Modeling of expansion and cracking due to ASR with a 3D lattice model

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ABSTRACT: It is generally possible to consider modeling of ASR damage in concrete in two main groups: modeling of gel formation and its expansion; modeling of ASR related damage. In this paper, authors take an attempt to combine both: simulating the correct crack formation and the connected concrete expansion. It is aimed to simulate ASR damage in a cementitious material bearing reactive aggregates. The model that is used is a 3D lattice type model. It models concrete on a meso-scale in which particles embedded in a cement matrix are taken into account. The particle structure is obtained by CT-scanning of samples. With the model the concrete expansion can be simulated. One of the inputs in the model is the local expansion of the gel. For that the mechanical properties of the gel should be known, which are obtained from an experimental procedure developed by the authors.

1 INTRODUCTION

Research in the past has resulted in insight on how to prevent ASR in structures. Mainly these measures focus on at least one of the three following aspects: (1) using aggregates without reactive silica; (2) using cementitious material that leads to a low alkali content in the pore water; (3) sealing the structure against water ingress. It is good, however, to understand the real mechanism behind ASR and the way it results in damage of concrete structures. The three measures described above are not always feasible, just because no other raw material to make concrete are available at a certain location or sealing the structure is not practical.

Modeling of ASR and ASR damage has attracted significant attention among the concrete science community [Capra & Sellier 2003, Multon & Toutlemonde 2006, Comby-Peyrot 2006, Ischiwaka & Miura 2007]. However, the community is still far away from using a single model for a complete simulation of the gel formation and generated damage mechanism. Alkali silica reaction modeling requires consideration of numerous parameters according to the state of art theories. Dissolution related characteristics of reactive silica, thermo dynamical aspects of gel formation, microstructure of concrete, random localization of the reactive sites, knowledge of the reaction mechanisms are just some of the examples among them [Capra & Sellier 2003].

It is generally possible to consider modeling of concrete in two main groups; (1) modeling of gel formation and its expansion; (2) modeling of ASR related damage. In this paper, authors take an attempt to combine both: simulating the correct crack formation and the connected concrete expansion. It is aimed to simulate ASR damage in a cementitious material bearing dissolved reactive aggregate. The model that is used is a lattice type model [Schlangen & van Mier 1992]. It is applied for ASR in concrete as described in [Schlangen & Garboczi 1997, Schlangen & van Breugel 2005, Copuroglu & Schlangen 2007]. It models concrete on a meso-scale in which particles embedded in a cement matrix are taken into account. With the model the concrete expansion can be simulated. One of the inputs in the model is the local expansion of the gel. For that the mechanical properties of the gel should be known. In this paper a test procedure, test results and a method to fit the model-parameters are described.

Recently the model is upgraded to a fully 3D version [Schlangen & Qian 2009]. Procedures to model ASR fracture in 3D materials are presented.

2 MODELING ASR DAMAGE

Heterogeneous materials have complicated fracture mechanisms, which are related to their microstructure. The use of linear elastic fracture mechanics to analytically describe these mechanisms is very hard, since fracture patterns consist of a main crack, with various branches, secondary cracks and micro cracks. To model concrete fracture these models were introduced by Schlangen and van Mier [1992]. Lattice models are now used quite a lot to model concrete crack patterns, mainly because the simulated cracks are very realistic and resemble to a great detail the cracks observed in laboratory tests and in practice. In these models a material is discretized as

a lattice consisting of small beam (or spring) elements that transfer forces.

The meshes used in this paper are 2D regular triangular meshes or 3D square meshes. Other options like random meshes are sometimes preferable, see [Schlangen & Garboczi 1997], however, for the present application the influence of the mesh is small. Each of the beams in the lattice can transfer, in general, normal force, shear force and bending moment. In 3D shear forces, bending and torsion moments in different directions are added. For a lattice with a regular geometry, the quantities for cross sections and stiffness and strength parameters are in principle, equal for all elements. However, these parameters can be varied, either element by element or according to a superimposed microstructure, in order to implement heterogeneity.

