Formation of eigenstress and cracks due to autogenous shrinkage

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ABSTRACT: Numerical modelling on the micro and meso-level of concrete is presented. The formation of the microstructure, including the matrix and the interfacial transition zones between aggregate particles is modelled explicitly on the micro-level. The outcome of these simulations are used in a meso-level model (lattice model) to study the formation of (micro-)cracking in concrete consisting of particles embedded in a matrix. The different matrix and interface properties as well as the level of restraining of deformations is included in these simulations. Three concrete mixes with different water-cement ratio are investigated. A lower w/c shows more autogenous shrinkage, higher eigenstresses and thus a higher tendency for cracking. From the simulations it is found that eigenstresses caused by autogenous shrinkage reduce the tensile strength of the concrete. However, it is also concluded that the local material properties are very important and influence the outcome of the simulations to a large extent

Keywords: fracture simulation, autogenous shrinkage, lattice model, multi-scale modelling, eigenstress

1 INTRODUCTION

The basic properties of the concrete are already formed during the development of the microstructure when the concrete hardens. During the lifetime of the structure these properties will change due to impact of various mechanisms. The development of the microstructure of concrete will be different if comparing the bulk part of the structure and the material in the cover zone. Wall effects, large particles will not be present at the surface, and also temperature and moisture variations during hardening will influence the formation of the microstructure in the cover zone. As a result, the properties of the concrete in the cover zone and the core of a structure are completely different. The concrete properties are also a function of the water-cement ratio (w/c). Lower w/c gives higher stiffness and strength. On the other hand it also leads to more internal shrinkage.

In this paper one aspect of the formation of the microstructure is investigated, i.e. the internal shrinkage and the resulting eigenstresses. During the hydration moisture will move trough the microstructure, simply because of variations in packing density close to aggregate particles and matrix. This movement of moisture will lead to autogenous shrinkage and also will influence the hydration and local mechanical properties of the material. Modelling of this mechanism on the micro-level is performed with HYMOSTRUC (van Breugel 1991).

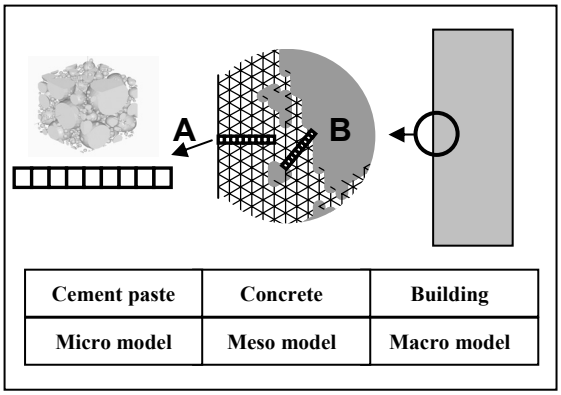


Figure 1. Schematic representation of micro- meso- and macro-level modelling.

The outcome of this simulation is used as input in the lattice model developed at Delft University to simulated fracture (Schlangen & van Mier 1992). The lattice model acts at the meso level (Fig 1). The model is extended in order to be able to apply internal loading which varies in time and study the development of eigenstresses and progressive damage (Schlangen et al. 2003).

The outcome of the meso model could be used to derive material properties for modelling concrete as a homogeneous material to analyse building elements on a macro level (van Beek & Schlangen 2000).

2 TOWARDS MODELLING MICROSTRUCTURE

The microstructure of a cement paste consists of a network of hardening cement particles that are glued together by a variety of hydration products. Modelling this kind of structure formation requires a broad scale of mathematical formulations and numerical techniques. At Delft University of Technology, a numerical simulation model has been developed, called HYMOSTRUC (van Breugel 1991), which has the potential to calculate the hydration process of cement-based systems. This model takes into account the formation of the interparticle contacts in the hardening cement paste matrix. In the model hydrating cement particles are considered to grow gradually in outward direction.

In the HYMOSTRUC model, on contact with water an arbitrary cement particle starts to dissolve under formation of reaction products. These products are formed partly inside and partly outside the original surface of the cement particle. The outward growing hydration product makes contact with neighboring particles. Ongoing hydration of the particles goes along with ongoing expansion and even embedding of neighboring particles. The embedding of other particles causes an extra expansion and, as a consequence, embedding of even more particles. An algorithm has been developed for the expansion mechanism of continuous expansion and embedding of particles through which the stereological aspect of micro-structural development can be simulated.

