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GREYSCALE MARKER FOR THE MODELING OF THE FRACTURE PROCESS OF CEMENT MORTAR CONSIDERING THE HETEROGENEITY OF THE MICROSTRUCTURE

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Abstract: Cement-mortar is a type of particulate ceramic composite which is widely used as a binder in the construction industry. The complex fracture behavior of the structure depends mainly on the fracture characteristics of the cement in the mortar. Here, we have explored the microstructural characteristics of the cement-mortar using a novel X-ray computed tomography (XCT) technique. The cement mortar has been prepared using standard Madras sand and ordinary Portland cement. A specimen of size 20X20X20 mm^3 has been reconstructed with a resolution of 21.2 µm. A reconstructed 2D image of the cement -mortar is used for the mesoscale finite element simulations of the crack propagation. In the proposed model, the material properties of the mortar have been distributed among the finite elements based on the greyscale histogram of the reconstructed image to represent the heterogeneity of the material. The correlation between the material properties and grey scale values covered by an element has been established using a grayscale marker. Here, the greyscale marker has been defined by averaging the grey levels of the image covered in the finite element grid/window using in-house MATLAB code. Later, the cohesive interface elements (CIEs) were inserted in the finite element mesh to simulate the complex nonlinear fracture behavior of mortar in tension. The mechanical and fracture properties of the CIEs have been used from the literature and are also mapped to the same distribution. The effect of the window size has been studied on the stress-strain response and fracture pattern of the specimen. Finally, an optimum size of grid/window is recommended for the cement mortar.

1 INTRODUCTION

The main cause of failure in both natural and man-made materials is crack propagation till fracture. Fracture mechanics originated in the early 20th century through the pioneering efforts of Inglis [1] and Griffiths [2]. This scientific field has emerged to thoroughly investigate and understand how materials fail, providing critical insights for improved safety and performance of any design component [3-5]. The fracture mechanics field is not only limited to the mechanical field; people from civil engineering backgrounds also started using it to understand the failure behavior of cementitious materials, e.g., concrete [6,7].

The infrastructural development of any country mainly depends on the civil engineering industry. Concrete is a key cementitious material in civil engineering and possesses different phases, e.g., cement-mortar, aggregate, and interfacial transition zone (ITZ) etc. [8-9]. The concrete usually displays complex and nonlinear behavior even under simple loads. This complexity arises from its heterogeneous hierarchical microstructure [10,11]. Therefore, concrete failure is a multiscale phenomenon that requires careful consideration of its internal material properties [12]. Numerous numerical models i.e., Lattice model [13], Particle model [14], distinct finite element method (DEM) [15], Boundary finite element method (BEM) [16], finite–discrete element method (FDEM) [17], finite element model [18], and Cohesive Zone Modeling (CZM) [19], etc. have been developed for mesoscale concrete analysis. Each method has its pros and cons.

In more recent studies, concrete is explored at the mesoscale, predicting its failure behavior under various loading conditions using the image-based finite element method and digital image correlations [20]. The behavior of cement mortar significantly affects the fracture process of concrete. Therefore, there is a need for a robust model that can accurately represent the mechanical behavior of cement mortar, considering its microstructural characteristics and the associated uncertainties. Recently, we developed a model for the homogenization of cement mortar, where the mechanical behavior of particles is correlated with grayscale values using an image-based finite element approach. This study has demonstrated that the homogenization window has a significant impact on the effective properties of the material [21].

This study builds upon the author's earlier work on the grayscale distribution of mechanical properties for material points and use of CZM for crack propagation [22]. In this investigation, grid size effect on the 2D micro-scale finite element model has been studied.

2 IMAGE-BASED MODELLING

The cement mortar has been prepared using standard Madras sand and ordinary Portland cement. The water-cement ratio is 0.2. A 2D slice of the reconstructed microstructure of specimen (size 20X20X20 mm^3) with a resolution of 21.2 µm has been considered. The details of the reconstruction process of the cement mortar from XCT can be found in [21]. Figure 1 shows reconstructed the 2D image. A mesh/gride is superimposed on the images to generated microstructurally informed finite elements as shown in Figure 2. The microstructure information has been transferred to the finite elements using grey scale marker (*GSM*). GSM approximates the grayscale intensity distribution as a discrete function based on the area covered by the pixels within the elements. For simplicity, we employ the average function of the grayscale values of pixels as a marker for the element. Thus, we can say that

$$E^{ele} = \oint(x, y, Gm) \tag{1}$$

Here, E^{ele} is the elastic modulus of the finite element which is a function of co-ordinates in *x* and *y* directions, and gray scale marker *Gm*. Where *Gm* can be written as an average function of the grey scale values of the pixels curved in a finite element.

$$Gm = \frac{\sum_{i=1}^{np} G_i}{np} \tag{2}$$

Here, G_i is the grey scale value of the individual pixel within the element. Thus, the elastic modulus of the element can be expressed as

$$E^{ele} = \frac{Gm \times E'}{\langle Gm \rangle} \tag{3}$$

Here, $\langle Gm \rangle$ represents the average of the grey scale markers for all the elements and $E'$is the homogenous elastic modulus of the material.