To construct the system of equations for the complete lattice, each element matrix has to be multiplied by the appropriate rotation matrix and positioned correctly in the system.

When solving the set of linear elastic equations for a lattice under an applied load, the load vector and stiffness matrix are known and the displacement vector is to be determined. The mechanism of ASR is modeled in this research with this meso-mechanical lattice type model (Delft Lattice model) in which the aggregate structure is taken into account using digitized images of the real material. The simulation of fracture is realized by performing a linear elastic analysis of the lattice under loading and removing an element from the mesh that exceeds a certain threshold. In the present simulations the normal stress in each element is compared to its strength. Details on the elastic equations as well as the fracture procedure of the model are explained in Schlangen & Garboczi [1997] for the 2D version and in Schlangen & Qian [2009] for the 3D version of the lattice model.

3 EXAMPLE OF ASR MODELED IN 2D

ASR damage was characterized in a concrete microbar specimen to be used in the numerical model. Concrete microbar was prepared with aggregates between 4.75 mm and 12.5 mm, dry aggregate/cement ratio of 1.0 by weight and W/C 0.33. Aggregate type was an ASR reactive clinopyroxene-olivine andesite and named as basaltoid in [Garcia-Diaz al. 2007]. Prismatic 40×40×160 mm microbar specimen was cured 1 day in 80°C water and in 80°C 1 N NaOH solution for 14 days. The expansion of the specimen was registered at 0.8% and showed significant cracking. It should be noted that the proposed expansion limit at 30 days is 0.14% for siliceous limestones and 0.04% for other aggregates. Further details of this test can be found elsewhere [Grattan-Bellew et al. 2003, Andic-Cakir et al. 2007].

After accelerated testing thin section prepared from concrete microbar was studied with a Leica DMRXP microscope using polarization techniques. In order to use in the model, the location shown in Figure 1 was selected and an image in florescent mode was captured. ASR damage in the specimen was further characterized using a Philips XL30 ESEM. The instrument was operated at 20kV accelerating voltage, beam current 20mA, 0.5Torr pressure and at 10mm working distance. Typical gel formations and damage patterns are given in Figure 2.
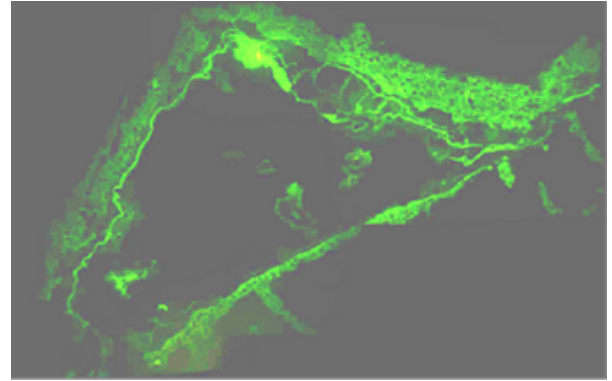

Figure 1. Optical microphotograph of a damaged basaltoid aggregate and surrounding paste due to ASR. The width of the total image with this single particle is in reality 9.66 mm.
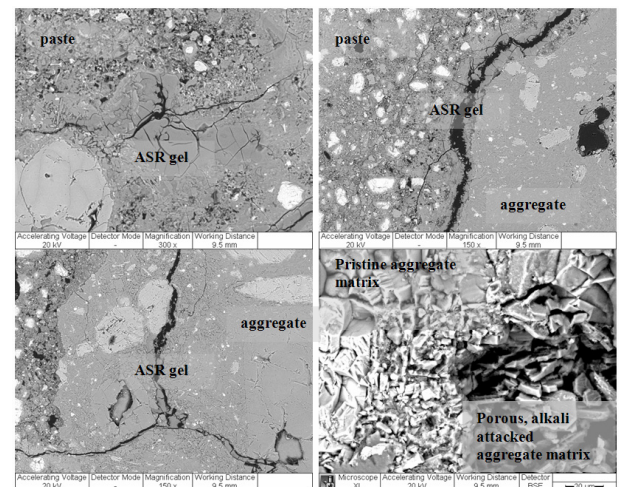

Figure 2. Variations of ASR gel formation and damage. A) Gel formation in the paste B) formation at the interface between aggregate and paste C) in the aggregate. D) Crack can easily develop or penetrate into the aggregate because of extreme dissolution of reactive aggregate matrix (volcanic glass) and its consequently reduced micromechanical properties.

