

VIRTUAL TESTING OF CONCRETE

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Abstract: The concrete is one of the oldest materials used in the building industry for ages. The models of this material are often designed to capture the behaviour of real constructions. To use these kinds of models the loading curves and basic experimental tests are needed. Since these experiments are expensive and often time consuming there is a new trend of replacing them by virtual numerical tests. This paper concentrates on one particular step towards developing such virtual laboratory – construction of a suitable representative volume element (RVE). Preliminary results addressing the influence of grain size distribution and their discretization inside RVE on finite element simulations of compressive damage of concrete sample are discussed.

Keywords: Concrete, finite element method, virtual testing, isotropic damage.

1. Introduction

In civil engineering, computational modeling is widely used in the design process at the structural level. Powerful commercial packages based on the theory of beams, plates and shells and on the finite element method (FEM) have been developed for structural analysis and are nowadays considered as one of the fundamental design tools. In contrast to that, an automated support for a selection or design of construction materials is currently not available. Specification of material properties and model parameters needed for structural analysis is not an easy task, yet it has a strong influence on the accuracy of the results. This is especially important if the influence of the mix composition, processing steps and environmental conditions during the construction stage on the long-term durability of the structure needs to be evaluated. Values of model parameters could be determined by experiments, but this is a time-consuming, tedious process that can considerably slow down the design process. Therefore, a virtual testing tool, i.e. integrated set of models, algorithms and procedures for the prediction of mechanical properties of materials, seems to be an attractive alternative.

Today, the most important construction material is concrete, which is a complex composite material over a wide range of length scales from nanometer to meter. The main objective of our work is to develop the virtual testing tool for concrete which will provide the material parameters for existing numerical models. Hence this paper serves as a preliminary study and is focused on the mesoscopic level of concrete where shapes of grains (aggregates) and their distribution play an important role. To assess their influence on numerical predictions of damage processes taking place in a concrete sample under compressive loading is the main objective of this contribution.

The paper is organized as follows. In Section 2 the preprocessing of numerical simulations is outlined. The comparison of numerical results of compression cube tests, for which the isotropic damage model is used, is demonstrated in Section 3. The concluding remarks and future extensions are presented in Section 4.

2. Preprocessing of numerical simulations

It has been demonstrated that creating a numerical model presents a crucial step influencing reliability and accuracy of numerical predictions, see e.g. (Zeman & Šejnoha, 2001; Zeman & Šejnoha, 2007). Here, preparation of a concrete sample at a mesoscopic level suitable for three-dimensional numerical

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simulations is described next with emphases on two essential steps: geometry preparation and generation of finite element mesh.

2.1. Geometry preparation

Generation of a numerical model in a realistic way follows a "take and place" method to place aggregates with a specific orientation one by one at the right position. The generation mechanism is designed here to fulfill the following requirements:

- The size distribution function of aggregates (grading curve) in real concrete should be matched.
- Shapes of grains should be approximated in a realistic way. Note that only convex shapes of aggregates and the shape factor (Eq. 1) are assumed.
- The minimum distance and volume control should be implemented.
- The periodicity of the grains crossing the model boundaries should be taken into account.

The generation procedure basically follows the steps mentioned above. First, the set of aggregates is created in accordance with a grading curve. The shape and size of grains is defined in this step. The grain shape can be seen as sphere, ellipsoid or polytope (polyhedron for 3D) and the breadth of the particle has to pass through a given upper sieve size and cannot be smaller than the lower sieve size, see Fig. 1 and (Mora et al., 1998) for more details. The length of the particle is given by the shape factor

$$\alpha = \frac{\text{length of particle}}{\text{breadth of particle}}.$$
 (1)

Dimensions of all shapes are generated purely randomly with the only constrain to fit the prescribed interval of the specific part of the grading curve. Moreover, for the polytope shapes the number of vertexes is also randomly generated in the appropriate limits. Whereas our interest is to obtain reasonably good agreement of the response of virtual testing sample with the true laboratory measurements, we still have to bear in mind the computational cost of such a simulation. Therefore, it is inevitable to implement into the generation procedures some control mechanisms which reduce the unsuitable small facets and angles in the particle.



Fig. 1: Definition of grain: a) Breadth, b) length.

When all aggregates are produced, they are taken out one by one from the aggregate base and randomly assigned positions and orientations and placed in the packing region. The larger aggregates are placed first to reduce overlapping and computational time. However, even if doing so the packed aggregates inevitably overlap each other, so that overlapping judgment is necessary for a successful 3D numerical modeling. If some minimal distance between grains is required each particle is first slightly enlarged before placing and after a successful positioning it is brought back to its original shape.

The last control mechanism is employed only when the grain exceeds the model boundaries and the periodicity condition has to be fulfilled. In such a case the aggregate is divided into the required number of parts placed at relevant positions. In addition, to provide conforming meshes a checking

procedure is invoked to ensure that the fractions of a given particle are not under some specified limits. The whole procedure described herein was implemented into the MATLAB high-level language and interactive environment (MathWorks, 2010). The multi-parametric toolbox for MATLAB (Kvasnica, 2009) is used to perform all operations with volumes including copying, merging, splitting, intersecting, etc.

2.2. Mesh generation

This technique implies the use of conforming finite element meshes easily enabling the implementation of periodic boundary conditions if needed. This might seem daunting in that it requires not only incorporation of an arbitrary number of aggregates, but also a complicated structure of cement paste around. In the present study these obstacles are overcome by employing the volumetric modeling capacities of the ANSYS package (ANSYS, 2005).

3. Numerical simulations

To address the influence of shapes of aggregates on the prediction of compressive damage, three different approximations (polytopes, ellipsoids and spheres) are considered for simulations, see Fig. 2. To that end, five different cube samples (50 x 50 x 50 mm) of each shape are constructed and used in the numerical analysis performed in the OOFEM finite element code with object oriented architecture for solving mechanical, transport and fluid mechanics problems (Patzák & Bittnar, 2001). Note that the volume of stones for all samples is considered equal to 15% of the total volume (4 – 8 mm = 30%, 8 - 16 mm = 70%) and the shape factor is set equal to 1.5.



Fig. 2: 2D cuts through 3D samples: a) Polytopes, b) ellipsoids, c) spheres.



Fig. 3: Average stress-stain diagrams: a) Comparison, b) sample with the polyhedron grains.

The isotropic damage material model with the exponential softening is assumed for both the stones and cement paste. The required parameters are taken from (Wittmann, 2002). The obtained average stress-strain diagrams are compared in Fig. 3a. Fig. 3b then presents one selected loading diagram for the grains substituted by polyhedrons. The evolution of damage parameter in reference steps for the 2D cut depicted in Fig. 3a is shown in Fig. 4.



Fig. 4: Evolution of damage parameter for the sample with aggregates approximated as polytopes (Fig. 3a): a) Step no. 26, b) step no. 40, c) step no. 100.

4. Conclusions

The comparison of the compression cube tests was presented in this paper. As can be seen from Fig. 3a no significant difference appeared between the simulations for various shapes of grains. This information should be verified for miscellaneous types of loading and material models as well. It is noteworthy that the approximation with polyhedrons required lower number of elements substantially influencing the computational time. Bear in mind that no interface elements have been used so far. This task we will be addressed in a forthcoming study. The following work will also focus on the possibility of introducing smaller fractions of stones into the calculations by means of some homogenization procedures (Vorel & Šejnoha, 2009; Sýkora et al., 2009).

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