DETERMINATION OF THE RVE SIZE OF QUASI-BRITTLE MATERIALS USING THE DISCRETE ELEMENT METHOD

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Abstract. Within a general multiscale scheme, it is necessary to define the representative volume element (RVE), over which a measured value becomes representative of the material. In the present work, the RVE size is determined by means of discrete element method (DEM), namely a three-dimensional lattice-particle model. These type of models have been proved to be efficient for simulating fracture processes in quasi-brittle materials. The model is used to perform the numerical simulations for different specimen sizes, aggregate distributions and material regimes. The resulting information is submitted into a statistical analysis and the chi-square test seems to be the best approach to determine the RVE size.

1 INTRODUCTION

Recent advances on computational performance have led to the development of multiscale models in order to tackle large and complex multi-field problems that were not solved formerly due to technical limitations. A wider spectrum of resolution is now available but previous studies are still necessary to carry out multiscale simulations.

Within a general multiscale scheme, the determination of the representative volume element (RVE) is of great interest. For homogenization techniques, the RVE is the cell to which homogenization is applied or the attached cell to a macro integration point in nested schemes [1].

The determination of the RVE size for random heterogeneous materials has been studied by some authors [1, 2, 3] with continuum-based models. In the present work, the discrete element method (DEM), namely a three-dimensional lattice-particle model, is used to perform the numerical simulations for cubic specimens of concrete. This type of models have been proved to be efficient for simulating fracture mechanics in cement composites.
This model has been used extensively to perform the statical procedure proposed by Gitman [2]. Two aggregate distributions are generated to study its effect on the RVE size. A simple way to apply boundary conditions by means of boundary particle is used to obtain less sparse results. Simulations are carried out until the hardening regime. RVE sizes varying from 25 mm to 100 mm are considered.

The RVE size for quasi-brittle materials has been successfully determined with the discrete element method. Results have shown a good agreement with the experimental observations and continuum-based model solutions. The main advantages of discrete models are also discussed in this work.

2 DISCRETE MODELS IN QUASI-BRITTLE MATERIALS

Several discrete models have been successfully implemented for the simulation of multiphysics problems in quasi-brittle materials. Cundall [4] discretized the continuum into circular particles with superficial interaction, with main applications in granular materials and fluid mechanics. Using a similar approach, Kawai [5] implemented the rigid-body-spring network (RBSN) to solve structural problems. Bolander [6], based on Kawai’s model, replaced the disk elements by a Voronoi tessellation to study fracture mechanics of concrete. In Zubelewicz and Bažant [7], the interacting elements are defined by the aggregates and their surrounding area.

Another type of discrete model is the lattice-based. In such a way, Bažant [8] developed a random particle model with axial interaction between the aggregates where a softening behavior is implemented. In the so-called Delft lattice model by Schlangen [9], on the other hand, the continuum is replaced by a truss whose minimum length is lower than the smallest inclusion so that different phases can be taken into account. After reaching a certain stress threshold, the failed beams are removed and microcracks are generated. Based on previous work by Bažant, Cusatis [10] presented a lattice-discrete particle model, an enhanced model achieved by implementing a more complex formulation based on the microplane models with very satisfactory results.

With the enhancement of computational power, new formulations of the problem are now possible, improving the model response. One issue concerning the discrete models is that, depending on the type, an important number of degrees of freedoms may be required. Therefore, multiscale techniques seems attractive in this case.

The authors’ lattice-particle model is based on some concepts of the aforementioned works and is successfully used to simulate fracture processes in concrete.

2.1 Material model

At the mesolevel, concrete is a random heterogeneous quasi-brittle material with three main phases: mortar, aggregates and interfacial transition zone (ITZ). In the RVE size determination, tensile tests on cubic specimens of length $D$ will be performed. This will set the domain where the aggregates must be placed. Aggregates are assumed to
be spherical-like particles and only coarse aggregates are taken into account. Particle generation is made according to a Fuller’s distribution, \( P(d) = (d/d_{\text{max}})^n \), where \( P(d) \) is the cumulative percentage passing a sieve aperture diameter \( d \) with respect to the maximum aggregate size \( d_{\text{max}} \); the exponent in the equation is \( n = 0.5 \). The total volume of coarse aggregates is assumed to be 40% of the whole concrete volume [11].

