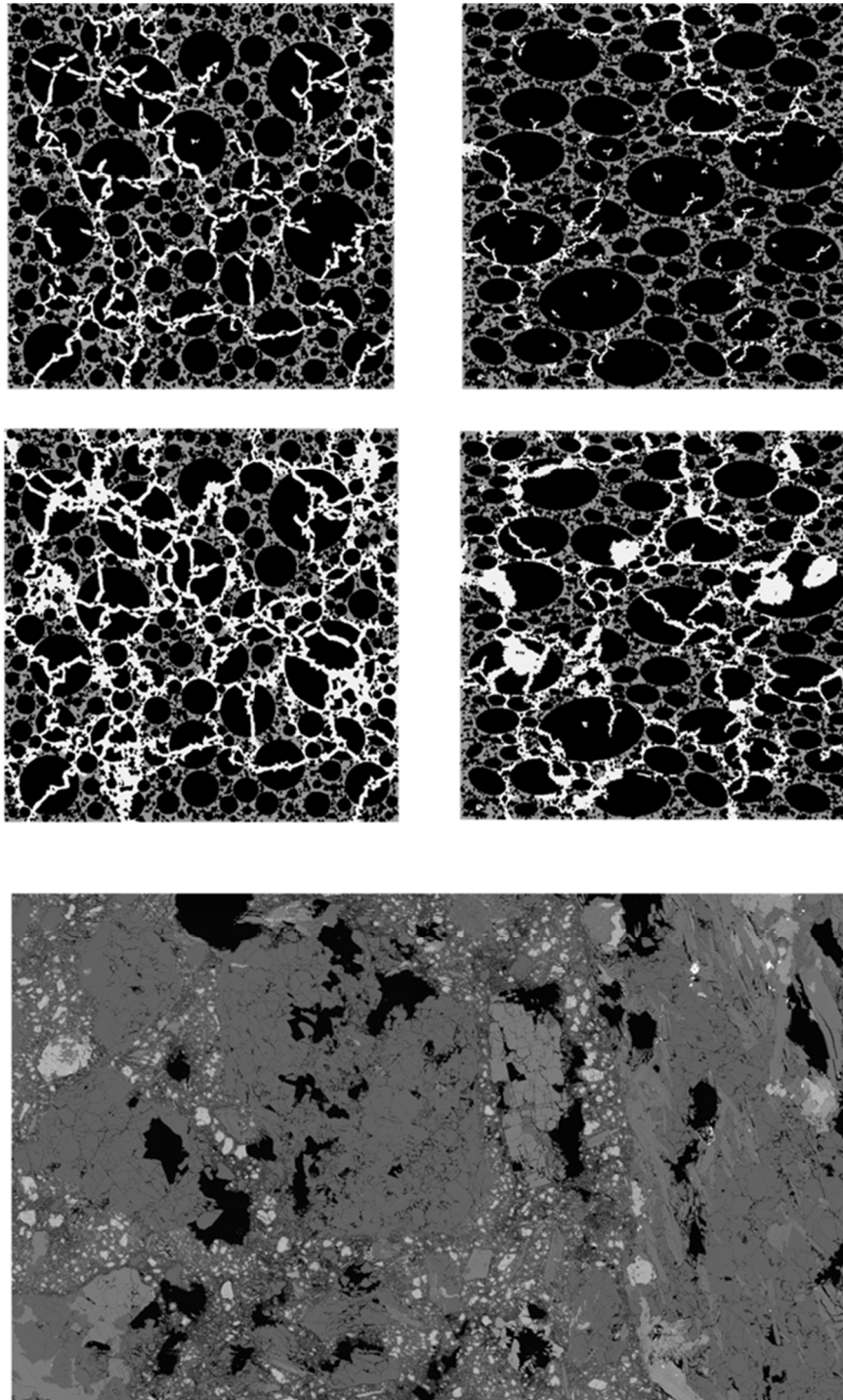


Figure 20. Effect of aggregate shape on damage

The figure illustrates the principal effect of the microstructure: the ellipsoidal aggregates favour fewer, larger cracks oriented along their principal axes, whereas the fracture pattern in the case of round aggregates is more diffuse. This is visible at the beginning of the reaction (top) where more damage is seen in the round aggregates than in the ellipses, which have higher apparent fracture toughness, and in the later stages (bottom) where the crack networks formed in the round aggregates are more intricate.



