Porous mesoscopic model and its application to the analysis of cement mortar properties and fracture

SUN XiaoXiao\(^1\), GUO XiaoMing\(^2\)\(^b\), CHEN XiangYu\(^3\)\(^c\) and DU JiaYu\(^3\)\(^c\)

\(^1\)No. 2 Southeast University Road, Jiangning District, Nanjing 211189, China
\(^2\)No. 2 Southeast University Road, Jiangning District, Nanjing 211189, China
\(^3\)No. 2 Southeast University Road, Jiangning District, Nanjing 211189, China
\(^a\)230169364@seu.edu.cn, \(^b\)xmguo@seu.edu.cn, \(^c\)220170969@seu.edu.cn

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Abstract. The porous mesoscopic model with high pore delivery quantity is established by the method of secondary development with the code of PYTHON. The process of damage evolution and mesoscopic fracture mechanism of cement mortar is studied. The result agrees well with the experiment and shows the stress concentration around micro-voids is the main reason contributing to damage of the surrounding cement paste, thus results in the convergence of micro-voids stripes which are vertical to loading direction to be cracks, and eventually leads to the fracture of specimen. The mesoscale parameters such as cement paste strength and porosity influence the mechanical properties of cement mortar.

Introduction

Cement mortar is one of the widely used materials in engineering construction and an important part of many kinds of composite materials. At mesoscopic level, cement mortar can be considered as a multiphase material consisting of cement paste, fine aggregates and a large number of initial defects in the form of micro-cracks and micro-voids \([1,2]\). Both the difference in mechanical properties between different constituents and complex internal structures will influence its macroscopic properties. According to the research \([3]\), as the defects in cement mortar, stress concentration will happen near micro-voids under external loads, which results in material damage, what’s more, leads to cracks initiation, growth and fracture of specimen. So it is necessary to analyze the mechanical behavior of cement mortar under mesoscopic level.

For decades, a large number of scholars have done various researches on cement-based materials. Ju Jiann-Wen \([4]\) proposed a cement mortar elastic damage constitutive model that takes the influence of micro-voids and fine aggregates into consideration, which confirmed that micro-voids and fine aggregates play a significant role in cracks initiation and propagation. This kind of constitutive considered the effect of meso-structure on material mechanical behavior, but the corresponding FEM model was still established in macroscopic scale, and there were still some gaps between actual situations. Sagar \([5]\) studied the crack propagation process in concrete and cement mortar by acoustic emission technology, and Ning Bao-Kuan \([6]\) analyzed the mesoscopic failure mechanism and bearing capacity of cemented soil by experiments. In addition, the Separate Hopkinson Pressure Bar Experiment was also applied to the study of dynamic performance of cement asphalt mortar \([7,8]\). In aspect of numerical simulation, anisotropic damage characteristics of cement mortar under impact load \([9]\) and the damage nucleation phenomenon in cement mortar under uniaxial compression load and sulfate attack \([10]\) were both studied deeply, which indicated the conclusion that the formation of cracks in cement mortar relating to the stress near surface of micro-voids. Under a finer scale, the coarse-grain model based on Gay-Berne free energy theory \([11]\) was applied to realize the simulation of cement mortar performance from nanoscale to mesoscopic scale.

According to the internal structural characteristics of cement mortar, a porous mesoscopic model with high pore delivery amount is established in this paper, considering the influence of fine aggregates and micro-voids on its macroscopic properties. The tensile failure process of cement
mortar is simulated and the mesoscopic mechanism of cement mortar fracture is studied. The results show that the porous mesoscopic model can accurately simulate the whole process of cement mortar fracture caused by damage evolution and the formation of cracks is closely related to the stress concentration near micro-voids.

