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MESOSCALE MODELING OF CONCRETE: MICROPLANE-BASED APPROACH

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Abstract: In the paper mesoscale model for plain concrete, based on the microplane theory [1] is presented. In the model concrete is treated as a bi-phase composite material, consisting of coarse aggregate and mortar matrix. The presence of interfacial transition zone (ITZ) between the two phases is neglected. The numerical study is based on the experimental tests performed by Wang and Wu [2] on small square concrete columns confined with CFRP and subjected to uniaxial compressive loads. The tests results, reported in terms of axial stress-strain relationships and failure modes, represent useful data base for the calibration of numerical models. In the first step of the study, only the unconfined concrete cylinder (R75) has been modeled at mesoscale. An important aspect of the proposed model is the generation of a random aggregate structure in concrete, which is based on a generation procedure implemented in Matlab R2013b. The mesoscale analysis of the unconfined cylinder is performed by using the finite element code MASA [3]. The constitutive law for mortar is based on the microplane model, while aggregates have been considered linear elastic. It is demonstrated that the numerical model is capable to correctly reproduce the mechanical behavior of the unconfined cylinder, confirming the predictability of the used approach.

1 INTRODUCTION

Concrete is composite, highly heterogeneous material, with randomly distributed defects of different sizes and shapes. The internal structure can be considered as a multi-level hierarchical system. According to [4], at least 4 levels of observation can be identified, namely: *macrolevel*, *mesolevel*, *microlevel* and *nanolevel*. At the *macrolevel*, concrete is treated as a homogenous material and its behavior is described by macroscopic quantities. The other levels consider concrete as a multi-phase medium characterized by coarse aggregate and paste, which morphology and properties depend on the considered level, so that: 1) at the *mesolevel*, the paste is considered as homogeneous material (with fine aggregates dissolved into it); 2) at the *microlevel*, the paste is constituted by cement paste (with pores embedded inside) and fine aggregates; 3) at the *nanolevel*, the paste is further subdivided into a) big pores (air voids), b) cement past with only small pores (capillary pores) in it and c) fine aggregates.

Most of the engineering studies available in the literature for the non-linear analysis of concrete, consider concrete as a homogeneous material, formulated within the framework of continuum mechanics. Although non-linear macroscopic models for concrete can give a realistic description of its global behavior, under specific conditions they fails in capturing important phenomena of the microstructure, determined by the randomness of the material heterogeneity. In this case, it is necessary to perform numerical analysis at the lower scales. With the type of computer facilities available today, mesoscopic analysis appears to be an important tool for evaluating the behavior of concrete.

To clarify the influence of meso-structure on global behavior of concrete, a number of numerical studies at mesoscale were carried out so far. In the 2D model proposed by [5], a procedure to generate a bi-phase composite structure in concrete (coarse aggregate and mortar matrix) has been proposed. The authors used an appropriate morphological law to generate two-dimensional structures with a given size distribution of: a) spherical aggregates; b) broken aggregates; c) aggregates with given shape characteristics. The generated material meso-structure has been mapped into a finite element grid to analyze processes and properties in concrete such as shrinkage, creep, fracture and non-linear stress-strain behavior. The model has been used by [6] to study the drying behavior of concrete at mesoscale.

In the 2D model proposed by [7] concrete has been modeled as a tri-phase composite material (coarse aggregates, mortar matrix and interfacial zones). Their study is based on the generation of a random aggregate structure, for rounded and angular particles, based on the Monte Carlo random sampling principle. Shape, size and distribution of the particles have been set to realistically reproduce the composite structure of concrete in a statistical sense.

The generated composite structure has been meshed to obtain the FE model. The main results obtained from mesoscopic study of concrete, based on the applied methodology are presented in [8]. In [9] a meso-structural model for the mechanical behavior of quasi-brittle materials, such as concrete, has been proposed. The model is based on interface elements (associated with a constitutive law representing non-linear fracture) coupled with linear elastic continuum elements. The approach proposed by the authors for fracture analysis of concrete is based on the Fictitious Crack Model (FCM) introduced by [10]. In order to reproduce general crack paths in the material, the interface elements have been inserted along selected inter-element boundaries.