These simulations further showed that the anisotropy observed in ASR depending on the direction of casting can be easily explained by a small bias in the orientation of the aggregates.

2.8 Effect of load

Another critical aspect for ASR models when comparing with field results is that they can capture the effect of applied load. The loads applied on dams, even large ones are no more than 2-5 MPa from the self-weight of the structure. ASR models are most different in the way they consider the effect of load. A number of them rely on large numbers of experiments for calibration, which is not in general practical. This is because the underlying assumptions cannot be used to satisfactorily predict the effect of load: they assume a conservation of the volume expansion, and a simple redistribution of the expansion, using coefficients fit from the experiments.

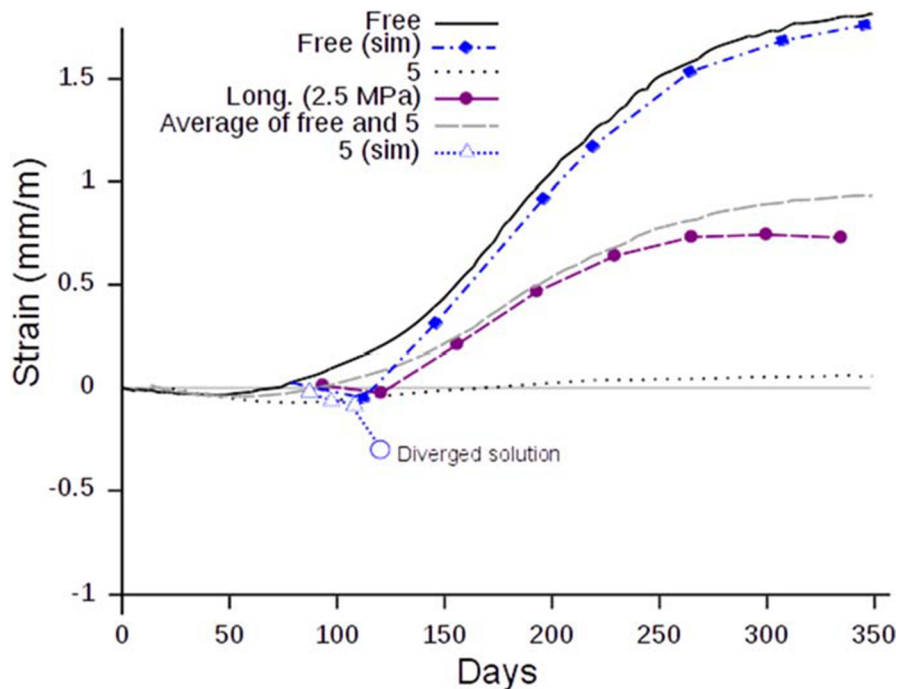


Figure 21. Simulation of effect of load

The LMC model relates the expansion to the damage morphology at the micro-scale. This is critical as micro-cracks become strongly oriented under load, explaining most of the phenomenology described in the literature. Crucially, it shows that there is no general link between expansion, damage and load in the case of ASR: therefore, the free expansion cannot in general be used to predict the loads ASR imposes on structures.

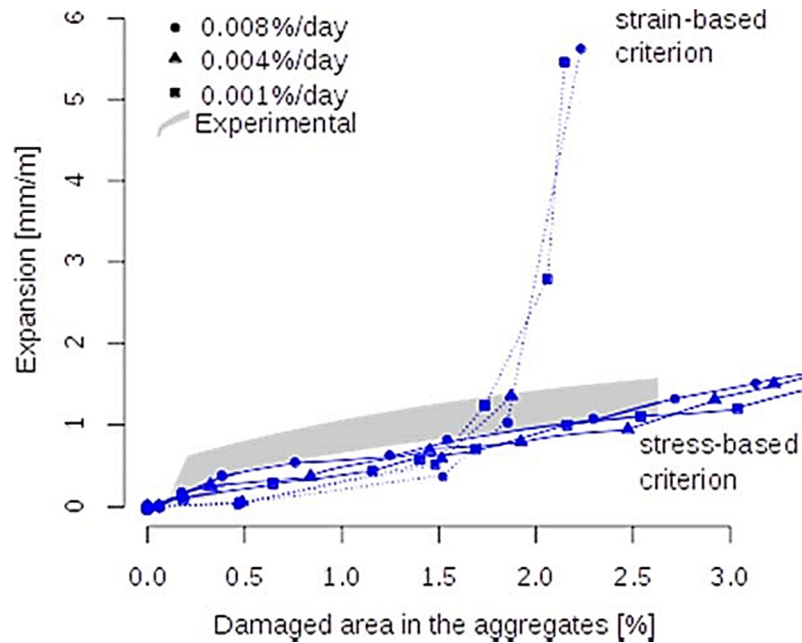
The model works well for loads up to 2.5 MPa, but the percolation of cracks in the paste is greatly accelerated under load, making simulations above 5 MPa impossible to run beyond the first steps.