Once the particle distribution is generated following the sieve curve, these are randomly placed using the take-and-place method [8]. The largest particles are placed first so that the smaller particles can be placed reasonably. A normal probability distribution is used to place the particles. For a given particle, the new position must meet the following requirements: a) not only the center but all the particle must remain inside the domain and b) particles must not overlap. The first issue is immediately satisfied by a simple coordinate transformation. For the second one, the take-and-place suggests to relocate the overlapping particles into a void.

The mesh is constructed following the actual aggregate arrangement by means of Delaunay’s triangulation (fig. 1), therefore it will only depend on the actual material mesostructure. Every connecting element represents the interaction between two particles. The area of the element is found so as to preserve the volume distribution of adjacent tetrahedra [10].

2.2 Elastic formulation

Every element of the mesh represents the mechanical interaction between the particles as shown in fig. 2. This is modeled by spring elements acting in normal and tangential directions, with stiffnesses: \( K_{ij}^N = k_1 E_{ij} A_{ij} / L_{ij} \) and \( K_{ij}^T = k_2 E_{ij} A_{ij} / L_{ij} \). Parameters \( k_1 \) and \( k_2 \) are used to adjust the macroscopic elastic modulus and Poisson’s ratio, respectively. In general, values of \( k_1 = 5 \) and \( k_2 = 0.3 \) lead to satisfactory results. \( A_{ij} \) and \( L_{ij} \) are directly obtained from Delaunay’s triangulation [10].

Local elastic modulus \( E \) will depend on the three phases of the heterogeneous material: mortar (\( E_m \)), aggregates (\( E_a \)) and ITZ (\( E_{\text{ITZ}} \)) [8]:

\[
\frac{L}{E} = \frac{L_{a1}}{E_a} + \frac{L_{\text{ITZ1}}}{E_{\text{ITZ}}} + \frac{L_m}{E_m} + \frac{L_{a2}}{E_a} + \frac{L_{\text{ITZ2}}}{E_{\text{ITZ}}}
\]

(1)

In the numerical simulations, the material properties are:
This formulation appears to be sufficient to reproduce the mechanical behavior at the meso- and macroscale under the elastic regime.

### 2.3 Fracture behavior

Different fracture laws can be found in the literature (i.e. linear or exponential softening laws in tension, hardening rules in compression) to account for the fracture behavior. However, for the present work, a simple brittle failure law (fig. 2c) has been tested in different configurations and provided satisfactory results. Brittle failure at local scale leads to quasi-brittle failure at global scale.

For a given load step, element stresses are computed and compared to their corresponding failure surface. The element with maximum stress-to-strength ratio is supposed to fail. Since shear interaction is also present, a Mohr-Coulomb failure surface (fig. 3) is used to account for other failure modes [6]. For the simulations, the following fracture parameters are used: $\phi = 35^\circ$, $c = 2f_t$ and $f_t = 4$ MPa.

### 3 DETERMINATION OF THE RVE SIZE

Many definitions for the RVE can be found in the literature, the most important are reviewed in [2]. Although there is not a single and exact definition of the RVE for an arbitrary heterogeneous material [3], the main idea is that the RVE should be large enough to keep the microstructural (meso- in our case) information, and small enough with respect to the macroscopic structural dimensions [2]. Moreover, to determine an RVE it is necessary to have (a) statistical homogeneity and ergodicity of the material; these two properties assure the RVE to be statistically representative of the macro response, and (b) some scale $L$ of the material domain, sufficiently large relative to the micro-scale $d$ (inclusion size) so as to ensure the independence of boundary conditions [12].
In any case, the determination of the RVE size depends on the material under consideration and the structural sensitivity of the physical quantity that is measured [1]. The definition of the governing parameter is quite important because different governing parameters may lead to different values for the RVE size. In general, macroscopic quantities such as elastic moduli or mesoscopic quantities such as peak stress can be taken.