Wriggers and Moftah [11] performed a 3D mesoscale model for concrete based on the generation of a random aggregate structure, in which the shape, size and distribution of the coarse aggregates closely resemble the real concrete structure. The generation procedure is based on the Monte Carlo method. Damage and fracture processes in concrete have been simulated using an isotropic damage model applied to concrete specimens loaded in uniaxial compression. Although the numerical models showed a good agreement with the experimental data, the authors recognized the importance to consider also an interfacial transition zone (ITZ) between aggregates and mortar matrix.

The mesoscale models described so far are formulated in the framework of continuum theory and they are mostly used to perform 2D or 3D small-scale simulations due to their high computational cost. For this reason, in the recent years several discrete models, such as "random particle model" and "lattice model" have been introduced for studying softening-damage and fracturing in concrete [12-17].

2 RANDOM AGGREGATE STRUCTURE

Aggregate takes up 60-80% of the total volume of concrete and it can be divided into fine and coarse fractions. Fine aggregates are usually constituted by natural sand with a maximum diameter smaller than 5 mm, while the majority of the coarse aggregates used in concrete consist of gravels and crushed stones, with diameter greater than 5 mm. As shown in [7] the shape of the aggregate particles depends on the aggregate type. Usually crashed stones are characterized by an angular shape, while gravel aggregates have approximately a rounded shape.

The generation of random aggregate structure plays an important role in the mesoscale analysis of concrete. In fact, several parameters, such as the shape, size and spatial distribution of aggregates greatly influence the mechanical behavior of concrete. The influence of the aggregate shape on the global behavior of concrete has been studied by many authors. Wittmann et al. [5] performed 2D analysis considering different shape of aggregates. Arbitrary composite structures are generated with the computer-generated particles and the geometry of the aggregates is simulated by using an appropriate morphological law. As explained by the authors, one possibility for analyzing a section of a given particle is to transform the contour into polar coordinates.

In [7] a procedure for generating aggregate structures for rounded and angular aggregates, based on the Monte Carlo random sampling principle, has been proposed. In order to shape the particles with a prescribed elongation ratio the authors established a criterion to define the width and the length of the particles. The width of the particle is defined as the minimum width of all described rectangles, which are big enough to contain entire particle inside. Having identified the described rectangle which gives the minimum width, the length and elongation ratio of the particle coincide with the length and length/width ratio of this described rectangle.

Regarding 3D models, Garboczi [18] introduced spherical harmonic functions, based on X-ray tomography, to characterize concrete aggregates particles. The original 3D particle images are taken from an X-ray tomography of a real concrete sample. Given the global image it is possible to extract individual aggregates, which are stored in a database together with the coordinates of each voxel, relative to the center of mass of the particle. These coordinates are then used to generate a surface function of the 3D particles, which is analyzed with spherical harmonics functions.

Determination of the aggregate size distribution is another important parameter which influences the properties of concrete, in terms of workability, strength and total cost of hardened concrete. Usually, the aggregate size distribution is determined by means of "ideal" grading curves, worked out on the basis of practical experiments and theoretical calculations, such as Bolomey's, Fuller's and Graf's curves. One of the most known and acceptable grading curve is the *Fuller curve* which optimize the aggregate packing and concrete properties.

To perform mesoscale analysis of the unconfined cylinder tested by [2], a simple procedure to generate a random aggregate structure in concrete has been implemented in Matlab R2013b. The procedure is based on a minimum distance criterion which avoids any intersection between two or more aggregates. In this study, only spherical particles are used, considering two different aggregate volume fractions (see Fig. 1).