The mechanism of ASR is modelled with the lattice model in which the aggregate structure is taken into account using the digitized images of the real material shown in Figure 1. In the model, the material is discretized as a lattice consisting of 42000 small beam elements.

In Andic-Cakir et al [2007] examples are shown of simulations of larger concrete samples with aggregates in which the swelling of the material is ana-

lyzed by simulating the expansion of either aggregates or interface. In this paper focus is on the mechanism of ASR. Three spots are selected in the sample with a single aggregate in which swelling ASR-gel is placed, i.e. inside the aggregate, inside the interface between aggregate and cement matrix, and inside the cement matrix. The three locations are shown as black dots in Figure 3. It is assumed in the analysis that the ASR-gel in the three locations swells in time with the same rate. The force or expansion is unknown and should be measured as explained in the next section of this paper. Random values are assigned as input parameters for the beam elements in the specific locations for strength (and stiffness). The values are randomly chosen in the range given in table 1. For the stiffness of each element the strength value is multiplied by 10.000.

Three different stages of cracking are shown in Figure 3. The deformations are scaled with the same factor.

Table 1. Strength [MPa] and Stiffness of components used in lattice simulation.

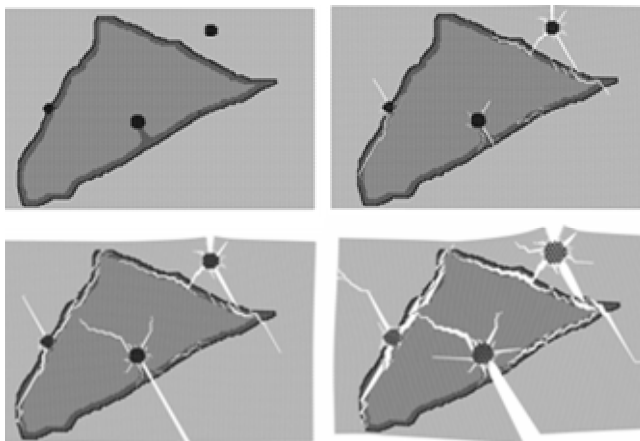|	Aggre-gate	Dissolved rim of aggregate	ITZ	Cement matrix	ASR gel
Strength	7.0-13.0	1.0-2.0	1.5-2.5	3.0-5.0	1.0

Figure 3. ASR damage sequence   (0, 500, 100 and 1500 elements cracked) according to Delft Lattice Model. Gel formations are created in various locations as observed in the microscopy study (see Fig.1 & Fig. 2).

4 MEASURING ASR-GEL PROPERTIES

4.1 *Description of device*

The swelling of the gel is the mechanism that creates the internal damage in the concrete and leads to the expansion of the concrete. As described above there is a need to know the force that is generated by the swelling of the gel, since that is the main missing input parameter for modeling the mechanism of mechanics involved in the ASR process. ASR is a slow process, which means an accelerated test is needed to obtain results in a short period of time. Similar conditions are used as in the accelerated mortar bar tests or concrete microbar tests [Andic-Cakir et al. 2007]. The specimens tested have a cross section of 15x15 mm^2 and a length of 20 mm. To make the specimens first an aggregate particle is sawn to the size of 15x15x10 mm^3. This specimen is placed in a mould and the remainder of the length of the final specimen is filled with cement paste (see Fig. 4). The specimens are cured in the mould for 1 day at 20°C and 99% RH, then they are placed in 80°C water for one day and tested in 80°C 1M NaOH solution for the following test period. Note, that during the testing also further hydration of the cement will have some influence on the results. This will be investigated at a later stage in this ongoing research. To test the specimens they are glued to a stainless steel frame as shown in Figure 4. Note that the steel frame has also a certain stiffness, which can influence the results. It is assumed that the stiffness of the frame is high enough

