Simulation of concrete fracture by using mesolevel truss and particle models

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ABSTRACT: In order to study the influence of the concrete composition and the loading conditions on the material behavior, fracture processes were simulated on the mesolevel. For generating the mesolevel concrete structure consisting of aggregate particles and the surrounding mortar matrix a new stochastic-heuristic algorithm has been developed. The algorithm attains comparably high aggregate contents in 2D as well as in 3D models. Two approaches for simulating cracking were used. A 2D particle model based on linear-elastic fracture mechanics allows to separately investigating some influences of the concrete composition on the fracture process under compression. Furthermore, compression as well as direct tension tests have been simulated using 2D and 3D truss models. In addition, 2D simulations of wedge splitting tests were carried out. For describing the element behavior, different non-linear constitutive relations were applied. Steel fiber reinforcement was modeled by introducing additional truss elements into the mesh.

Keywords: concrete, mesolevel, particle model, truss model, steel fibers

1 INTRODUCTION

For studying the influence of the concrete composition on the macroscopic properties mesolevel models have proved to be applicable. On this structural level, the material is modeled as a three-component system consisting of the coarse aggregate particles, the surrounding homogeneous mortar matrix and the interfacial transition zones between them. Phenomenological models describing the concrete as a homogeneous material nowadays allow to realistically simulating fracture processes but do not account for the effects of the concrete composition on the macroscopic material behavior. For deeper understanding of the physical processes determining the macroscopic material behavior, models considering the inhomogeneous nature of concrete are required.

In the study presented here, two different approaches for simulating cracking on the mesolevel were used. A fairly simple 2D particle model based on linear-elastic fracture mechanics was utilized for investigating influences of the concrete composition on the fracture process under compression. Furthermore, 2D and 3D truss models were applied for simulating compression as well as tension tests. In extensive parametric studies, the models have been tested and optimized. Experimental observations on mechanical concrete properties could be confirmed by the simulation results (Slowik & de Barros Leite 1999).

This study presents a comparison between the different approaches by evaluating the applicability of the different models, and proposes some model improvements and refinements.

2 GENERATION OF MESOLEVEL MODELS

Mesolevel models require the generation of the aggregate-mortar structure in realistic way. Corresponding generation algorithms should, therefore, fulfill the following requirements:

- a) Location, also shape and size, of the aggregate particles should be determined at random;
- b) Spatial aggregate distribution should be uniform;
- c) Given content and size distribution of the aggregates should be exactly matched;
- d) Aggregate contents as high as in the real concrete should be achievable.

The first requirement implies the usage of a random generator. For fulfilling requirement c) it is recommended generating all the particles first and

then, in a second step, placing them in the test volume. In this way, the specified aggregate content as well as the size distribution can be exactly matched. Furthermore, this approach conforms to the making of real concrete. The last requirement is the most problematic.

A trivial way of placing aggregate particles in the test volume is to obtain their locations purely at random. When a particle is placed partially outside of the test volume or when it is overlapping previously allocated particles the trial location is dismissed and a new one is obtained. Although the simplicity of such a scheme is fairly attractive, the efficiency is very poor. Such mechanisms are only capable to achieve comparably low aggregate contents, and the approach is extremely redundant and time-consuming. The resulting mesolevel structure is a very coarse idealization, which in general does not resemble the real concrete.

Vervuurt (1997) used an improved mechanism that simulates a process in which circular particles are dropped into a mould. When a particle reaches a minimum distance to at least one of the previously allocated particles, the location is fixed. By simulating the "falling" process of a particle several times and taking the deepest position found, the reachable aggregate content may be increased. A disadvantage of this effective algorithm is that the aggregate content cannot be exactly predetermined. Another possibility of generating an aggregate-mortar structure is to discretize the test volume or test area similar to a finite element meshing. Then, the particle volumes/section areas are shrunk forming the matrix structure (Stankowski 1990). Hence, in theory, aggregate contents near to 100% may be achieved. However, the obtained mesolevel structure is quite different from those in real concrete samples.

A new algorithm for generating a realistic aggregate-matrix structure is proposed here. The stochastic-heuristic scheme for allocating the aggregates, which has been embodied in the algorithm, allows generating aggregate contents comparable to the ones in real concrete and equivalent spatial distributions. In addition, the generation mechanism successfully meets all other requirements outlined above.