The C30 concrete mixture used by [2] is composed by Ordinary Portland Cement (OPC). River sand has been included as the fine aggregate, while crushed granite stone with a maximum size of 10 mm has been used as the coarse aggregate. Additional information for the C30 composition have been provided by the authors by means of a private communication: aggregates occupy 65% of the total specimen volume, 34% of which is constituted by coarse aggregates (5 mm ≤ D ≤ 10 mm), while the remaining 31% is constituted by fine aggregates (D ≤ 5 mm).

a) b)

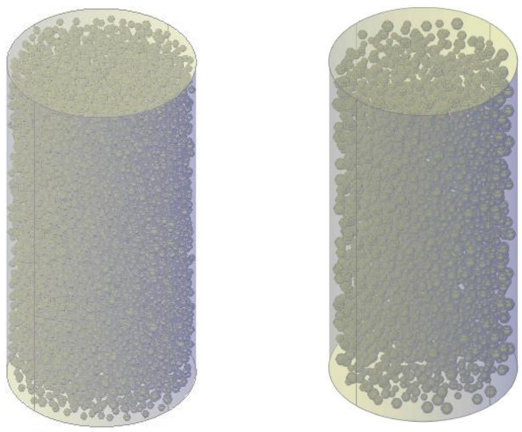

Figure 1: C30 Concrete composition: a) 20% of coarse aggregate; b) 10% of coarse aggregate.

In the implemented model, concrete is treated as a bi-phase composite material (coarse aggregate and mortar matrix that includes the fine aggregate). The size distribution of the coarse aggregate (34%) has been determined by means of the *Fuller curve*. Once evaluated the complete aggregates composition, a simple procedure to randomly generate the centers of the aggregate particles has been implemented in Matlab R2013b. The particles centers have been placed inside the specimen in such a way that any intersection between the particles is prevented. Once defined the spatial distribution of the particle centers, the corresponding solid spheres (with a given diameter) have been generated within the column. Then, all the spheres have been subtracted from the external solid to obtain the two distinct phases of the concrete specimen: 1) coarse aggregate; 2) mortar matrix. The geometry of the obtained meso-model has been finally imported into the FE program MASA [3] and meshed with 3D solid four-node finite elements.

Numerical analysis performed at mesoscale in the framework of continuum mechanics theory can be rather expansive, from a computational standpoint, especially for 3D simulations. To highlight this aspect, two different concrete compositions (Fig. 1) have been considered to generate the FE model for the cylindrical specimen (R75): a) composition I (Fig. 1a), where a coarse aggregate volume fraction of 20% has been guaranteed with the correct size distribution (5 mm ≤ D ≤ 10 mm); b) composition II (Fig. 1b), where a 10% of the coarse aggregate has been obtained with the same size distribution. It is worth noticing that the FE model obtained by composition I (Fig. 1a) is from the computational point of view rather expensive (more than 10^6 of 3D solid elements). For this reason, only the composition reported in Fig. 1b has been here considered for the FE analysis of the concrete cylinder (R75).

3 MICROPLANE MODEL

The finite element analysis has been carried out using the FE program MASA [3]. The most relevant part of the code for the non-linear analysis of concrete is the constitutive law, which is based on the microplane theory [1]. The background of the “microplane modeling approach” can be traced back to the pioneering idea of Taylor [19] dealing with plasticity of polycrystalline metals. The basic idea behind this formulation is that the stress-strain relation can be defined independently on various planes in the material, assuming that the stresses calculated on such planes are the resolved components of the macroscopic stress tensor (static constraint), or that the strain components on such planes are the resolved components of the macroscopic strain tensor (kinematic constraint). The term "microplane" [20,21,22] refers to the fact that the material behavior is characterized on the weak planes of various orientations that are found in the microstructure (e.g. the inter-aggregate contact planes).

The microplane model formulated in [1] is based on the so-called relaxed kinematic constraint concept. It is a modification of the M2 microplane model proposed by [23]. Each microplane is defined by its unit normal vector components n_i (see Fig. 2).

a) b)

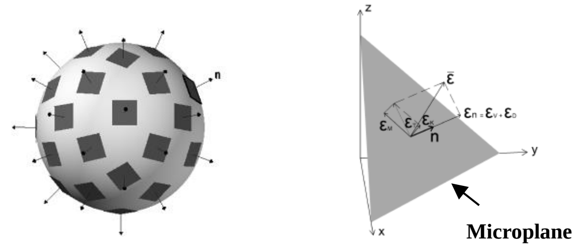

Figure 2: (a) Integration points on the unit radius sphere and (b) Decomposition of the macroscopic strain vector into microplane strain components – normal (volumetric and deviatoric) and shear.