The steel frame is attached to a micro tensile-compression testing device (developed by Kammrath & Weiss). The shape of the testing frame is such that the specimen can hang inside a pool with the solution at 80°C and that the loading and measurement-parts are outside this pool, see Figure 4. The solution in the pool is covered with a layer of oil to prevent evaporation. The deformation of the specimen is measured with a displacement gauge mounted on to the steel frame. The test can either be run in deformation (zero deformation) or in load control (zero load). In this way it is possible to test the free deformation that will take place due to the ASR formation, but also the stress that is generated if this deformation is restrained. Also different loading regimes are possible, for instance first a restraining of the deformations until a certain stress is reached and after that a free deformation to simulate the situation inside a concrete. Here first a stress has to be created to overcome the strength of the material and then the deformation due to the swelling of the gel can take place.
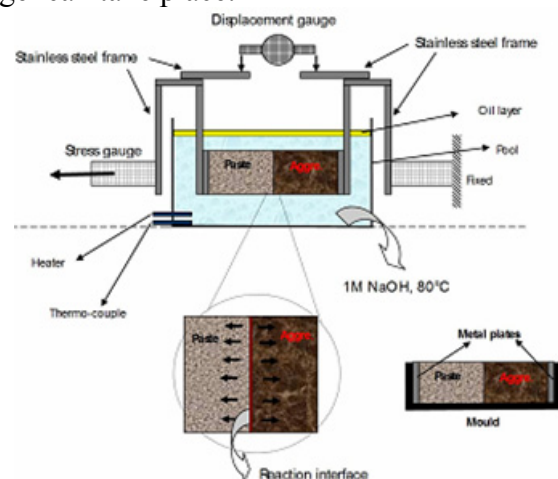

Figure 4. Principle design of device to measure mechanical properties of ASR-gel.

4.2 The first results

The first tests are performed on olivine basalt aggregates, the same material as in the tests on concrete microbars described in section 3. From the chemical composition of the basalt, described in detail in Copuroglu et al. [2007], it was found that the basalt consist of 44% of SiO_2, which makes the material highly reactive. In Figure 5 two typical results are shown. The first result is of a test in load-control, where actually the load is kept to zero and the free deformation is measured in time. In the graph (Fig. 5a) the free deformation of the specimen during the test is given. The measurement in the graph starts, a few hours after the specimen has been submerged into the pool containing the solution, from the moment the temperature in the specimen was 80^oC and the temperature in the frame and the machine reached a stable value. What can be seen is that the specimen elongates during the first 5 days to a total value of about 70 µm.

The second test (Fig. 5b) is performed under deformation control. To be able to control this test properly, first a compression load (of 120 N) was applied to the specimen. Then the system was switched to deformation control (zero deformation). It can be seen in the graph that at first the load decreases due to relaxation. Subsequently the reaction starts, the gel is formed and tries to expand. Because the deformation is restrained, the compression load increases again.
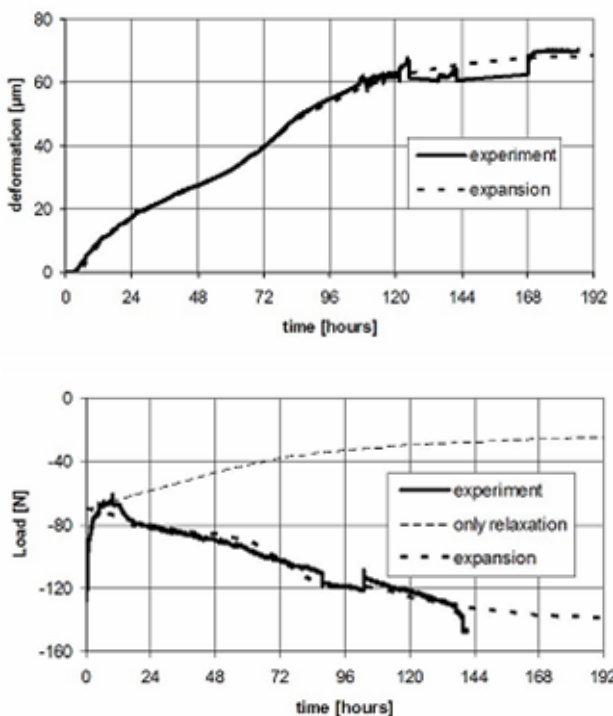