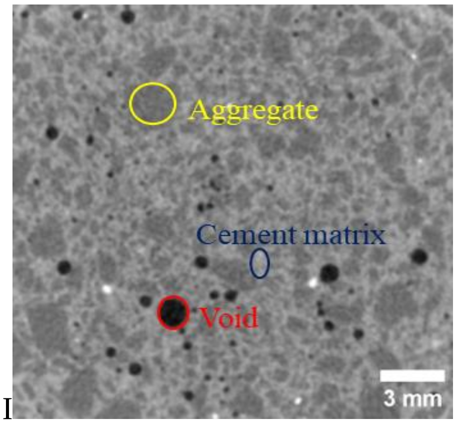

Figure 1: Reconstructed 2D image of Cement mortar

This correlation of the elastic modulus is caried out using an inhouse MATLAB script, which involves defining a Grayscale Marker (GSM).

Next, cohesive interface elements (CIEs) are inserted in the finite element mesh to model the crack initiation and propagation in the mortar. The four-nodded cohesive interface elements (known as CPH2D4 in Abaqus) with zero in-plane thickness are incorporated into the initial mesh to simulate the fracture process with the help of in-house MATLAB code. The final image-based 2D mesh is shown in figure 2.

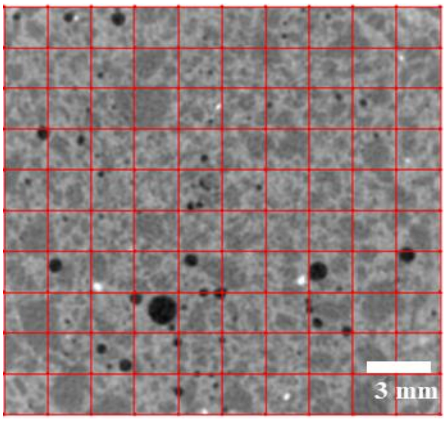

Figure 2: Mesh overlayed on the image

The material properties of the CIEs are also assigned using a normal distribution to include the uncertainties associated with the local strengths of the material points. The properties used for the 2D simulations are shown in Table 1 and Table 2.

3. NUMERICAL SIMULATIONS

Three mesh sizes 5×5, 10×10, and 25×25 are used to conclude the grid size sensitivity of the method. For all three cases, the uniaxial tension test is simulated using the boundary conditions shown in Figure 3. A displacement-controlled load simulation is conducted using the Abaqus/Explicit solver. A time step of 0.01s is utilized to resolve nonlinear equation systems, ensuring that the loading condition is quasi-static. The results are discussed in detail in the next section.

Table 1: Elastic properties of cement- mortar [23]

Elastic Modulus (GPa)	Poisson's ratio	Density (kg/m3)
30	0.2	2300

Table 2: Damage properties of CIE_INT [12]

Initial stiffness (MPa/m)	Tensile strength (MPa)	Shear strength (MPa)	Fracture energy (N/m)
10^9	3±0.5	1.5±0.5	30

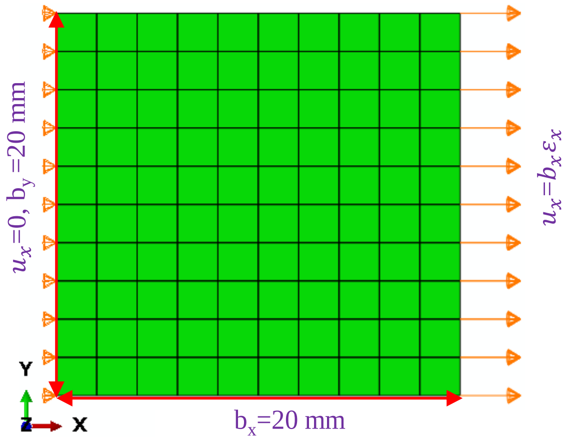

Figure 3: Boundary condition for uniaxial tension test

4. RESULTS

Figure 4 shows the mean stress-displacement curves of each grid size. The effective stress is calculated by dividing the total reaction force of the left edge node by the specimen height. It is observed that grid sizes 5X5 and 10x10 have a small nonlinear regime before the peak stress. Whereas, the finer grid 25x25 is mostly linear initially and has a small nonlinear regime near the peak. The peak stress is maximum in the case of the finer mesh (i.e. 25x25) with a sharper descending slope. On the other hand, the behavior of the other two grids is more or less similar.