2.9 Role of creep

One of the important questions still open at the end of the Dunant thesis was why the damage predicted in the paste was so much larger than the loss of stiffness observed experimentally. As mentioned in the introduction, the damage in the paste has much larger consequences than the damage in aggregates. Therefore, the prediction from the LMC model are already more conservative than predictions of other physics-based micro-mechanical models where damage initiates in the paste rather than the aggregates. However, the damage being still too high, two hypotheses were put forward to explain the discrepancy. The first one was that 3D percolation of cracks is different from 2D,



and the second was that creep dissipated the stress from ASR.



Indeed, expansions predicted as a function of the damage in the aggregates are closer to the experimental observations: the overprediction of the expansion disappears as the damage in the paste is considerably reduced. The space-time model therefore has a larger domain of validity than the quasistatic one and is probably usable for long-term predictions.

An important finding from the visco-elastic simulations was that damage in the paste depends on the rate of the expansion. Therefore, experiments at higher temperature should exhibit steeper losses of properties for the same amount of reaction than field concrete. This illustrates how physics-based models help interpret observations.

Nonetheless, simulating the expansion under load does not work better than in the quasistatic case, because although fewer cracks are formed in the visco-elastic matrix, they do not propagate much slower. This allowed us to conclude that the effect of ASR at later stages is dominated by the percolation of cracks in the cement paste.

This finding is unique in the currently published ASR models, as the others are based on experiments subject to leaching, meaning this regime is never reached before the reaction is exhausted. In real dams, there are no reasons to believe exhaustion happens until long after the planned useful life of the structure.