Before placing the aggregate in the test volume the whole set of particles is generated according to the given aggregate content and size distribution. The aggregate particles are designed as ellipsoids and by controlling the ratio between their three middle-axes a variety of different shapes may be obtained. The placement of the particles is performed successively starting with the largest ones. Initially, a random position of the particle is obtained. If the particle is completely inside the specimen and does not overlap previously placed ones the position is fixed. Otherwise, the particle is shifted or rotated in order to get away from the specimen boundary or overlapping particles. If this does not solve the conflict new movements are attempted. Direction and magnitude of the movement are calculated by using a certain algorithm, which will be described in a separate publication.

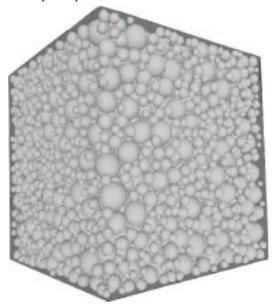


Figure 1. Three-dimensional mesolevel model (maximum aggregate size 16 mm, minimum aggregate size 4 mm).

In the real process of placing and compacting concrete the particles hit each other and bounce back until they have reached their final position. Therefore, the proposed mechanism of placing the particles is more realistic than a purely random procedure.

Figure 1 shows a 3D mesolevel model created by using the proposed stochastic-heuristic algorithm. The maximum ratio of the smallest to the largest half axis of the elliptical aggregate particles amounted to 0.9, i.e. the particles were nearly spheres. For a minimum particle size of 4 mm the maximum aggregate volume contents which could be reached were 52 % for a maximum aggregate size of 16 mm, 61 % for 32 mm and 66 % for 64 mm. By using a personal computer the model generation can be accomplished within a few minutes. Two-dimensional concrete models are easily obtained by slicing three-dimensional models. The resulting sections of the aggregate particles are elliptic.

A first version of the proposed algorithm has been used for creating 2D mesolevel models with polygonal aggregate particles (see Fig. 2). Such models are required for the simulations described in the next section.

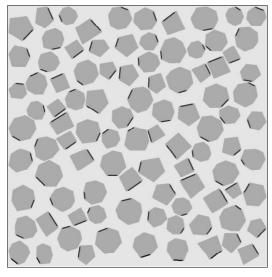


Figure 2. Two-dimensional mesolevel model (aggregate content 45 %, maximum aggregate size 16 mm) with initial cracks.

3 PARTICLE MODEL

Zaitsev (1982) proposed a model based on linearelastic fracture mechanics for simulating the crack propagation in concrete on the mesolevel. The concrete is considered to consist of polygonal aggregate particles and a homogeneous mortar matrix, see Figure 2. In the contact zones, straightline initial cracks are assumed. These cracks might result from shrinkage taking place during cement paste hardening. Usually, about one initial crack per aggregate particle is generated in the numerical experiments. By using criteria of linear-elastic fracture mechanics for loading modes I and II, the propagation of the initial cracks under increasing external load is simulated. When a certain geometric constellation of two neighboring cracks is reached these cracks coalesce. Global failure occurs if a crack completely splits the specimen.

An extended and refined version of the original Zaitsev's model (Slowik & de Barros Leite 1999) has been employed in the current study. For determining the stress intensity factors a more

general solution by Cotterell & Rice (1980) is used (see Figure 3), allowing the simulation of crack propagation under various loading conditions. The stresses in the uncracked specimen are at first determined under the assumption of homogeneity and then corrected in the vicinity of the aggregate particles for taking into account their effects on the stress distribution. These effects are estimated using continuum mechanics solution for a circular elastic inclusion in an infinite elastic plate. Crack propagation is controlled by a mixed mode criterion considering the stress intensity factors K_I and K_{II} and the principal stress direction. For the coalescence of neighboring cracks a criterion based on solution for crack interaction (Kachanov 1985) is applied. Furthermore, the model accounts for fiber reinforcement. The effect of the fiber reinforcement is considered by applying pairs of crack closing forces to the crack surfaces. These forces are crack opening dependent according to a bond-slip relation for fibers embedded in mortar.