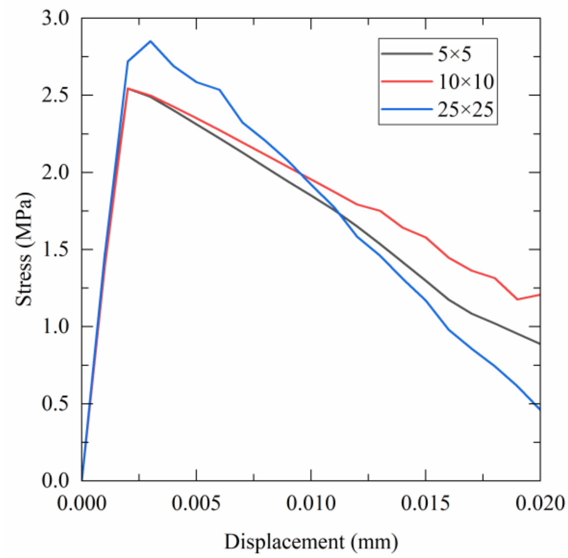

Figure 4: Stress–displacement curve for a cement mortar sample with different mesh size.

To explain the difference of the behavior of the stress-displacement curves the final crack pattern of all three cases are presented in Figure 5.

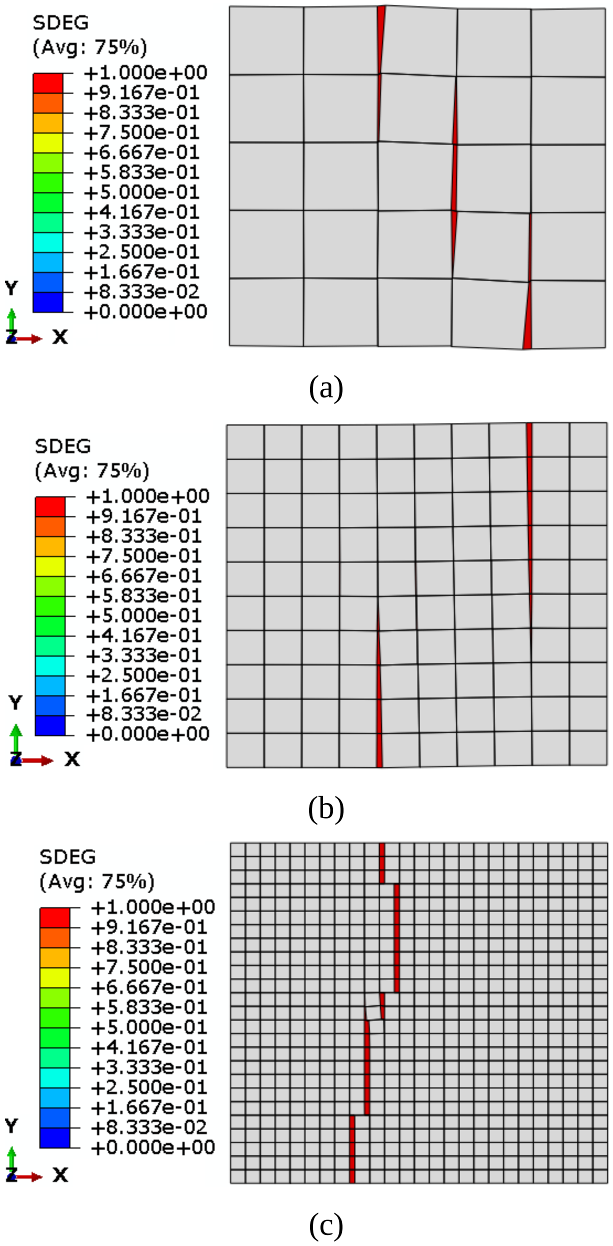

Figure 5: Cohesive fracture paths for a cement mortar sample with different discretization size (a) mesh size: 5×5 (b) (a) mesh size: 10×10 (c) mesh size: 25×25

The propagation of macrocracks is visualized by examining the scaler damage variable (SDEG) of cohesive interface elements in Abaqus/ODB. A displacement scale factor (DSF) of 15 is applied in all distorted crack patterns to improve the clarity in the images. There are three cracks appeared at different places in the case of 5x5 mesh (refer the red areas at top middle and bottom of the grid in figure 5a). In the case of grid sizes of 10×10, there are two cracks at distinct places (see the red color regions in Figure 5b). In the case of 25x25 grid size, the one crack has propagated through the RVE in a zig-zag fashion. As the grid size gets finer the local heterogeneity increases which gives the rise to different crack patterns that are responsible for the difference in the stress-displacement behavior of curves.

6. CONCLUSION

This study emphasizes the essential role of heterogeneity in stress localization and the crack propagation process. As the heterogeneity of the microstructure increases the local stress concentrations give rise to micro-cracks at distinct places that later emerge into micro cracks. The heterogeneity is diluted for larger sizes of the meshes as we have utilized the mean grey marker for the definition of the properties. Therefore the stress-displacement response is more or less similar in the case of courser mesh sizes. This shows that the proposed method is very effective in transferring the local behavior between the length scales.

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