The original modelling work was based on a homogenous distribution of the particles in cement paste. In later work the model has been extended to include randomly stacked particles in a predefined envelope shape, representing an initial cement paste system. The hydration algorithm of the extended HYMOSTRUC 3D model (Koenders 1997) is now applied to the randomly stacked particles, calculating the growth of the particles as hydration proceeds. This forms the basis for the so called ribbon model. The extended model also provides information about the capillary pore structure that remains after hydration of the cement particles through the inverse space that remains from a hydrating cement paste volume. This pore structure is the basis for the moisture transport calculations that determined the movement of capillary water through the hardening cement paste system during hardening.

3 THE RIBBON MODEL

The ribbon model is a three-dimensional model for simulating cement paste between two aggregate particles. Going from a concrete level to a modelling level (Fig. 2), the hardened cement paste between two aggregates can be represented by a tubular volume, or ribbon. The way of simulating the microstructure in this ribbon is based on a cement paste volume in which spherical cement grains are stacked randomly in a tubular volume.

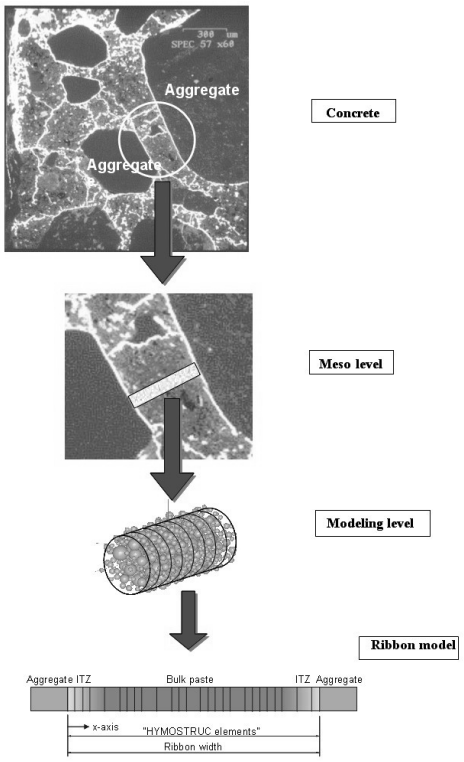


Figure 2. Overview of the ribbon model, (Koenders et al. 2003).

The initial distribution set up this way is, in fact, a representation of the initial stage of the mixed water-cement emulsion (cement particles in the aqueous phase). The tubular volume is then subdivided in slices, each of them having a certain water-cement ratio, obtained by dividing the amount of water present in the slice by the amount of cement present in that slice. For each slice the hydration process can be simulated with the HYMOSTRUC software, starting with the initial water-cement ratio of the slice in view.

The generated initial microstructure can be characterized by its geometrical properties, like water-cement ratio or paste density. This reflects the distribution of the cement grains over the ribbon width, while taking into account the packing restrictions at the regions close to the aggregate surface. The HYMOSTRUC simulations for each of the subsequent slices of the ribbon provide information about the evolution of the microstructure and the associated moisture movements in the subsequent slices. This might influence the microstructural properties like porosity, permeability etc. and influence the movement of moisture during hardening.

The movement of capillary water through the hardening cement paste system is explicitly modelled within the HYMOSTRUC 3D model (Koenders et al. 2003). As hydration proceeds, water is chemically and physically bounded to the cement while forming hydration products that contribute to the development of a load bearing microstructure. Capillary water is consumed and taken out of the system, causing unbalances in the capillary surface tensions. These unbalances are forcing capillary water to move from the water-rich area's (e.g. ITZ) towards the water lacking area's in the central parts of the cement paste ribbon matrix. This process redistributes the capillary water in the paste, while influencing the materials properties development.