Figure 5. Measured mechanical properties of ASR-gel: Free deformation under zero load (a) and measured load under restrained deformation (b). In the graphs also the simulated results are shown after fitting the input parameters.

4.3 Fitting the ITZ parameters

In this section the procedure is described to fit the ITZ parameters for a 2D model. However in 3D the procedure is similar. In the model it is assumed that the gel is mainly formed in the ITZ between aggregate and cement matrix. It is not important for the model if this is exactly on the boundary between the two or that the expanding gel forms cracks inside the matrix or in the aggregates. The beam elements located in the ITZ just describe the expanding mechanism in this zone. So basically it is assumed that the elements in the ITZ crack, become gel and start swelling. Where exactly this crack starts is not important, it can be in the cement matrix, inside the aggregate or just at the interface between them. It can also be a mixture of cracking on the different phases. Important is only that the zone around the aggregate expands following a certain rate, which is determined from the experiments. To determine the properties of these elements the tests described in paragraph 4.2 are modeled with the mesh shown in Figure 6. In the mesh three different elements are used, i.e. matrix, ITZ and aggregate. The modeling of the first test, the free expansion is simple. The elements in the ITZ are given a strain in time such that the total deformation of the specimen corresponds with the measured deformation. Since the specimen is not restrained, the stiffness of the elements are not of influence. The second test, restrained deformation, is used to determine the stiffness of the ITZ beam elements. In this simulation the strain of the first test is applied to the elements and the stiffness in time is chosen such that the reaction load in the simulations corresponds with the measured load in the test. The stiffness of the beam elements has to decrease in time to have the correct fitting. This stiffness is then a combined stiffness and relaxation of the complete zone around the real interface between aggregate and cement matrix. Thus it includes the gel, but also the maybe partly cracked cement matrix and aggregate.

In Figure 5 the resulting curves of the fitting are compared with the experimental curves. In Figure 5b also the simulated load is plotted versus time in case that there is only relaxation (in the elements) of the initial pre-stressing load on the specimen. This means only a decrease in stiffness in time and no expansion of the elements.

Examples of simulations in which this modeling technique is used can be found in Schlangen et al [2008].
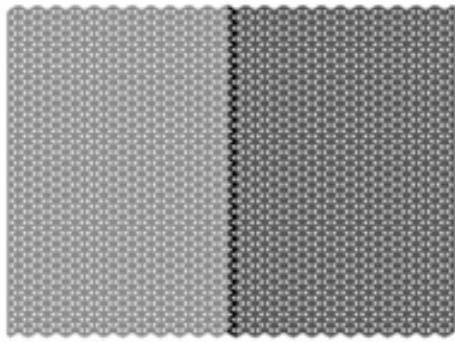
Figure 6. Modelization of specimen with lattice elements to fit gel properties.

5 3D MODELING PROPOSAL

The modeling on 3D is a bit more complicated. The equations of the beam elements have some more comp0nents. The stiffness matrix of a single element is a 12x12 matrix and there are 6 degrees of freedom in each node. The equations are further explained in Schlangen & Qian [2009].

In 2D it is easy to use the real microstructure of the material to implement heterogeneity. The image of figure 1 can for instance be used to decide the properties of the single beam elements. In Andic-Cakir et al. [2007] and Schlangen et al. [2008] an image of a cross section of a specimen containing several aggregates is taken as a starting point. In 3D this is not straightforward. In Comby-Peyrot [2006] 3D generated particles with some kind of irregular shape are used. However these particles still far from real aggregates and also the shape of real particles will depend on the type of aggregate and will vary a lot.