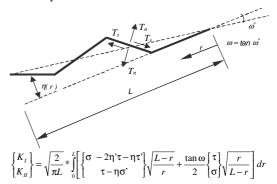


Figure 3. Stress intensity factors for kinked cracks, Cotterell & Rice (1980).

Figure 4 shows the crack pattern obtained in a concrete specimen under uniaxial compression. In the upper left corner the initial crack pattern, i.e. prior to loading, is shown. The other crack patterns correspond to different load levels.

In extensive parametric studies, the influences of material composition and loading conditions on the fracture process have been studied (Slowik & de Barros Leite 1999). It could be shown that the fracture behavior becomes more brittle with decreasing aggregate size whereas the compressive strength is nearly independent on the aggregate size of normal strength concrete. Increasing stiffness of the matrix results in a strength increase. An advantage of mesolevel models is the opportunity to separately study the influences of individual properties of the mesolevel components on the global material behavior. For example, modifying

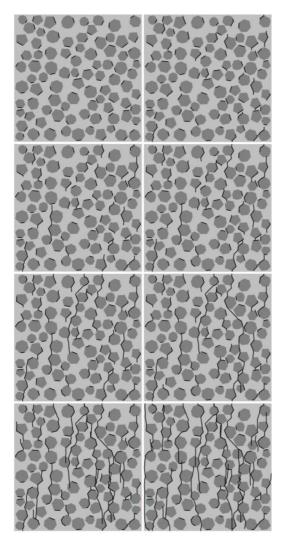


Figure 4. Simulation of the crack propagation under increasing compressive load by using the particle model.

the matrix stiffness without changing the interface properties is nearly impossible in real experiments. Furthermore, effects of the concrete component properties on the global mechanical behavior may be studied at exactly the same structure, i.e. with the same spatial arrangement of aggregates and initial cracks.

When simulating steel fiber reinforced concrete failure, for 1% fiber volume content an increase of the compressive strength by about 5% was observed for normal-strength concrete. At its current stage the particle model does not allow to simulate the post-peak range of concrete fracture tests. Therefore, the influence of fiber reinforcement on the ductility could not be demonstrated.

Effects of loading conditions and specimen geometry on the fracture process have been studied as well. Figure 5 demonstrates that the compressive strength generally decreases with increasing specimen slenderness. This effect appears to be dependent on the boundary conditions. As expected, confined end faces resulted in a strength increase when the slenderness ratio is low.

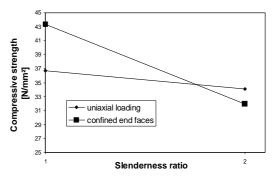


Figure 5. Effect of the specimen slenderness on the compressive strength, mean results of numerical simulations by using the particle model, 100 samples per series. The slenderness ratio is the specimen height divided by the specimen width.

The numerical results appeared to be insensitive to the minimum aggregate size in the particle model. This observation justifies the simplifications made by considering only the large aggregate particles in the generated mesolevel models.

4 TRUSS MODEL

During the last 30 years, the use of discrete models to describe the nonlinear behavior of materials such as rock or concrete has gained growing popularity (Burt & Dougill 1977, van Mier 1995). Each of such discrete models presents a set of different assumptions with regards to material idealization, structural idealization, mechanical properties and material behavior of discrete elements (fracture law). In addition, these models may differ in the consideration of the material behavior (pure brittle or more ductile) as well as in the consideration of the loading condition (tension or compression). Consequently, all of these models have been reported fairly successful in their specific purposes, but hardly efficient in describing the material behavior in situations other than the ones on which they have been tailored. In the particular case of cementitious composites, this suggests that general-purpose tools may require certain level of

flexibility to accommodate the effects caused by differences in the material compositions.

4.1 Model Idealizations

The model developed in this study combines many of the successful features of existing models and some supplementary new features. The corresponding simulation tool allows the selection of different softening functions, mechanical properties and probabilistic scattering for each material. It also allows selection among 4 different framework type elements: planar truss (4 degrees of freedom), planar frame (6 d.o.f.), space truss (6 d.o.f.) and space frame (12 d.o.f.) elements.

The meshes are initially generated as perfect lattices. However, small perturbations may be imposed to produce irregular meshes. The 2D grid consists of 4 nodes interconnected by 4 lateral elements and 2 diagonals, while the 3D grid consists of 8 nodes interconnected by 12 edge elements, 12 diagonals on faces and 4 inside.