In addition to this, the volumetric changes of the hardening cement paste system will be affected as well. Using the phenomenological relation of Bangham (Koenders et al. 2003), the shrinkage of the ribbon paste could be quantified. The autogenous shrinkage for the mix with w/c is equal to 0.3 is plotted at three stages in the hydration process in figure 3. The results of the simulations for the three mixes (w/c=0.3, 0.4 and 0.5) are presented in figure 4, where the autogenous shrinkage and the development of E-modulus is plotted after 20 hours of hydration. The mix with the lower w/c shows the highest shrinkage. From figure 3, it can be observed that at the ITZ the shrinkage is larger, leading to larger microstructural deformation close to the aggregates. The denser packing in the central bulk paste is causing a slight increase of the shrinkage in that particular region. It appeared that a denser initial particle structure is causing higher internal pore pressures, causing larger potential deformations, but that on the one hand, these deformations are opposed by the higher elastic modulus (Fig.4).

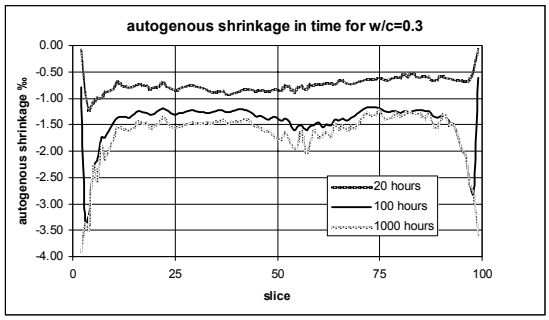
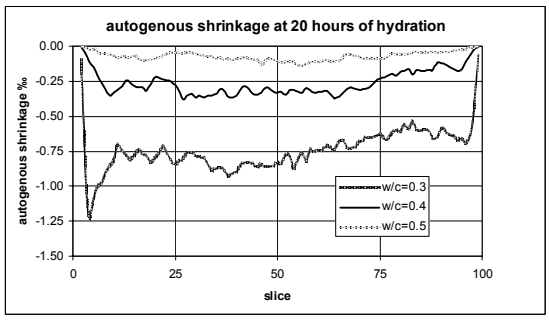


Figure 3. Autogenous shrinkage for mix with w/c=0.3 at three stages of hydration: 20, 100 and 1000 hours.



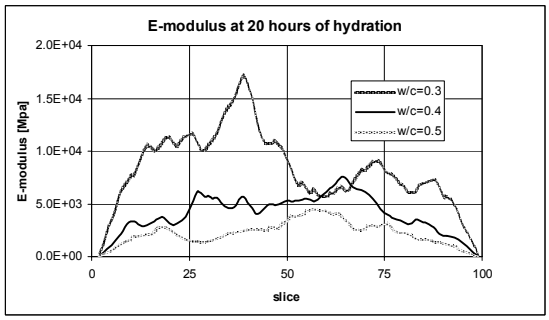


Figure 4. Autogenous shrinkage (top) and development of E-modulus (bottom) after 20 hours of hydration for three mixes, with different w/c.

4 MODELLING FRACTURE ON A MESO-LEVEL

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 the fracture patterns consist of a main crack, with various branches, secondary cracks and microcracks. To gain some more insight into the problem the use of numerical tools is a good option.

Studies in theoretical physics indicated that lattice type models can be quite successful for the simulation of fracture processes in heterogeneous materials, see, for instance (Herrmann & Roux 1990). These models were adopted for specific applications such as to simulate fracture in concrete, see, for instance, (Schlangen & van Mier 1992, Bolander & Saito 1998, Ince et al. 2003). In these models a material is discretized as a lattice consisting of small beam (or spring) elements that can transfer forces, see Figure 5.

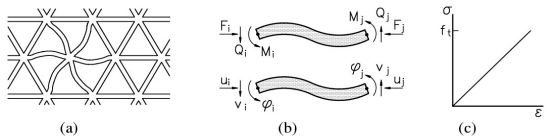


Figure 5. Lattice of beam elements (a), definition of forces and degrees of freedom (b), stress-strain relation of beam element (c).