Microplane strains are assumed to be projections of the macroscopic strain tensor ε_{ij} (kinematic constraint). On the microplane are considered normal (σ_N; ε_N) and two shear stress-strain components (σ_K, σ_M, ε_K, ε_M). Unlike phenomenological models for concrete (e.g. plasticity or damage based models), which are based on tensor invariants, the microplane model is characterized by scalar stress-strain relationships independently defined along pre-selected spatial directions. The macroscopic model response comes automatically out as a result of the numerical integration over such planes.

To realistically model concrete, the normal microplane stress and strain components have to be decomposed into volumetric and deviatoric parts ($\sigma_N = \sigma_V + \sigma_D$, $\varepsilon_N = \varepsilon_V + \varepsilon_D$). Unlike most microplane formulations for concrete, which are based on the kinematic constraint approach, in the present model the kinematic constraint is "relaxed" in order to prevent an unrealistic model response for dominant tensile load and to prevent stress locking phenomena.

To generate the macroscopic stiffness and stress tensor from known microplane strain and stress components, the principle of virtual work is used to approximately enforce the equivalence of stresses on the microplane scale and the macroscale:

$$\sigma_{ij} = \sigma_V \delta_{ij} + \frac{3}{2\pi}\int_S \left[\sigma_D\left(n_i n_j - \frac{\delta_{ij}}{3}\right) + \frac{\sigma_m}{2}\left(m_i n_j + m_j n_i\right) + \frac{1}{2}\left(k_i n_j + k_j n_i\right)\right] dS \qquad (1)$$

where S denotes the surface of the unit radius sphere and δ_{IJ} denotes Kronecker delta, ni is direction of the microplane and ki and mi are directions of shear microplane components. The integration is performed by numerical integration using 21 integration points (symmetric part of the sphere, see Fig. 2a).

To account for large strains and large displacements, Green-Lagrange finite strain tensor is used. Furthermore, to account for the loading history of concrete, the co-rotational Cauchy stress tensor is employed. Detailed discussion of the features and various aspects related to the finite strain formulation of the microplane model are beyond the scope of the present paper. For more detail see [1].

4 MATERIAL PROPERTIES AND FE MODEL

The numerical study is based on an extensively experimental campaign performed by Wang and Wu [1] to investigate the influence, on strength and ductility, of the corner radius when concrete specimens are confined with CFRP. The specimens tested by [1], characterized by constant ratio width/height (150/300 mm), have the following characteristics: 1) 6 different cross section corner radius, which varies as 0, 15, 30, 45, 60 and 75 mm (see Fig. 3); 2) three different configurations: a) unconfined columns; b) 1ply CFRP-confined columns (with a nominal fiber thickness equal to 0.165 mm) and c) 2ply CFRP-confined columns (with a nominal fiber thickness equal to 0.33 mm) ; 3) two different concrete grade: C30 and C50; 4) two types of CFRP for C30 and C50. In the present numerical investigation only the unconfined cylinder (R75) made of C30 concrete has been analyzed at mesoscale.

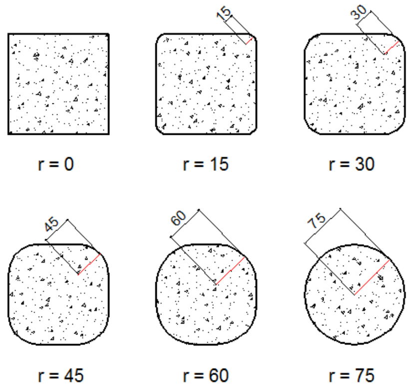

Figure 3: Corner radius variation of the columns.

In a first step of the study the 12 internal *microplane parameters*, characterizing the model [1], have been calibrated for mortar matrix to correctly reproduce the macroscopic mechanical properties of C30 concrete (see Tab.1).