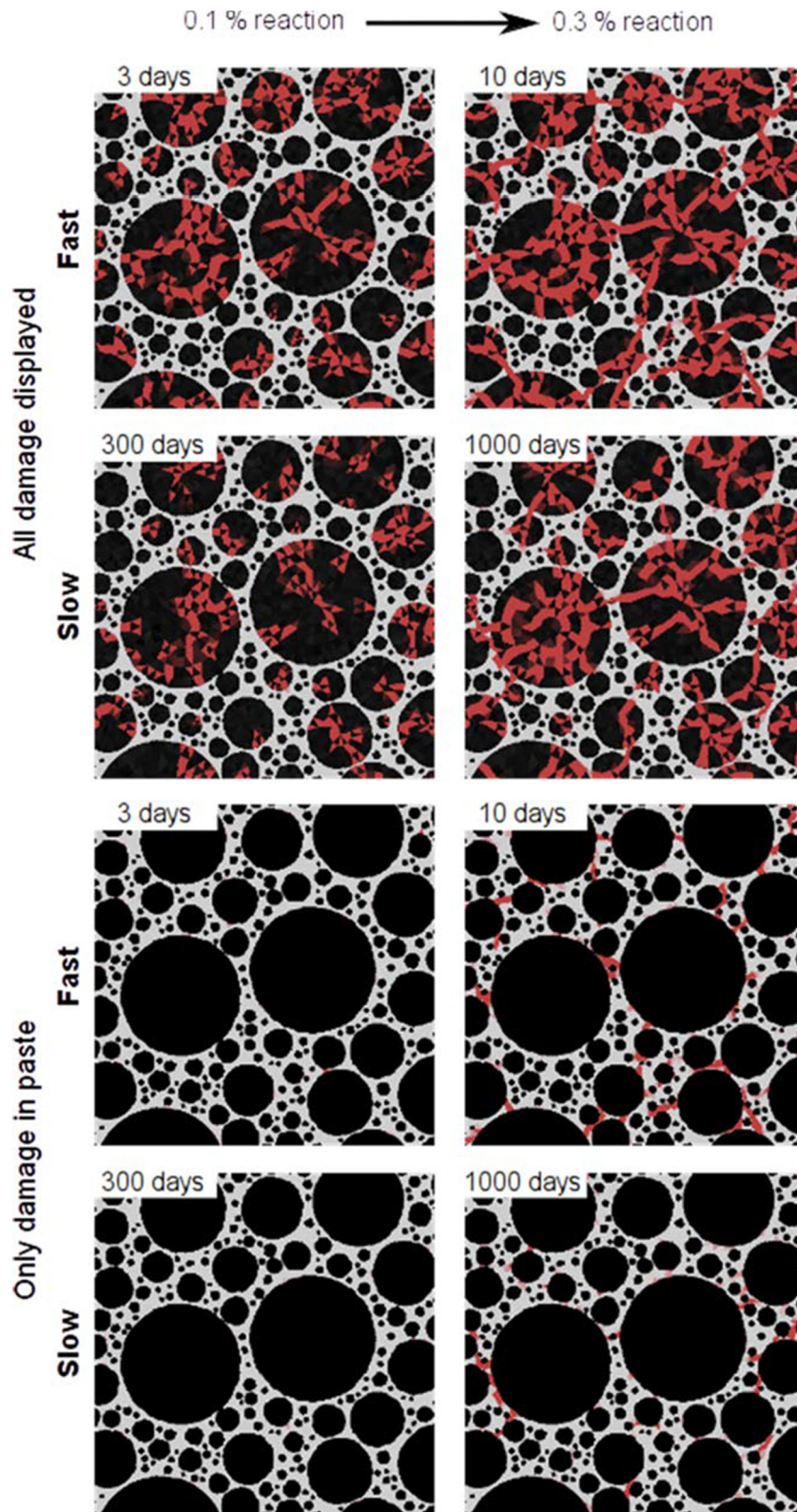


Figure 22: Impact of creep on damage



3 Summary

During the course of the 3 theses carried out at LMC a fundamental basis was laid linking the microscopic processes occurring during alkali silica reaction to the macroscopic consequences. The construction of model was crucial to establishing these links.

In most aggregate types the reaction occurs within the aggregates. The model based on this phenomenon enables the relationship between microscopic damage and free expansion to be understood. It is also possible to simulate the effects of different aggregate sizes. This provides the possibility to upscale results from lab concrete to dam concrete.

The model does not implicitly consider the kinetics of the reaction. However the assumption of a constant rate of gel formation fits well the experimental results. The activation energy for the reaction is known so the kinetics can then be adjusted for different temperatures.

The model clearly shows that creep must be taken into account, otherwise the loss in stiffness is very much overestimated.

The thesis of Aurelia Cuba Ramos in LSMS with Prof. Molinari has parallelised the code and extended it to 3D. It was also demonstrated that the microscale could be linked to the structural scale. Nevertheless it remains to integrate creep in this version.

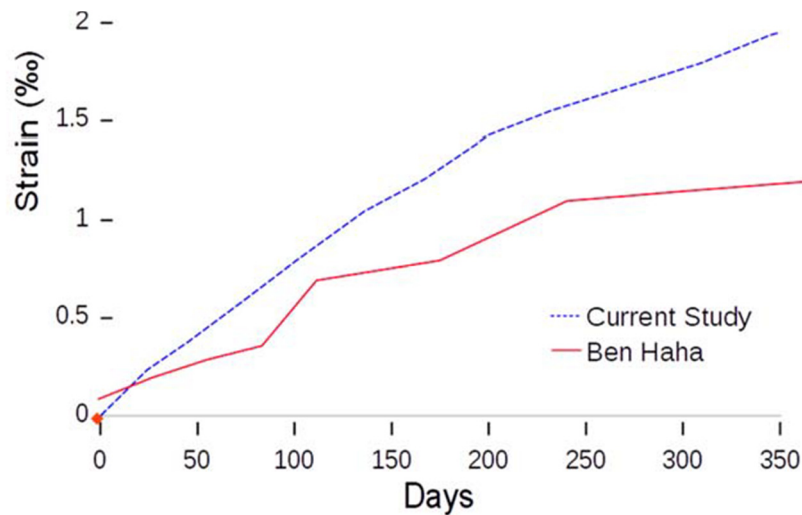
Further experimental results are needed to complete our understanding of the effects of constraint on expansion.