In the present work, the elastic and hardening regimes are accounted for, hence macroscopic and mesoscopic are used, respectively.

3.1 Problem description

The authors’ lattice-particle model described in section 2 is used extensively in different tension tests until the peak-load, so that elastic and hardening regime variables can be measured (fig. 4).

Four different RVE sizes are taken into account, $D = 25, 50, 75$ and $100$ mm as represented in fig. 5; with two different aggregate distributions, $d_{max} = 8, 16$ mm referred to as $d8$ and $d16$, respectively (fig. 6).

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<th>Aggregate distributions</th>
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<td>d (mm)</td>
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When dealing with RVE tests one main issue is the definition of the boundary conditions. Commonly used boundary conditions include (a) linear displacements, (b) uniform traction and (c) periodic boundary conditions [13]. This choice will affect the results of homogenization methods including homogenized properties [3]. In this work, the boundary conditions are imposed according to [1, 3] as shown in fig. 4a. So far, in the author’s model particles are only randomly distributed within the domain, then two ways for applying constant displacement at one end are used: (i) as a linear variation in a thick layer of the specimen [10] and (ii) through strategically placed particles at the surface, these particles are quite smaller than the others resulting in elements mostly of mortar.
Therefore, two different meshes will be obtained, as shown in fig. 7, and will be referred to as $b0$ for (i) and $b1$ for (ii).

An event-driven algorithm as in [9] is numerically implemented to solve the system until the peak-load. The stress-strain curve is obtained by homogenization of the surface reactions and the imposed displacement. From this curve, the elastic modulus $E$ and peak stress (tensile strength) $f_t$ can be obtained, the former a macroscopic quantity, the latter a mesoscopic quantity. For the statistical analysis under the elastic regime another macroscopic parameter such as Poisson’s ratio $\nu$ is considered. A simple procedure to measure $\nu$ can be found in [8, 10].

### 3.2 Material regimes

Under tensile loading, concrete is a softening material in which three different consecutive regimes are present: (i) elastic, (ii) hardening and (iii) softening until failure.
According to Gitman [2], RVE can be found both in the linear-elastic and the hardening regime. But once in the softening regime, material loses its representativity and cannot be found. This is caused by the damage localization and therefore loses statistical homogeneity. On the other hand, Nguyen [3] specifies that an RVE does exist in the post-peak regime for softening materials but it should be emphasized that in this case the RVE refers to a localization band.

In the present work, the elastic modulus \( E \) is the chosen quantity for the elastic regime and the tensile strength \( f_t \) for the hardening regime.

3.3 Statistical analysis

A statistical analysis is performed with the information provided by the previous simulations. Two series of samples are taken, corresponding to the elastic and hardening regimes. For both series, four different configurations are considered: two boundary conditions type (b0 and b1) and two aggregate distributions (d8 and d16).

For the elastic regime, four RVE sizes are produced (\( D = 25, 50, 75 \) and 100 mm) and
nine tests are performed for each size. This is repeated for each configuration, resulting in a total number of 144 simulations.

On the other hand, three RVE sizes are produced \((D = 25, 50\) and \(75\) mm). Since the numerical resolution under the hardening regime is computationally more expensive, only five complete tension tests are submitted to analysis. As for the elastic regime, this is repeated for each size and configuration, resulting in a total number of 60 simulations. For both regimes, a total number of 204 simulations have been carried out.

With all these data, it is now possible to perform a statistical analysis. In the literature many considerations can be found: (a) expectation can give a measure of the convergence but for some variables this is not possible; (b) standard deviation which does give a measure of how sparse the results are for a given size, but still requires a criterion and (c) chi-square which gives a measure of the deviation with respect to the mean value and can be compared to the corresponding value for a 95\% accuracy test.

Let \(x\) be a given variable and \(\langle x \rangle\) its expectation, for a total number of realizations \(n\), the chi-square value can be obtained by the following equation:

\[
\chi^2 = \sum_{i=1}^{n} \frac{(x_i - \langle x_i \rangle)^2}{\langle x_i \rangle}
\] (2)

For an accuracy test of 95\% and the statistical degree of freedom equal to 2, the table value is \(\chi^2_{95\%} = 0.103\). The test is positive for \(\chi^2 \leq 0.103\), therefore the RVE size is found.

