Computational Materials Science 90 (2014) 157–170

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Mesomechanical characterization of porosity in cementitious composites by means of a voxel-based finite element model

Francisco Montero-Chacón [a,b,*], Jorge Marín-Montín [b], Fernando Medina [b]

[a] Abengoa Research, Campus Palmas Altas, Calle Energía Solar 1, 41014 Seville, Spain
[b] Escuela Superior de Ingeniería, Universidad de Sevilla, Camino de los Descubrimientos s/n, 41092 Seville, Spain

ARTICLE INFO

Article history:
Received 16 September 2013
Received in revised form 27 March 2014
Accepted 29 March 2014
Available online 4 May 2014

Keywords:
Mesoscale characterization
Voxel-fem
Multiscale modeling of concrete

ABSTRACT

At the mesoscale, concrete is regarded as a heterogeneous material with two main phases, namely mortar and coarse aggregates. However, the presence of pores at this scale may play an important role on the macromechanical properties of the material. Due to their complex geometry, these mesostructures usually require a large number of discretization elements. In this paper, a voxel-based (volumetric pixel) model is used in order to account for porosity while reducing the number of elements on the characterization of the mesomechanical properties of concrete. In order to validate the voxel model, a comparison to an equivalent tetrahedralized mesh is carried out, showing an important reduction in computational times but with similar results. For such validation, the effect of the voxel size and the consideration of the interfacial transition zone are also accounted for. Finally, uniaxial tension tests are carried out in order to characterize the elastic (i.e. elastic modulus and Poisson's ratio) and fracture (i.e. tensile strength) properties in concrete mesostructures of different sizes (25, 35 and 50 mm). The effect of porosity is analyzed by considering different pore fractions and validated with analytical and experimental results.
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1. Introduction

Traditionally, concrete has been treated as an ordinary homogeneous material. However, at the naked view, it is possible to observe that its structure is more complex and, therefore, opens a large number of possibilities to improve its performance. Certainly, at the mesoscale (i.e. ~10 mm), concrete is regarded as a heterogeneous material, namely a composite material with two distinguished phases (a matrix made of mortar and coarse aggregates as inclusions from 4 mm up to 30 mm). Secondary phases such as pores, interface transition zone (ITZ), fibers, or any other kind of additives can be accounted for at this level if they remain within the aforementioned scale.

Multiscale strategies [25,45,28,15] can be applied for the development of materials completely *in silico*. In fact, nowadays it is possible to create virtual labs in which performing tests is cheaper and quicker. In such way, many different material configurations and designs can be rapidly tested, providing a specific range where experimental tests must be carried out. Needless to say, experiments are a complementary yet important part of multiscale analyses that should not be disregarded.

In the literature, there exists a large number of numerical models for the analysis of concrete at the mesoscale, which can be classified into two main groups: discrete and continuum. The origin of the former type of models can be found in the seminal work by Hrennikoff [19], in which the continuum is discretized by a truss network. Later on, Cundall [11] proposed the so-called *distinct element method* (DEM), using circular particles with superficial interaction to simulate fracture in granular materials. Based on these earlier discrete models, several extensions have been successfully achieved for the analysis of fracture mechanics of concrete and other quasi-brittle materials [22,7,2,12]. On the other hand, in continuum-based models, the heterogeneous mesostructure of concrete is treated as a composite material, being the mortar and aggregates the matrix and inclusions, respectively. One of the first continuum models is that from Wittmann and coworkers [38]. More recently and based on this philosophy, new continuum models both in 2D and 3D have been proposed, being the material behavior [46] and the matrix-aggregate interface [24] the most important tackled issues.

Initially, the development of mesostructural continuum models for concrete was focused on the material law for the mortar phase. Different types of constitutive models have been proposed in the literature, brittle or smeared cracking [5], strong discontinuities

* Corresponding author at: Escuela Superior de Ingeniería, Universidad de Sevilla, Camino de los Descubrimientos s/n, 41092 Seville, Spain. Tel.: +34 95 448 72 93.
E-mail addresses: francisco.montero@research.abengoa.com (F. Montero-Chacón), fmchacon@us.es (J. Marín-Montín), medinaencina@us.es (F. Medina).

http://dx.doi.org/10.1016/j.commatsci.2014.03.066
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[3], or damage models [14,46], among others. As pointed out before, the use of cohesive elements has been found to be an efficient way to model the ITZ behavior in many applications [34,9,24]. On the other hand, with the increase in computational power, new particle shapes, explicit modeling of the ITZ or more advanced material laws have been formulated.