CT-scanning is a useful technique to obtain the shape of real particles. Garboczi [2002] proposed a method to obtain the shape of aggregate particles with CT-scanning and then give a mathematical description of the shape. In this way a database of various shaped aggregate particles can be set up. This database could then again form the basis for a packing program to generate 3D microstructures. However this packing algorithm is not easy and not available yet.

In this paper another approach is used. A number of irregular shaped aggregate particles are mixed together with low density plastic flakes. These flakes actually work as a distance-holder between the particles. The total amount of aggregates in the mix is about 50%. However this can be varied. This specimen is scanned in a CT scanning machine and 3D image is obtained after reconstruction. Using high density particles combined with low density plastic flakes makes the scanning easy. If the aggregates are put in real concrete mix then it is hard to distinguish between cement paste and aggregate particles. A similar trick is used by Schlangen & Qian [2009]

where low density aggregates are used in a concrete to be able to locate the particles in the cement paste.

From the scanned image a digizited voxel image of 40x40x40 mm is cut in which each voxel is a 1 mm cube. The result is shown in figure 7.
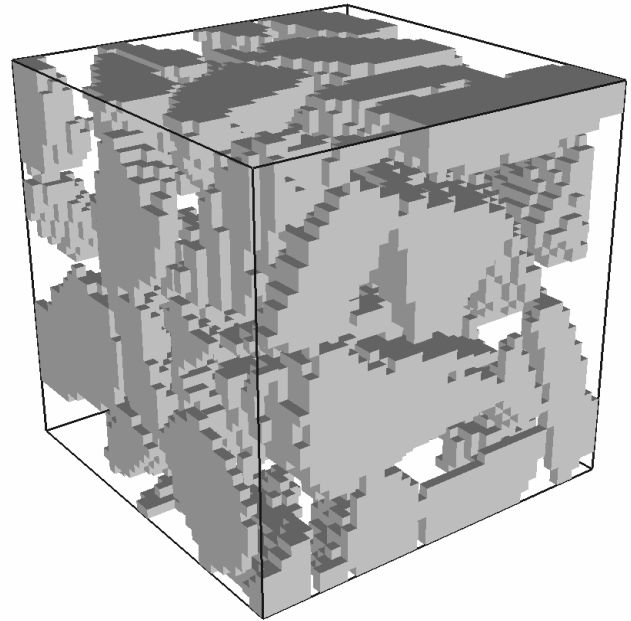

Figure 7. Digitization into 40x40x40 voxel image of CT-scan of aggregates.

On top of this image a square lattice is projected of 40x40x40 beam elements. Subsequently the beams are given properties of aggregate, matrix and ITZ depending of their location as shown in figure 8.
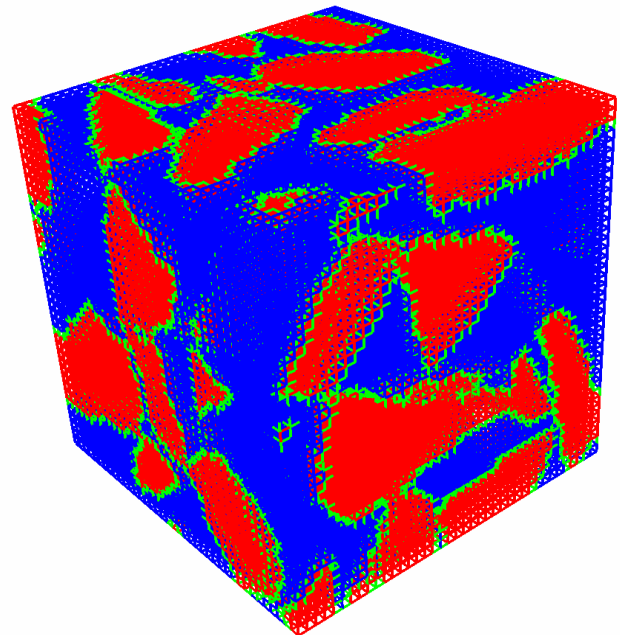

Figure 8. 3D square lattice network of showing aggregates, interface and matrix.