Table 1: Macroscopic mechanical properties of concrete

Mechanical properties	C30
Modulus of elasticity E_{cm} [MPa]	29500
Poisson's ratio	0.2
Compressive Strength [MPa]	30
Tensile Strength [MPa]	3
Fracture energy [J/m^2]	90

The numerical values of the used parameters are summarized in Tab.2, while the corresponding constitutive law for mortar is shown in Fig. 4.

For the aggregate the linear elastic behavior is assumed. Both concrete phases have been discretized with 3D solid four-node finite elements. The spatial finite element discretization of unconfined cylinder (R75) is shown in Fig. 5.

To assure objective results with respect to the adopted mesh, the crack band method [24] has been used. The load is applied by displacement control. The loading and reaction surfaces are assumed to be confined in the horizontal directions, similar as in the experiments.

Table 2: Microplane parameters for mortar matrix

a	0.0002
b	0.05
p	0.6
q	0.3
η	0.6
e1	0.000048
e2	0.0013
e3	0.0008
e4	5
m	0.528
n	1.0
k	0.6

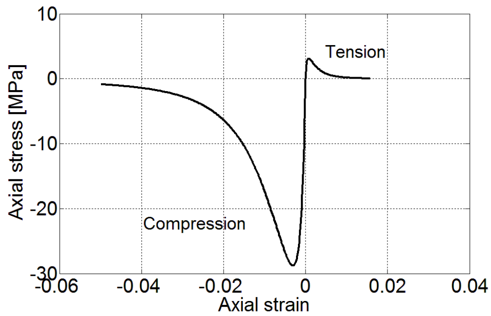

Figure 4: Microplane parameters and constitutive law for mortar matrix (element size of h = 6 mm).

a) b)

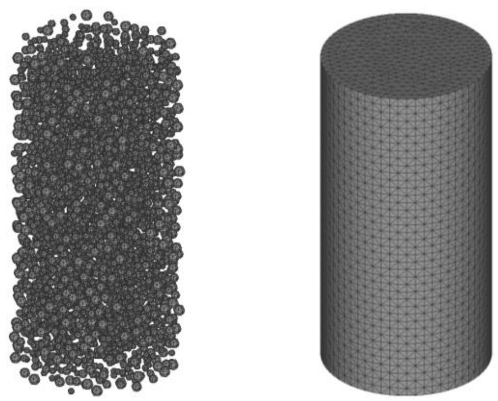

Figure 5: FE model used in the analysis of R75: a) aggregates; b) mortar matrix.

5 RESULTS AND DISCUSSION

The uni-axial stress-strain curves obtained for R75 are reported in Fig. 6, where the numerical and experimental results, in terms of axial and lateral strains, are shown. The same as in the experiments, the stress is obtained by dividing the global axial force over the concrete section area. Note that the experimental data are average of three experiments. The axial strain has been evaluated over the localized zone on the middle side face of the specimens. The measurement base approximately corresponds to the length of the vertical LVDT used in the experiments (200 mm). Consequently, the axial strain in the analysis is obtained by dividing the difference between the axial displacement at the top and at the bottom of the localization zone by its length.

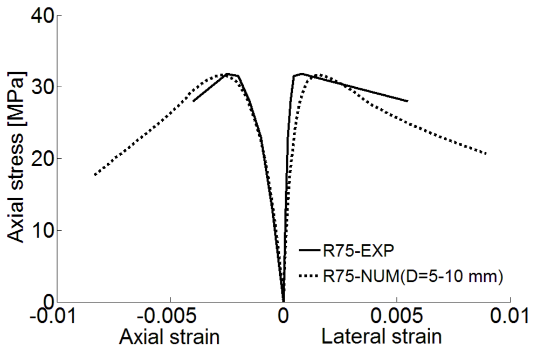

Figure 6: Stress-strain curves.