Notwithstanding, the ensemble to work carried out over the past 15 years provides a solid foundation which can be applied, in the future, to understanding the consequences of alkali silica reaction in dams.



Appendix I: Detailed protocol for curing and expansion at LMC

The ASR testing methods around the world tend to offer many variations on the same basic idea: samples cast with the aggregate being tested are cured in warm conditions to accelerate the expansion which is recorded with time. The expansion measure can be complemented by other observations.



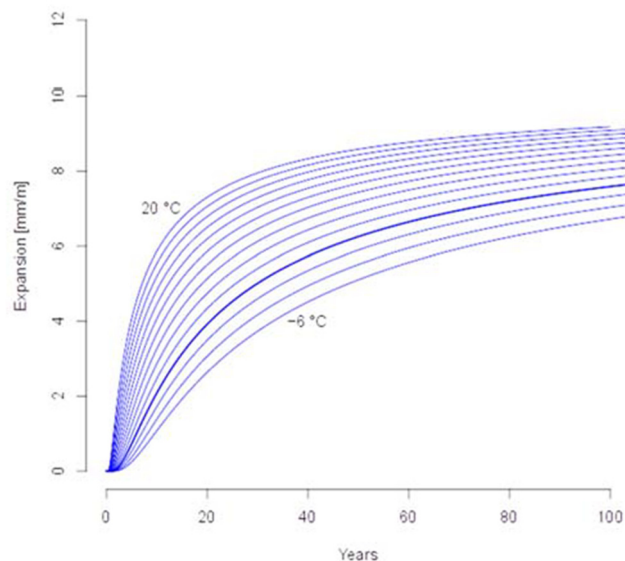
Mix design

- The cement content was tested by Ben Haha, it doesn't affect significantly the results. Therefore, expansion tests can be performed using a wide range of mixes.
- The role of the PSD on the expansion and degradation of mechanical properties is important. Therefore
 - ↘ For the purpose of screening an aggregate, mortar suffices: aggregates crushed to sand can be used for testing in mortar bars. These are smaller and easier to manipulate and expand faster.
 - ↘ To test a mix for the purpose of diagnostic or prognosis requires reproducing the PSD as exactly as possible. This is necessary as the shape of the expansion curve depends strongly on the PSD.
- The w/c does not affect the development of the reaction, but paste strength affects the degradation of the properties, therefore:
 - ↘ Using a standard mortar mix is recommended for the purpose of screening aggregates. This allows comparison between mixes.
 - ↘ To test a mix for the purpose of diagnostic or prognosis requires reproducing the w/c: the expansion in the later stages of the reaction depends on the strength of the cement paste, therefore it is necessary to reproduce this in the laboratory.
- The alkalis can slightly change the kinetics of the reaction in aggregates commonly found in Switzerland. However, some aggregates have what is called a "pessimum effect". This is notably the case for very reactive aggregates. This factor has not been found to significantly affect the aggregates typical of the Swiss Alps.



Cure

- The strength of the paste changes the expansion and degradation. It is important that samples be cured at least 28 days before they are put in hot conditions. This pre-cure allows the cement microstructure to stabilise and helps the reproducibility of the measure. Further, the mechanical properties of paste hardened for 28 days are much closer to that of field concrete, making observations more relevant for the purpose of prognosis.
 - ↘ It is well established that the expansion follows an Arrhenius-like law for reasonable temperatures. Reasonable temperatures range from 5 to 60 degrees, although temperatures above 50 C can alter the reaction mechanisms for some aggregates. At 80 C, unreactive materials, such as alpha quartz can start reacting.
 - ↘ Temperatures above 60 C should be avoided as they change the chemical nature of the reaction: the gel formed at these higher temperatures has different mechanical properties than the gels formed at lower temperatures.
 - ↘ Three temperatures should be tested for the purpose of establishing the apparent activation energy of a mix. This is necessary for the purpose of prognosis: using the apparent activation energy of the reaction and expansion curves obtained at 38 C, the expansion of dam concretes can be calculated.



- ↘ The temperature of 38 C, commonly used around the world, is recommended as it allows results to be easily compared to literature.
- Various methods have been proposed to avoid leaching.
 - ↘ 100% RH is not recommended as water condensates on the concrete and induces important leaching over the duration of the experiments.
 - ↘ Wrapping samples with cloths imbibed with sodium hydroxide solutions works. It is however difficult to do well, and has few benefits if the cement pore solution is known.
 - ↘ The recommended method is to perform the cure in a bath where the alkali concentration matches that of the cement pore solution. Without information, a value of 120 mmol/l of NaOH has been determined to work well.