The simulation of fracture is realized by performing a linear elastic analysis of the lattice under loading and removing (or partially removing, see Ince et al. 2003) an element from the mesh that exceeds a certain threshold, for example strength, strain or energy. The results that are obtained from simulations with lattice models, however, depend strongly on the used fracture criterion and the chosen element and/or mesh type. To obtain realistic results it is important that the relation between the implemented disorder in the model and the heterogeneity of the material that is to be simulated is as close as possible. Details on the elastic equations as well as the fracture procedure of the model are explained in (Schlangen & Garboczi 1997). In this reference also a description of the fast conjugate gradient solver implement in the Delft Lattice Model can be found.

In the present paper a fracture criterion based on normal force in the beams only is adopted. Various fracture criteria are used in the past, all having pros and cons (van Mier 1997).

In previous application of the lattice model mostly fracture of materials was studied due to an external loading or deformation on a specimen. Now attention is focused on the simulation of eigenstresses that develop in the material as a result of autogenous shrinkage. The simulation is performed in time. The time steps, development of E-modulus and shrinkage are taken from the ribbon model described in the previous section. The meshes (regular triangular lattices) shown in figure 6 are used in the simulations. The 2D meshes have a total width and height of 600 μm. They consist of circular aggregates with diameters between 40 and 200 μm embedded in a matrix. The size of the beam elements in the mesh is 8 μm. The average distance between the particles, the width of the matrix, is 100 μm. This corresponds with the size of the ribbon in the ribbon model. The ITZ (arbitrarily taken a width of 15 μm) is plotted in a different color just to distinguish between aggregate and matrix. In reality the material (matrix and the two ITZs) between aggregates is modelled as a continues matrix as explained below.

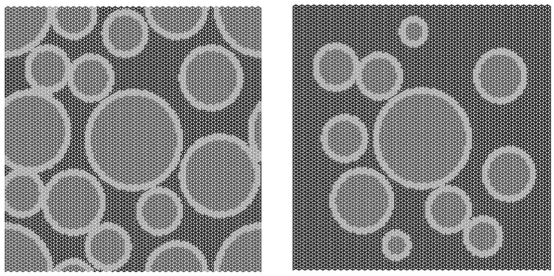


Figure 6. Lattice meshes used; periodic boundary lattice (left), free boundaries (right).

The aggregate is given a stiffness of 70 GPa and a strength of 10 MPa. The matrix is given the stiffness according to the E-modulus in the various slices obtained from the ribbon model, shown in figure 4. The elements close to the particles get a lower stiffness and the elements far away from the particles a higher stiffness. In every time step the stiffness is increased. Relaxation is taken into account by assuming that 50% of the stress that occurs in the elements relaxes immediately. Time effects should be taken into account. Further research is required to study this effect on a local scale. The tensile strength (f_t) is taken proportional to the stiffness values ($f_t = E/10000$).

In the simulation of autogenous shrinkage, the loading that is applied on the mesh is the internal shrinkage of the matrix in every time step that followed from the ribbon model. After applying the strain on the mesh the deformations are allowed to relax (Schlangen & Garboczi 1997). For all the beams the ratio of stress/strength is calculated. The beam element that has the highest ratio, and in addition a ratio higher than 1, is removed form the mesh. Next, the deformations are allowed to relax again, after which the next beam is removed. This procedure is repeated until all beams have a ratio of stress/strength lower than 1. Then the timestep is increased and the stiffness, strength and strain of all the beams are adjusted. This procedure is repeated for all time steps.

5 ANALYSES WITH LATTICE MODEL

5.1 *Simulation of shrinkage*

Simulation of autogenous shrinkage is carried out on the lattice with periodic boundary conditions. This case represents the situation in which deformations of the material are fully restrained (like in an infinitely large specimen, or specimen with external restraining).

Applying the shrinkage of the matrix to the mesh results in cracking as shown in figure 7. Due to the low stiffness of the elements in the ITZ close to the particles, at this spot localization of the deformations takes place.

Eigenstresses are the result of restrained deformations. The strength of the elements determines the formation of cracks. In the case of the low w/c (w/c=0.3) first crack localization in the ITZ occurs already in the early time steps (after 2 hours of hydration). After about 50 hours of hydration localized cracks in the matrix form, which splits the mesh in several parts (Fig. 7a). In the simulation of the mortar with w/c=0.4 cracking of the ITZ starts at a later stage, after 12 hours and localization of cracking in the matrix is also found after 50 hours (Fig. 7b). For the mix with w/c=0.5 after 1000 hours of hydration only some cracking in the ITZ occurs and no failure of the matrix is found. Experimental evidence of cracking of concrete with low w/c caused by autogenous shrinkage can be found in many references, see for instance Baroghel-Bouny & Aïtcin (2000).