An RVE determination procedure is proposed in [2]. It consists of the following steps:

i Set an initial size, \(D_i = D_0\)

ii Generate \(n\), five at least, cubic specimens of size \(D_i\)

iii Perform the numerical simulations and obtain the stress-strain curve

iv Compute the corresponding \(\chi^2\) value

v Perform the accuracy test: if \(\chi^2 \leq 0.103\) then RVE size is achieved: \(D_i\); otherwise increase \(D_i\) and go to (ii)

4 RESULTS

There are many estimations of the RVE sizes by different approaches. Generally, following a theoretical estimation, Lemaitre [14] proposed a value of 100 mm for concrete. Experimental observations [15, 16] refined the RVE size to, approximately, \(D = (3 - 5) \, d_{\text{max}}\) and \(D = (7 - 8) \, d_{\text{max}}\). Using the concept of characteristic length [17, 18], another value of the RVE is proposed as \(D = (2.7 - 3) \, d_{\text{max}}\). Analytical approaches [19] suggest an RVE size to be \(D = 4.5d_{\text{max}}\).

Chi-square test results are presented below for the accounted regimes. The chosen quantities are the elastic modulus \(E\) for the elastic regime and tensile strength \(f_t\) for the hardening regime. Two cases are presented for each regime: \(b_0(d_{8-16})\), \(b_1(d_{8-16})\).
Figure 8: Chi-square tests for $E$ (upper), $\nu$ (medium) and $f_t$ (lower)
4.1 Elastic regime

From the results, we can clearly state that $E$ (fig. 8 - upper) seems to be a correct quantity. Results for $\nu$ (fig. 8 - medium) are also presented and shows very low values, passing the test for the first RVE size. Concerning the aggregate distribution, it can be seen that d8 converges before d16, as expected. For a same volume, d8 contains more particles allowing it to converge before. The use of boundary particles (b1) improves the results for smaller values of $D$. Boundary conditions on b0 are applied to a thick layer of particles and this is done sparsely for a low number of particles. RVE size results in 50 mm for this regime and shows a kink point at this value.

4.2 Hardening regime

In the hardening regime (fig. 8-lower), similar maximum chi-square values are obtained, although for the b0 configuration are slightly larger. In this configuration, d8 and d16 lead to similar results, but the chi-square criterion is firstly satisfied by the d8 specimen, as expected. Following this criterion, an RVE size of 45 mm results. On the other hand, for the b1 configuration this difference is larger and the RVE size for the d8 distribution is achieved from 35 mm and d16 from 45 mm.

5 CONCLUSIONS

In this paper, the determination of the RVE size in quasi-brittle materials, namely concrete, has been succesfully achieved by means of a lattice-particle model developed by the authors. The determination of the RVE size is of great interest within a multiscale framework.

Following Gitman’s procedure [2], satisfactory results have been obtained for the RVE size. Results show an RVE size of $D \approx 4d_{\text{max}}$, in accordance to experimental and analytical results presented in section 4. In general, an RVE size of 50 mm seems to be a good approximation.

Two different aggregate distributions have been considered to study the dependency on the RVE size. Larger RVE sizes are obtained for larger aggregates sizes, this is more evident for the b1 series. In any case, more aggregate distributions should be considered in order to state more defined conclusions. Also, two boundary configurations have been tested. The use of boundary particles (b1) has shown to be an efficient way to obtain more converging results. This is probably due to the way boundary conditions are applied. This paper should be considered a first approach and other periodic boundary conditions should be implemented. As pointed out in [3], the size of the RVE in the case of non-periodic boundary conditions is larger and the cases with and without wall-effect are relatively similar.

Discrete element models such as the lattice-particle model are very useful to gain insight in quasi-brittle materials. Lattice-particle models results attractive in the way that a large number of degrees of freedom are decreased contrary to large continuum-based models.
The extension to softening regimes and the use of other variables such as the energy dissipation are proposed for future research.

REFERENCES