The section areas of different elements (edge, diagonals, etc) are automatically set in manner that the mesh stiffness matches the continuum stiffness (assuming same elastic modulus for all elements). The system allows for different values for each class of elements being manually assigned.

The material types for the line elements are assigned by projecting the lattice onto the aggregate-matrix structure (Fig. 6) and detecting whether both element nodes lie inside of the same aggregate (aggregate element) or both element nodes lie in the matrix and the element does not intersect an aggregate (matrix element). Otherwise, the element is considered as bond interface between the two other materials. If perfect bonding is assumed, the material stiffness of each bond interface element is assigned proportionally to the amount of each of the two materials in the element. For weak bonding, the interface element is considered as a third and independent material.

Two different approaches have been employed by various researchers to simulate the material behavior and overall fracture process. In the first approach, a failure criterion is specified for determining the collapse of discrete elements, after which the elements are removed. Thus after an initial linear response, a nonlinear behavior is obtained as result of successive failure of elasticbrittle discrete elements. This approach seems apparently simple but also dependent on the size of the discrete elements. Other approach includes a tensile softening branch in the material law of the discrete element. The latter was preferred in this study, yet assigning different softening laws for

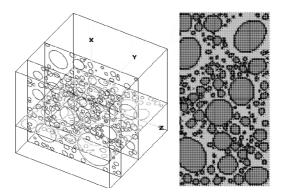


Figure 6. Idealized structure for 2D analyses: slice cutouts from 3D specimen (left) and idealized mesh structure (right).

tension and compression to different materials. The tensile softening functions are described on the basis of stress crack-opening laws. In order to adjust the elastic moduli of the softened elements at each step of the analysis, a number of procedures have been implemented for the different structural element types. The stress analysis is carried out in incrementally stepwise manner under displacement control using a direct solver.

The effect of fiber reinforcement was also modeled by introducing additional elements connecting distant nodes of the matrix media. Hence in the case of fiber-reinforced concrete, a softening function was derived on basis of a bondslip relation, in order to describe the behavior of the elements representing fibers.

4.2 Numerical Simulations and Discussion

Some selected results from extensive parametrical analyses and brief descriptions of the simulations are presented. In the initial set of the numerical simulations, the most common assumptions used by most models were investigated under different loading conditions. This first set was particularly useful in a development stage, in order to define or develop the features of the current model. The second set of simulations demonstrates features and applications of the model presented here.

4.2.1 Model Development Stage

The following conventional assumptions were investigated at this stage:

- *a)* The concrete composition constitutes of mortar, aggregate and interfacial zone (ITZ) elements;
- b) Specimen is assumed as homogeneous media (mortar) and coarse aggregates are placed inside;
- *c)* ITZ is assumed as homogeneous material with relatively weak mechanical properties;

- *d*) Common results of mortar and aggregate testing are assigned to element properties;
- *e)* Overall softening is obtained by the removal of elements which fail under a fracture law;
- f) The concrete (matrix-aggregate) structure and mesh topology are generated on the 2D space and scaled up by a thickness t of the fictitious slice;

Under limited conditions, the above-mentioned assumptions seem sufficient for capturing practical overall failure behavior and crack pattern, but inconsistencies appear as soon as different material compositions and load conditions are investigated.

Simulation results of direct tension tests of specimens with different aggregate content, assuming low strength values for ITZ elements, showed a considerable loss of overall strength, proportional to increasing of aggregate contents, which disagrees with experimental results. On the other hand, when the strength of ITZ elements was assumed equivalent to that of mortar elements, there was little increase in the global strength and cracking still developed along interfacial zones.

Figure 7 presents stress-strain curves of direct tension simulations, in which an exponential tensile softening function was used to bring the fracture process and aggregate shape and stiffness were varied. Strength values for ITZ elements slightly lower than those of mortar were sufficient to enforce crack bridging and development of the crack surface along ITZs, in agreement with experimental results. Aggregate shape/size effects were also captured in terms of ductility of stressstrain curves. The use of ellipsoidal aggregates with low sphericity (\mathbf{r} = ratio of the middle-axes, see Fig. 7) produced increase of fracture toughness, when compared to nearly spherical aggregates. Softer aggregates resulted in natural loss of global stiffness yet little increasing in the overall strength, possibly due to reduction of stress concentration along matrix/aggregate interfaces.