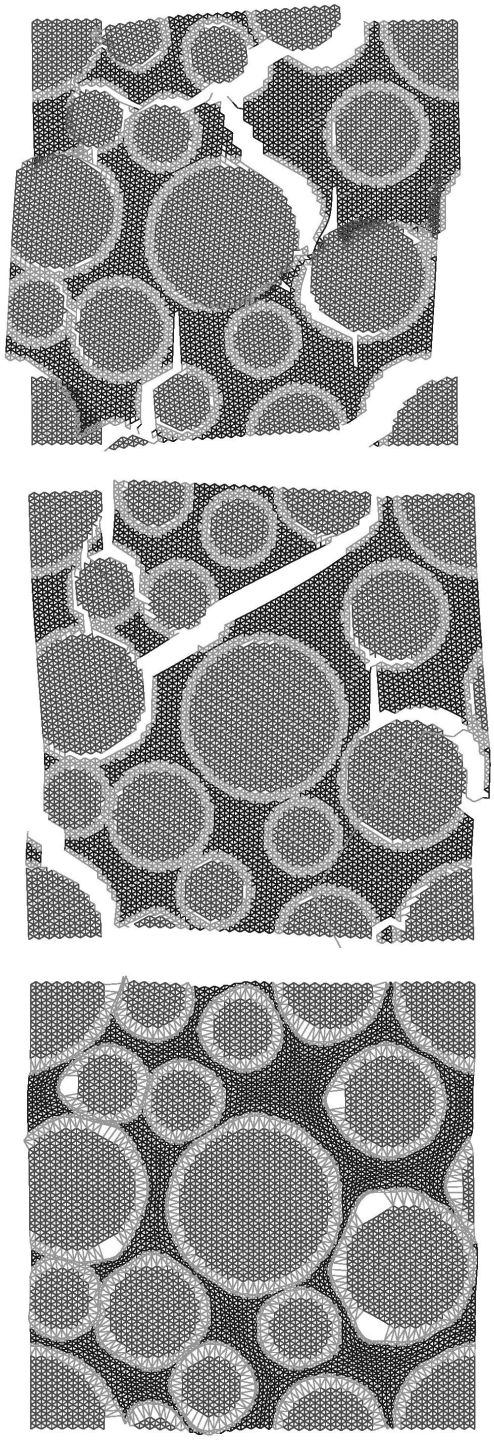


Figure 7. Cracking due to autogenous shrinkage in full restrained lattices (periodic boundaries); w/c=0.3 (top), w/c=0.4 (middle), w/c=0.5 (bottom).

5.2 *Simulation of tensile loading*

On the mesh with free boundary conditions a tensile loading is applied. The mesh is stretched in the horizontal direction. Fracture is simulated according to the cracking procedure in Schlangen & Garboczi (1997). Simulations are carried out for three mixes and at three ages (20, 100 and 1000 hours of hydration).

The results are plotted in figure 8-10. In figure 8 the load-deformation curves obtained after 20 hours of hydration for the three mixes are shown. The total deformation of the mesh is plotted in the graphs, which results in snap-backs in the descending branch.

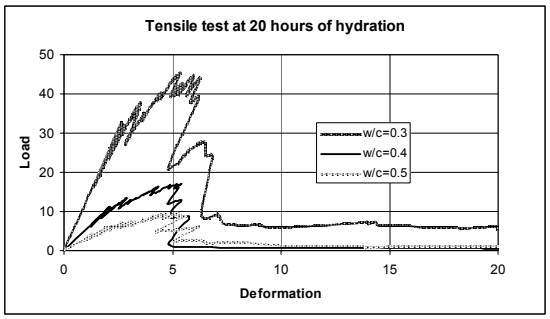


Figure 8. Load deformation curves in tension after 20 hours of hydration for 3 mixes.

Figure 9 gives the fractured meshes at pre-peak, peak load and at the end of the softening curve for the mix with w/c=0.3 and at 20 hours of hydration. However the cracking in the other simulations, with different w/c and at different ages show comparable crack patterns.