- The cure should last at least a year. Mixes prepared with some aggregates have been observed to only start expanding only after 150-200 days. The 28 day cure before the samples are put in their alkaline baths increases this “induction” period.

Measure of expansion

- Temperature variation should be minimised when doing the measure. It is recommended to have the measuring equipment in the hot room where possible. Dunant tried cooling the samples as well as measuring them immediately after they were removed from their hot room. A lower variability was observed when samples were allowed to cool, but this should be taken as an indication that temperature control is important, not that the samples need to be cooled. Indeed, measuring samples in the hot room has the lowest variability.
- RH variation should be minimised: samples should be taken out of their baths, wiped to remove the excess water and measured as fast as possible.

Supplementary measures

- Mechanical properties
 - ↘ Static modulus measures can be done non-destructively. It is therefore recommended that a sample be used throughout the expansion period to that effect.
 - ↘ Flexural and compressive strength are useful to track the effects of the reaction. These require the preparation of sacrificial samples.
 - ↘ For both these measures, a non-reactive sample with the same mix design should have been prepared.
- The most important measure is the direct measure of the degradation using polished sections and image analysis. This measure is the only way to detect reaction absent expansion or mechanical tests. At LMC a sample is cast for this purpose and sliced as the expansion progresses.

Appendix II: Detailed protocol for Image analysis

Principle

The direct measure of ASR developed at LMC uses image analysis on BSE polished sections. The measure is the fraction of the aggregate transformed to gel or cracks. These are identifiable as they are much darker than the rest of the aggregate.

Implementation details

Aggregates can have very varied textures, some even resembling cement paste. To be able to extract the aggregates from the image, a series of filters is used:

- Possible aggregate grains are identified by their grey levels
- They are filtered according to their shape and area
- Filtered grains are assembled using morphological operations to form potential aggregates
- Potential aggregates are filtered according to their shape and area

The result of these operations is a mask which separates aggregates from paste. It is possible to use a simplified procedure where only the ASR reactive phase of the aggregates is tracked. This phase is generally quartz.



Reproducibility of the measure

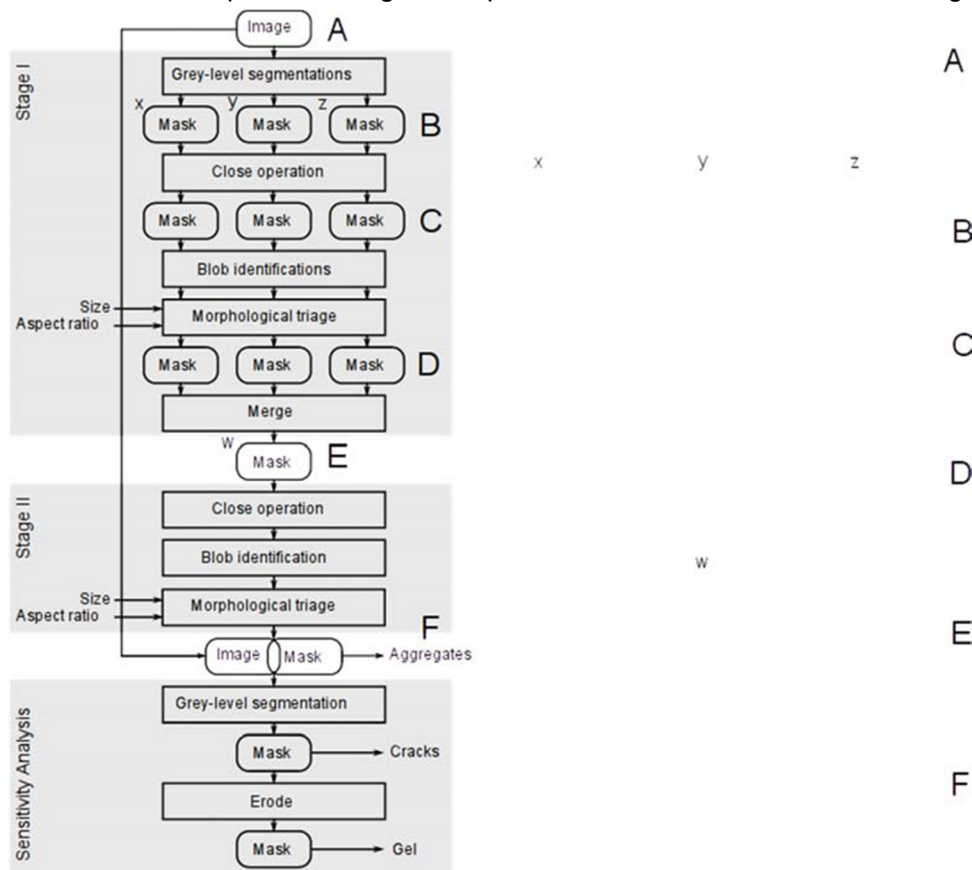
A key difficulty is that each image acquisition has different grey levels. A series of recommendation was developed to minimise the variation. The image parameters are adjusted such that the quartz peak, nearly always present from aggregates has grey level 100, and the cement grains 220