In simulations of compressive tests the abovementioned assumptions are insufficient to cast the diffuse cracking pattern. The observed failure in compression may be described as a shear crack band cutting diagonally through the specimen, which does not correspond to experimental results. The weak ITZs resulted in loss of global stiffness, and overall strength considerably underestimated and rather brittle failure. The application of a tensile softening function to decay the element stiffness was insufficient to produce overall failure.

Fracture of mortar specimens was simulated to investigate the assumption homogeneous material. The aggregate structure was generated and a

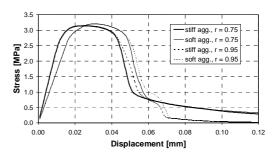


Figure 7. Simulations of tension test with conventional model assumptions and varying aggregate stiffness and shape.

standard deviation of 5% in values of the element properties was assumed. The obtained stress-strain curve (Fig. 8) does not vaguely resemble experimental curves of direct tension tests. The lack of a driving force for the crack resulted in development of cracking surface concurrently from both sides. The crack developed diagonally, straight from one corner to the other. In particular cases of concrete under compressive loading a shear failure may occur, but in most cases of practice the failure is caused by tensile stresses transversal to loading resulting in concurrent longitudinal cracks. The shear stresses are partially resisted and redistributed by the frictional forces in the composite granular material.

Mesolevel models usually generate only coarse aggregates representing usually less than 40% of the volume. Hence, the surrounding matrix (cement paste, voids and small aggregates), which is considered homogeneous, may be over 60% of the volume. Therefore, the assumption of mortar as nearly homogeneous material may be directly responsible or contributes largely to inconsistencies in the results. Inhomogeneities have been introduced in certain models either by a standard variation in the strength properties or by a randomly distributed decay in a percentage of elements. The effects of both approaches are also

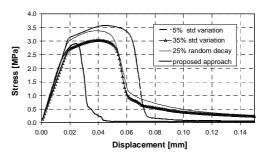


Figure 8. Comparison of various approaches for simulating inhomogeneities in mortar specimens.

shown in Figure 8. At high values of standard deviation (0.35) the shape of the curve only slightly improves but the overall tensile strength is still very high. The random decay seems to produce a better effect but still insufficient. Both approaches are merely based on distribution of chaos at random, which has little chance of using problem specific knowledge or bringing any enlightenment to the problem.

4.2.2 Model Settlement Stage

More rational ways of introducing weakness in terms of degree of inhomogeneity of interface and mortar elements, which take into consideration the aggregate size distribution and other admixture information, are required.

In this last implementation stage the properties of mortar elements were generated a priori over the entire mesh using a proposed approach, in which a media of fine aggregate particles is generated. This initial structure is employed to roughly estimate properties of matrix elements on basis of the aggregate properties considering: i) a decay in the properties somehow proportional to the fractions of different aggregates sizes in a fuller distribution, which constitute the volume of the mortar, taking into account the grid size of the mesh; and ii) the expected volume of the porous media. Standard deviations of a maximum 5% value were applied to the properties of the elements. This technique obviously introduces overheads in terms of computational effort, but it seems to pay off in performance. The resulting curve is considerably improved (Fig. 8).

The concrete structure was generated thereafter and superposed over the existent mesh of mortar elements in order to determine the aggregate and ITZ elements, i.e. elements that lie partially inside of the aggregate. For the aggregate elements the properties are completely reassigned but for the ITZ elements only a small reduction factor is randomly applied to the strength values.

In the proposed model, failure was simulated by assigning an insignificant value to the member stiffness and, therefore, no member is physically removed. It was assumed that in a locally closed strut-tie system, the "failure" of tensile ties artificially increases the stresses in the compressive struts resulting in plastic deformation and failure of the compressive struts. Therefore, a softening function was introduced to account for the effect of the plastic deformation and eventual failure.