As can be seen from Fig. 6, the numerical results are in good agreement with the experimental one. The model is capable to correctly reproduce the non-linear behavior of concrete in the pre-peak regime, as well as the strain-softening behavior of the post-peak. As regards the axial stress vs. lateral strain curve, the model shows a lower concrete expansion with respect to the experiments. This can be attributed to a simplified random aggregate structure assumed for concrete and to the absence of a Interfacial Transition Zone (ITZ) between aggregates and mortar matrix. All these aspects greatly influence dilatation properties of concrete.

The typical failure mode of the cylindrical specimen (R75) is shown in Fig. 7, where the maximum principal strains are plotted.

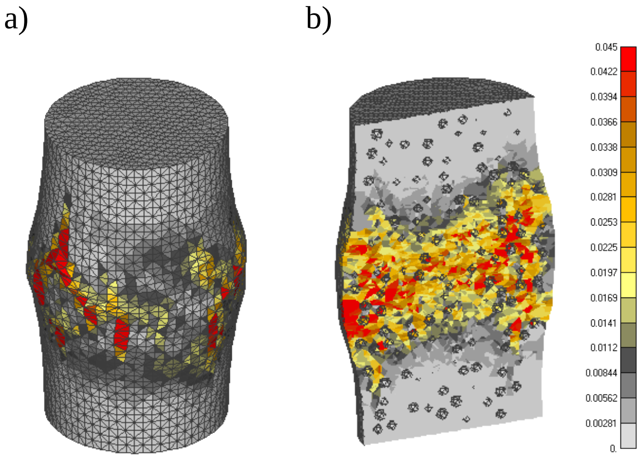

Figure 7: Failure mode of R75 (Maximum principal strains).

The red zones correspond to the crack opening greater than 0.25 mm. As can be seen damage localizes in the central part of the specimen where the crack pattern is characterized by several vertical and inclined cracks, which form a shear band at the end of the loading process (Fig. 7a). To show the internal damage distribution (Fig. 7b) the specimen has been cut at mid-section. Similarly to the experiments, it is possible to recognize the typical hourglass shape of concrete at a final stage of the loading history.

The volumetric strain evolution is reported in Fig. 8.

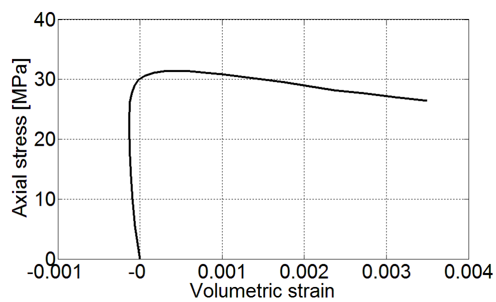

Figure 8: Dilatation properties of unconfined cylinder (R75).

On the curve, two different zones can be identified. The first one is characterized by the negative volumetric strains, which indicate volumetric compaction of concrete, while the second one is characterized by positive volumetric strains associated to concrete volumetric dilatation due to the cracking and damage.

6 CONCLUSIONS

In the article a mesoscale model for concrete, based on the microplane theory, is presented and discussed. Concrete is treated as a bi-phase composite material, i.e. coarse aggregates are embedded into the mortar matrix. The presence of interfacial transition zone (ITZ) is neglected. An important aspect of the proposed mesoscale model is the generation of the aggregate structure in the concrete cylinder, that is based on the random generation procedure implemented in Matlab R2013b. Due to the high computational requirement only the model with 10% of the total coarse aggregate volume fraction is discussed considering the realistic aggregate size distribution (5 mm $\leq$ D $\leq$ 10 mm). From the obtained numerical results, the following conclusions can be drown out: (1) The numerical results are in very good agreement with the results of experimental tests, confirming the predictability of the used approach based on the microplane theory [1]; (2) The modeling based on the mesoscale approach, in which concrete is discretized as a bi-phase composite material, is able to realistically replicate the response of plain concrete, both in terms of macroscopic stress-strain response and failure mode; (3) Dilatation properties of concrete are correctly reproduced, through a transition between "compaction" and "dilatation" of concrete; (4) From the computational point of view mesoscale model, formulated in the framework of continuum theory, can be rather demanding. Therefore, parallel processing computational schemes should be used.

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