Figure 10 shows the development of the tensile strength in time for the three mixes. In the graph the peak loads obtained at the three hydrations times (20, 100 and 1000 hours) are plotted.

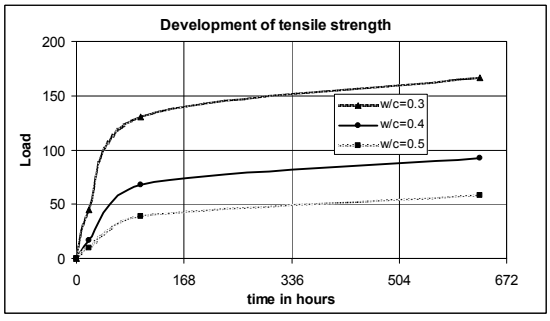


Figure 10. Development of tensile strength in time for 3 mixes.

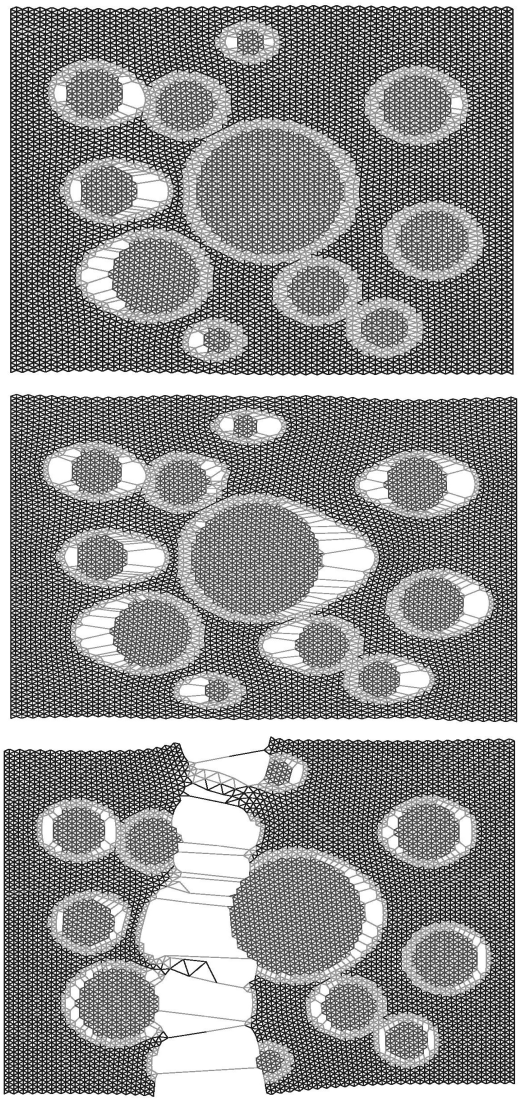


Figure 9. Simulation of tensile fracture; pre-peak (top) at peak load (middle); post-peak (bottom).

5.3 *Influence of eigenstress on strength*

Autogenous shrinkage of concrete that is not externally restrained does not lead to stresses, since the material can deform freely. However, internally stresses will develop. Stiff aggregates restrain the shrinking matrix. The aggregates will be compressed (Dela & Stang 2000, Stang & Ostergaard 2003). In the matrix, however, also tensile stresses will be develop as a result of the autogenous shrinkage. The tensile stresses

(eigenstresses) found with the lattice model in the three mixes after 20 hours of hydration are shown in figure 12. The light colors represent tensile and the dark colors compressive stresses.

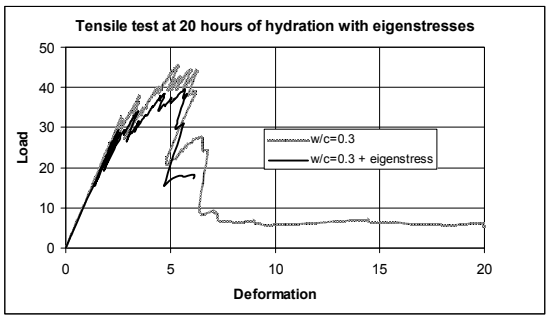


Figure 12. Load deformation curves for tensile test with and without eigenstress for w/c=0.3 after 20 hours of hydration.