Simulations of uniaxial compression, direct tension and wedge-splitting tests of FRC specimens were also carried out after the

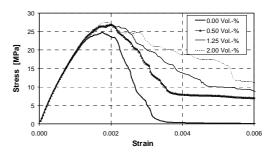


Figure 9. Stress-strain curves of simulations of FRC specimens with different fiber contents under compression.

adjustments in the settlement stage. For the 2D analyses, an effective length of the fiber was assumed considering only the projection of the 3D fiber on the plane of the 2D slice cutout. In the results, the maximum load is only slightly influenced by the fibers whereas the post-peak strength increases notably with the fiber content, yielding more ductile fracture (Fig. 9) and more diffuse crack pattern. Results agreed with experimental findings but the 2D model is limited to low aggregate content specimens. Increasing of aggregate or fiber contents produces jamming of fibers in localized areas and temporarily increases in strength. Such effects may be at certain extent observed in experimental testing, but using much higher aggregate and fiber contents than the ones employed in these simulations.

The 2D approach is commonly used not due to better performance, but due to difficulties in obtaining the 3D concrete structure. Since the proposed model is based on a 3D concrete structure, comparisons between 2D and 3D analyses could be performed. A specimen was cut in many subsequent slices along the two axes perpendicular to the loading direction. For each direction, average aggregate content of the slices is close to content of the specimen. However, the aggregate content of individual slices may vary considerably from one to another. Consequently, the curves from assorted slices may be also quite different. In direct tension tests, most cracking surfaces developed in the middle third part of the specimen and were roughly horizontal. Yet in some slices, the cracking surface developed concurrently from two opposite sides of the specimen. Thus clearly showing that, even considering only slices in a single direction, the cracking surfaces in the simulations were not the same. In fact, when the cracking surfaces of all slices in the two directions are plotted together in the 3D space, they form a diffuse band instead cracking surface. Therefore,

the curves obtained in 3D analyses have to be compared with the averaged curve of the slices of a same specimen. The averaged curve is more brittle and tends to overestimate the strength of the specimen as compared to the 3D curve. The 3D curves are less sensitive to variations of aggregate content when the interface is considered very weak, which suggests different assumptions from 2D material properties. In FRC simulations, the 3D curves are gentler than 2D curves and considerably less sensitive to variations in fiber and aggregate contents.

Figure 10 shows examples of cracking surfaces obtained in selected simulations of direct tension and uniaxial compression. The cracking patterns of simulations perfectly correspond to cracking surfaces obtained in experimental tests.

Figure 11 (left) describes the fracture behavior in wedge-splitting simulations. The dark color shows elements, which have collapsed, while the very light shades in the vicinity of the crack are elements that entered in softening process due to the rising of localized stresses. The crack runs along aggregates interfaces straight below the notch. In the right side of Figure 11, fiber reinforcement was used, resulting in change in the cracking path with slight increase in strength and considerable increase in ductility, as it has also been observed in experimental tests.

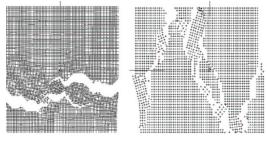


Figure 10. Typical crack patterns obtained in simulations of direct tension and uniaxial compression tests.

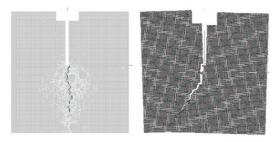


Figure 11. Comparison of fracture behavior in simulations of wedge-splitting tests for the same concrete structure without (left) and with (right) fibers.

5 CONCLUSIONS

Mesolevel models are prospective tools to describe both qualitative and quantitative effects of independent mechanical properties of material components on the global mechanical properties of the composite material. Experiments can only statistically estimate the independent effects, since a) two specimens with identical structure cannot be produced; and b) changes in one component result in adjustment on other components with simultaneous changes in the mesoscopic structure.

Most mesolevel concrete models have been developed for simulations under tension since this failure type is more clear and easier to implement, but models, which are valid only for a particular loading situation, are mere artificial maneuvers to mimic well-understood features, yet not able to describe real material behavior. Substantial effort should be made to enhance the performance of existing models under compression since there lie most applications for concrete. Comparisons between simulations of a same specimen under different loading condition proved to be useful for detecting inconsistencies in models and distinguishing assumptions that mimic the real material behaviour from those which are merely numerical manoeuvres.

Though 3D idealizations and analyses introduce more complexity and effort, they are clearly more accurate and suitable for practical applications. The 2D analyses may be efficient to spot out the inconsistencies for model development.

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