To simulate ASR damage part of the material has to be given an expansion. In Andic-Cakir et al. [2007] and Copuroglu & Schlangen [2007] it was already discussed that is highly depends on the type of

aggregates were the expansion takes place. In some types of aggregates the expansion takes place at the rim of the aggregates, in which case it is better to have the expansion reaction only in the interface elements (green elements in Fig. 9). While in other aggregate-types the total aggregate shows a swelling reaction, which makes it more logical to choose for an expansion in the aggregate (red) elements in figure 9.
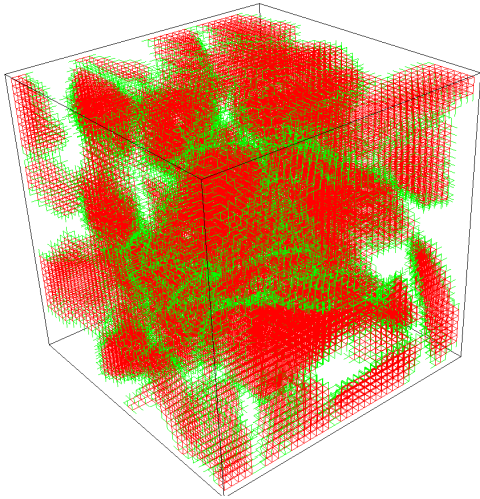

Figure 9. 3D Beam elements of aggregates and interfaces.

Most aggregate, however, have certain parts of the aggregates where the reaction takes place. Some planes insight the aggregate dissolve and the expanding gel is created in this plane after which a crack through the aggregate is formed. An option to implement this in the model is shown in figures 10 and 11. Here a 3D skeleton operation is performed on all the aggregates. The result of this that only major planes inside the aggregate are left after this operation. Giving these elements an expansion in time is most probably more realistic. The amount of expansion in time can be obtained from tests as discussed in section 4.1.
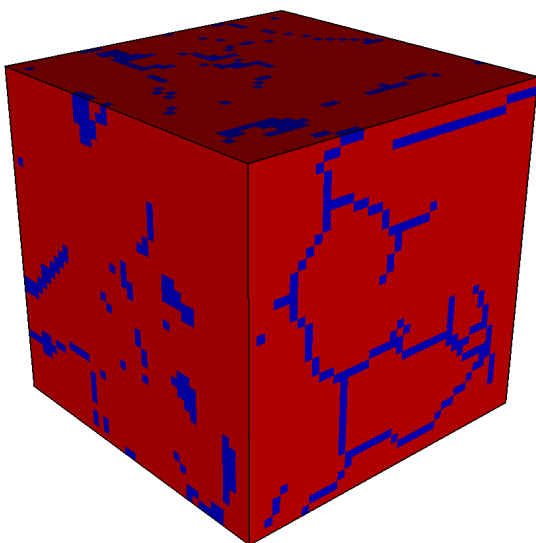

Figure 10. Cube showing aggregates at surface after performing a skeleton function on the aggregate particles.
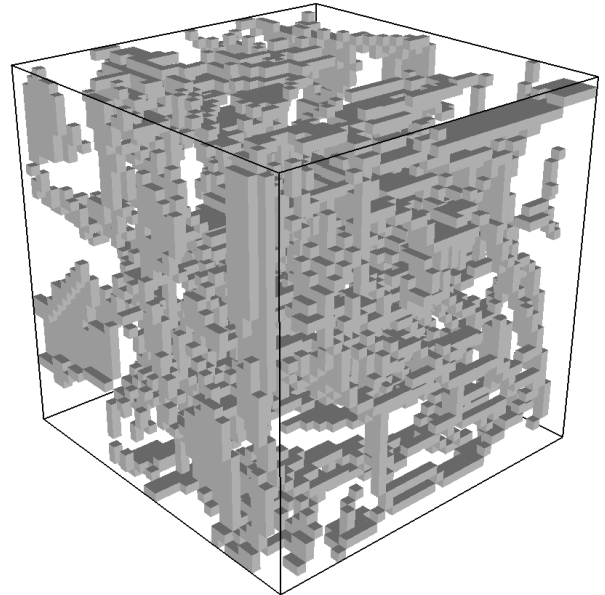

Figure 11. Cube showing aggregates voxels after performing a skeleton function on the aggregate particles.