The tensile eigenstresses introduce micro cracking in the ITZ in case of the low w/c (w/c=0.3). Due to these micro-cracks in combination with the eigenstresses the tensile strength is reduced by 15 % in case of w/c is equal to 0.3 (see Fig. 11). This is found from a tensile test simulation which is performed on the mesh after the eigenstresses due to autogenous shrinkage (Fig. 12a) are calculated. For higher w/c the reduction in tensile strength is less. For w/c is equal to 0.4 only a few percent an d for w/c is 0.5 no change in tensile strength is found. Note that these simulations are only performed after 20 hours of hydration. At other time-steps the results can be different. Shrinkage, stiffness and strength change with ongoing hydration. The change is not proportional for all the elements located in the different slices of the ribbon between aggregates. Furthermore, the difference between matrix and aggregates changes, because the properties of the aggregates do not change with hydration.

6 DISCUSSION AND CONCLUSIONS

In the paper simulations on two levels of concrete are presented. The outcome of a lower level is used as input at a higher level. Modelling the complete process of formation of microstructure, building up of eigenstresses, formation of local damage and structural performance in a single model is still not possible due to computational limitations.

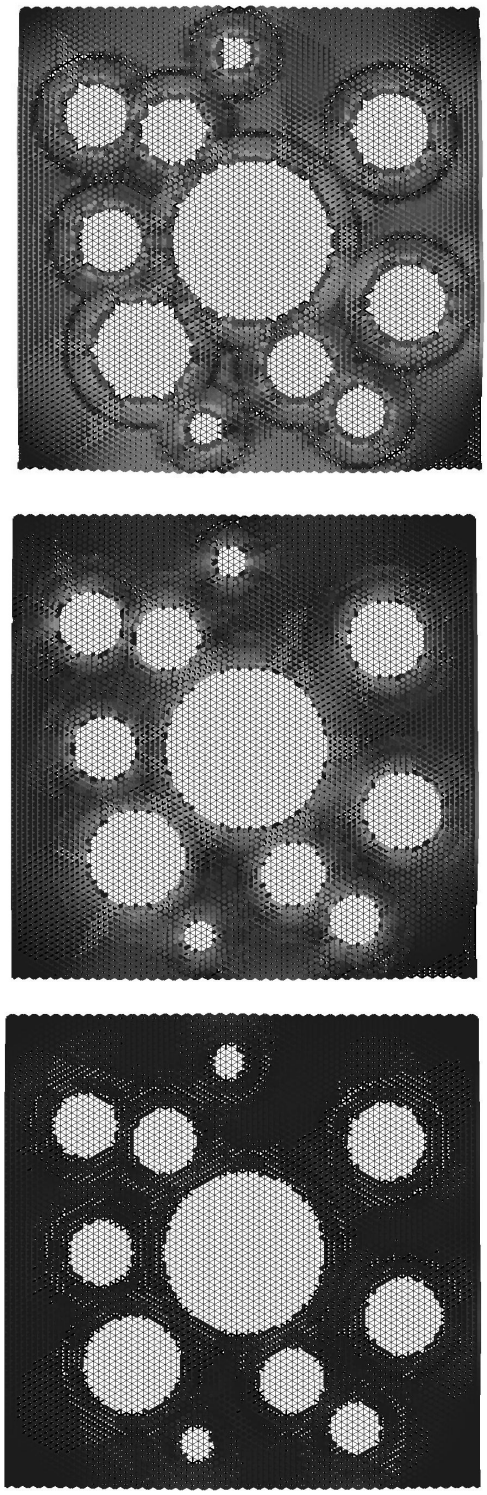


Figure 11. Eigenstresses in matrix after 20 hours of hydration; w/c=0.3 (top), w/c=0.4 (middle), w/c=0.5 (bottom); light colors = tensile stress, dark colors = compresive stress.

However, it will also be not practical. Zooming in on a level and studying the processes in more detail will increase the insight in the mechanism taking place.

The formation of the microstructure with HYMOSTRUC and the movement of moisture with the ribbon model resulted in local information of stiffness and strain in ITZ and matrix. Simulations for three mixes with different w/c are performed. Lower w/c gives higher autogenous shrinkage, but also higher stiffness and strength.