- The image parameters are adjusted such that the quartz peak, nearly always present from aggregates has grey level 100, and the cement grains 220
- Care is taken that the image acquired is saturated neither in the white nor the black.

As the contrast and brightness drift during the acquisition, they are further adjusted in post-processing. Then, the damage measure is performed at constant sensitivity: the grey level threshold below which the cracks are defined is such that:

$$1/\text{aggregate area} * d \text{ grey} / d \text{ crack area} = \text{cst.}$$

Combined, these precautions give a reproducible relative measure of the degradation.



Post-treatment, and accessory measures

Using morphological operators, notably erosion, it is possible to distinguish the fine cracks from the larger gel pockets. The programme used at LMC generates both these values.



Appendix III: List of publications

Ben Haha, M., Gallucci, E., Guidoum, A, Scrivener, K.L.

Relation of expansion due to alkali silica reaction to the degree of reaction measured by SEM image analysis

Cement and Concrete Research, 37 (8), 2007, pp. 1206-1214

Dunant, C.F., Scrivener, K.L.

Micro-mechanical modelling of alkali-silica-reaction-induced degradation using the AMIE framework

Cement and Concrete Research, 40 (4), 2010, pp. 517-525

Dunant, C.F., Bordas, S.P.A., Kerfriden, P., Scrivener, K.L., Rabczuk, T. An algorithm to compute damage from load in composites

Frontiers of Architecture and Civil Engineering in China, 5 (2), pp. 180-193

Cyrille F. Dunant, Karen L. Scrivener

Effects of uniaxial stress on alkali-silica reaction induced expansion of concrete

Cement and Concrete Research, 42 (3), 2012, pp. 567-576

Cyrille F. Dunant, Karen L. Scrivener

Effects of aggregate size on alkali-silica-reaction induced expansion

Cement and Concrete Research, 42 (6), June 2012, pp. 745-751

Giorla, A.B., Scrivener, K.L., Dunant, C.F

Finite elements in space and time for the analysis of generalised visco-elastic materials

International Journal for Numerical Methods in Engineering, 97 (6), 2014, pp. 454-472

Giorla, A.B., Scrivener, K.L., Dunant, C.F

Influence of visco-elasticity on the stress development induced by alkali-silica reaction

Cement and Concrete Research, 70, April 2015, pp. 1-8,

Dunant, C.F., Scrivener, K.L

Document Physically based models to study the alkali-silica reaction

Proceedings of Institution of Civil Engineers: Construction Materials, 169 (3), pp. 136-144

Appendix IV: List of theses

Ben Haha, M.

Mechanical effects of alkali silica reaction in concrete studied by SEM-image analysis

PhD-thesis no 3516, École polytechnique fédérale de Lausanne, 2006

Dunant, C.

Experimental and Modelling Study of the Alkali-Silica-Reaction in Concrete

PhD-thesis no. 4510, École polytechnique fédérale de Lausanne, 2009



Giorla, A.B.

Modelling of Alkali-Silica Reaction under Multi-Axial Load

PhD-thesis no. 5982, École polytechnique fédérale de Lausanne, 2013

Cuba Ramos, A. I.

Multi-Scale Modeling of the Alkali-Silica Reaction in Concrete,

PhD-thesis no. 7591, École polytechnique fédérale de Lausanne, 2017