Modeling heterogeneity of the microstructure is not a simple issue, and it depends mainly on the geometrical aspects of the former (e.g. characteristic size and shape of the phases, presence of voids in the domain). A summary of different methods to overcome such issue is presented in [30]. These methods can be classified into:

- *Direct*: a geometrical division of the domain is previously made in order to state boundaries between different phases. Then, the phases are directly meshed with an unstructured mesh [6], although other approaches are valid such as the Voronoi cell [31]. If the microstructure is obtained via digital imaging, rough interfaces may appear. Thus, smoothing of the surfaces [40] is an appropriate way to reduce the number of elements.
- *Voxel*: the domain is discretized in a structured grid in volumetric pixels (i.e. brick elements in the finite element mesh) and the microstructure is mapped onto this. The material properties are assigned thereafter. This approach is used in [30] and the present work.
- *Gauss point*: follow the philosophy of voxel methods but the heterogeneity is introduced at the Gauss point level [50], however this method works both for structured and unstructured meshes.
- *Octree*: refines the voxel mesh by the introduction of *hanging nodes* at the interfaces to improve the resolution therein; elsewhere the domain remains voxelized [23].

The heterogeneity of the mesostructure promotes the use of tetrahedral finite elements when tackling this problem through a continuum approach. Although direct approaches provides very high accuracy, they require a large number of elements for the phase transitions, and even more when these are size-graded. This is especially problematic when small phases, such as pores, are taken into account. Thus, a voxel approach reduces the number of elements while keeping the simplicity of the formulation. On the other hand, the Gauss point method although increases the accuracy over the voxel method, leads to discontinuities within the element and therefore requires more computational effort. Regarding the hanging nodes, this approach still improves the resolution over the latter method, but in the case of multiple inclusions of different sizes it becomes impractical in terms of computational efficiency.

Based on the aforementioned facts, the use of voxels is an appropriate approach in the case of heterogeneous structures of graded inclusions and with the presence of pores. Therefore, a new strategy based on the use of volumetric pixel [30], referred to as *voxel*, is presented for the analysis of these complex structures within the finite element method framework.

The principle of the method is tested in the first place with a simple 2D unit cell. Then, in order to validate the voxel method with respect to the direct method, a comparison between a tetrahedral and a voxel mesh is carried out. An analysis of the effect of the size of the voxel is performed in order to determine the correct resolution of the mesh. Finally, the voxel model is validated through analytical and experimental results.

With the present voxel-based model, it is possible to design a *virtual testing* facility in order to determine the elastic (i.e. elastic modulus and Poisson's ratio) and fracture (i.e. tensile strength) properties and their dependence on the specimen size, boundary conditions and pore fraction. This methodology can be used for the prediction of the material properties and the design of certain concrete mixes upon these.

2. Mesostructure generation

At the mesolevel, concrete is regarded as a random heterogeneous quasi-brittle material with three main phases: mortar, aggregates and interfacial transition zone (ITZ). For the simulation of the mesostructure, only coarse aggregates are taken into account and assumed to be spherical-like particles. This particle generation is made following a Fuller's distribution, thus the cumulative percentage, P, passing a sieve aperture diameter d is given by $P(d) = (d/d_{max})^n$, with n the exponent of the equation in the range of 0.4–0.7 (in this paper is set to 0.5), and d_{max} the maximum aggregate size. The total volume of coarse aggregates with respect to the whole concrete volume is assumed to be 40%, as discussed in [46]. The algorithm for the generation of mesostructure is based on the take-and-place method proposed by Bažant et al. [2]. In this method, the largest particles are placed in first place so that smaller particles can be placed reasonably. A uniform probability distribution is used to place the particles.

Once all the particles are arranged within the domain of the specimen, the mesostructure is voxelized by means of a geometrical discretization, as shown in Fig. 1. This procedure basically reads that if the distance from the aggregate center to the centroid of the element is less than the radius of the aggregate, the element is assigned aggregate properties; otherwise, the element is assigned mortar properties.

In Fig. 2, a 3D render for a given mesostructure is presented. The size of the element (voxel) has to be carefully chosen in order to better represent the discretization. For instance, a large element size will lead to an excessively distorted mesostructure and, therefore, representativeness loss. Therefore, a voxel size less than the diameter of the smallest inclusion is defined. Obviously, the voxel size has an influence on the global mechanical properties, for this reason an analysis of the effect of such parameter on the latter is carried out in Section 3.3.

The size and shape of the aggregates may affect the cracking patterns. Thus, in order to analyze the effect of the volume fraction and the aggregates size, two maximum aggregate sizes are considered: $d_{max} = 8$ and 16 mm, in the virtual tests.

2.1. Modeling of porosity

The presence of pores in the mortar matrix influences the global macroscopic material properties. Moreover, the presence of voids and pores in a material are directly related to the decrease of the strength, regardless the material mix, sieve curve or cement type [35]. Porosity is classified as active and nonactive, depending on its influence on mechanical properties with changing moisture state [47].

In general, porosity is defined as the fraction volume of voids in a given material. The experimental measure of porosity is described in the ASTM C642 standard and it consists in an awkward process that comprises oven-drying, water immersion and boiling of the specimen.

Thus, the characterization of porosity in concrete via numerical methods is of great interest since this phase is always present at the mesoscale (and other scales as well). As shown in Table 1, the size of the pore strongly depends on the scale of observation. At the mesoscale this value cover almost three orders of magnitude (from 1 to 1000 μm).

The modeling of porosity has been tackled mostly from the transport point of view. For instance, in [4], this problem is solved by means of voxels. Regarding the mechanical properties, an

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