This information is used as input in the lattice model to study deformations, eigenstresses and damage. The simulations with the lattice model have shown that autogenous shrinkage leads to cracking already at an early stage of the hydration for mixes with a low water cement ratio. Condition is the restraining of the deformations. A requirement for this to happen is the full restraining of deformations. In the case of free boundaries, however, internally a restraining will be present due to the stiff particles embedded in the matrix, which leads to (tensile) eigenstresses in the matrix. Furthermore, some eigenstresses in the material will always be present. This can either be externally or internally by temperature or moisture gradients or expanding mechanisms due to chemical reactions in the material. The tensile strength is reduced by these eigenstresses and thus the material has a lower load bearing capacity.

Cracks patterns as found in this study are of course found in many experimental investigations. Examples can be found most probably elsewhere in these proceedings. However the exact shape of the crack patterns (ITZ or localized matrix cracks) depends on the amount of eigenstress and the local properties, such as strength, stiffness and relaxation. The determination of local properties will be investigated in an experimental program which is currently being set up in the microlab.

In the simulations it is further assumed that bonds which break in the mesh will always form a crack. If these cracks are formed at an early stage of hydration, there is a chance that due to ongoing hydration and formation of microstructure these cracks will heal. The strength, stiffness but also the amount of shrinkage at these locations is then unknown and needs further research.

REFERENCES

Baroghel-Bouny, V. & P.-C. Aïtcin (eds) (2000), Shrinkage 2000, Rilem PRO 17.

Beek, A. van & Schlangen, E. (2000), Simulating the effect of shrinkage on concrete structures, in V. Baroghel-Bouny & P.-C. Aïtcin (eds), Shrinkage 2000, Rilem PRO 17, pp. 477-492

Bolander, J.E. & Saito, S. (1998), Fracture analysis using spring networks with random geometry, *Engineering Fracture Mechanics*, 61, (5-6): 569-591.

Breugel, K. van (1991), *Simulation of hydration and formation of structure in hardening cement-based materials*, PhD thesis, Delft University of Technology, Delft, The Netherlands.

Dela, B. & Stang, H. (2000), Two dimensional analysis of crack formation around aggregates in high-shrinkage cement paste. *Eng. Fracture Mech.*, 65**:** 149-164**.**

Herrmann, H.J. & Roux, S. eds (1990) *Statistical models for the fracture of disordered media*, Elsevier/ North Holland, Amsterdam.

Ince, R., Arslan, A. & Karihaloo, B.L., (2003), Lattice modelling of size effect in concrete strength, *Eng. Fracture Mech.* 70: 2307–2320

Koenders, E.A.B., (1997), *Simulation of volume changes in hardening cement-based materials*, PhD-thesis, Delft University of Technology, Delft, The Netherlands.

Koenders, E.A.B., Ye, G. & van Breugel, K. (2003), Numerical simulation of moisture flow through hardening cementitious cover, in F.A. Finger (ed.), proc. *IBAUSIL*, September 24-27, Weimar, 2: 917-926.

Mier, J.G.M. van (1997), *Fracture processes of concrete*. New directions in civil engineering. CRC Press, Boca Raton: 448.

Schlangen, E. & van Mier, J.G.M. (1992), Experimental and numerical analysis of micromechanisms of fracture of cement-based composites, *Cem. Conc. Composites*, 14: 105-118.

Schlangen, E. & Garboczi, E.J. (1997), Fracture simulations of concrete using lattice models: computational aspects, *Eng. Fracture Mech.*, 57(2/3): 319-332.

Schlangen, E., Koenders, E.A.B. & van Breugel, K. (2003), Multi-scale modelling of crack formation in the concrete cover zone, in D.A. Lange et al. (eds), *Advances in cement and concrete*, Proc. ECI conference, Copper Mountain, Co, August 10-14, 281-291.

Stang, H. & Ostergaard, L.(2003), Cracking and fracture in early age concrete, in D.A. Lange et al. (eds), *Advances in cement and concrete*, Proc. ECI conference, Copper Mountain, Co, August 10-14, 257-268.