An example of a simulation is shown in figure 12. This image shows a deformed and cracked 3D specimen. In the simulation only the interface elements are given an expansion in time.
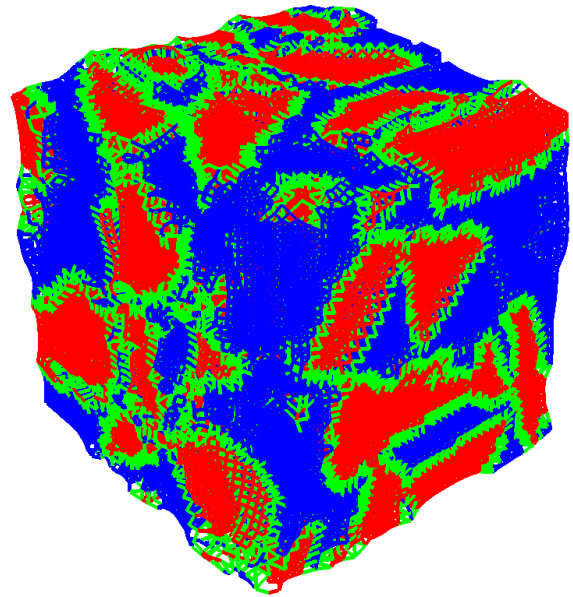

Figure 12. Deformed and cracked cube in lattice analysis in which ITZ-elements expand.

6 CONCLUSIONS

In this paper a model is presented to simulate expansion of concrete due to ASR. The model is a meso-mechanical model that takes the heterogeneous microstructure of concrete in 2D as well as 3D into account. The input for the model is the expansion of ASR-gel formed in at the boundary zone between aggregates and cement matrix. The expansion of the

gel is measured in a new test device. In this machine the expansion of gel formed in a single interface is measured. This is different from deformation measurements on mortar or concrete specimens that usually are performed to determine the expansion due to ASR of the material.

The stiffness including the visco-elastic behaviour of the gel is determined from measurements in the same device from tests with restrained deformation. Not only the visco-elastic behaviour of the gel is determined in this way, but actually the visco-elastic behaviour of the zone in which the gel is formed and (micro-)cracks occur. In literature also tests are reported in which the pressure is determined that develops in mortar and concrete specimens in which ASR takes place [Ferraris et al. 1997, Kawamura & Iwahori 2004]. However in these tests the complete material with many interfaces is tested. In these tests there is an external restraining from the test-setup, but also an internal restraining from the material (cement paste) itself. This makes the interpretation of the results very complicated. In the test setup used in the research presented in this paper, only one interface, one location where gel is formed and therefore also only one location where pressure builds up is present in the specimen. Which means it is a direct measurement of the properties.

After fitting the properties of the ITZ-elements from the experiments the model can be used to simulate expansions in real concrete samples.

It is the opinion of the authors that the procedure described in this paper can also be used to determine and predict the expansions in different concretes, with different aggregates. It should also be noted that the mechanism of ASR can be different for different aggregates. For the basalt aggregates used in this research it is known that they dissolve from the outside to the inside, which means that the gel formation and the expansion reaction take place at the rim of the aggregates. In other type of aggregates, i.e flint, it is known that the reaction takes also place inside the aggregate particles, which leads also to different fracture characteristics of the concrete. Further measurements to support this are ongoing. It can also be analysed which matrix strength or strain capacity is needed to be able to lower the strain or delay the expansion in the material so much that it does not lead to deterioration of the structure. In Ostertag et al. [2007] it is shown that this approach can be successful by adding micro-fibres to the matrix to enhance the strain capacity and with that decrease the rate of the alkali silica reaction.

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