**Organization of the Text**

**Establishment of porous mesoscopic model.** Cement mortar consists of fine aggregates, cement paste and a large number of micro-voids. The sizes of pores due to the use of the admixture or agitation process are usually $60 \sim 230\mu m$. For interlayer pores and capillary pores, the sizes are $0.5 \sim 2.5nm$ and $10 \sim 50nm$ respectively. The porous mesoscopic model established in this paper not only contains fine aggregates and cement pastes, but also takes micro-voids with sizes from $60\mu m$ to $230\mu m$ into consideration. The interlayer pores and capillary pores are not considered in the model because of the small sizes. The geometric shape of fine aggregates and micro-voids in the model is circular. Due to the small sizes, the geometric shape has little effect on results. So, circular is adopted to simplify the process of model establishment.

The fine aggregates and initial micro-voids distribute in cement paste randomly which occupy corresponding spatial positions and do not intersect with each other. Therefore, the delivery of aggregates and micro-voids in the model has to be carried out simultaneously with disjoint judgement. Taking Fig. 1 as an example, the boundary of cement mortar is determined by the rectangle area. When an aggregate is placed, a coordinate $(x_{ci}, y_{ci})$ is randomly generated in the rectangular area as the center coordinate of circle $A_i$, and its radius $r_i$ is randomly generated according to the grading of aggregates.

![Fig. 1 Fine aggregates and micro-voids delivery in the model](image)

Disjoint judgment is carried out based on Eq. 1 and Eq. 2. Firstly, Eq. 1 is applied to judge whether the generated aggregate $A_i$ is disjoint with the boundary. Here, $m$ is the parameter controlling distance between aggregate and boundary. If Eq. 1 is satisfied, Eq. 2 is applied to judge whether the aggregate $A_i$ is disjoint with any delivered aggregate $A_j$ $(j=0 \sim i-1)$. Here, $n$ in Eq. 2 is a parameter controlling distance between different aggregates. Although the distance between aggregates can be infinitely close, in order to form proper mesh, it is necessary to make the distance between aggregates greater than a suitable minimum.
\[
\begin{align*}
|x_i - x_n| &> r_i + m \\
|x_j - x_n| &> r_j + m \\
y_i - y_n &> r_i + m \\
y_j - y_n &> r_j + m \\
\sqrt{(x_n - x_i)^2 + (y_n - y_i)^2} &> r_i + r_j + n.
\end{align*}
\]

When the above conditions are satisfied, the randomly generated circular aggregate \( A_i \) is successfully delivered. The micro-voids are delivered in the model with similar method. The process is accomplished by secondary development in commercial FEM software ABAQUS.

The mechanical properties of the constituents in cement mortar are determined according to the following assumptions:
(1) The fracture toughness of fine aggregates is much higher than that of cement paste, so, it is assumed that the crack will not pass through fine aggregates and the damage of aggregates will not be considered.
(2) Cement paste is a quasi-brittle material with strain softening characteristics. Its mechanical behavior is simulated by a plastic damage model \([12]\) which can reduce the sensitivity of mesh scale to some extent.

**Simulation of cement mortar failure under tensile load.** Due to the small sizes of micro-voids, a large number of elements are needed to satisfy the requirements of calculation accuracy. Considering the computational efficiency, a small scale model is adopted in this paper. As shown in Fig. 2, a plane stress model with a size of 30 mm × 30 mm is adopted to simulate the process of cement mortar failure. The model contains enough fine aggregates and initial micro-voids and its size is much larger than three times of maximum aggregate’s size. So, it can reflect mechanical properties of cement mortar. The fine aggregates are river sands with particle size from 0.15mm to 4.75mm, and the apparent density is 2.6g/cm\(^3\). The diameters of micro-voids range from 60μm to 230μm, and the porosity is 7%. The elastic modulus of cement paste is 28.30GPa, its compressive strength, tensile strength and Poisson's ratio are 32.50MPa, 5.0MPa and 0.2 respectively. The elastic modulus of fine aggregate is 50.40GPa, and its Poisson's ratio is 0.16. The load is applied on right side of the specimen with velocity of 0.02 mm/s.

![Fig. 2 Cement mortar under tensile load (white circular: fine aggregates, black circular: micro-voids, gray region: cement paste)](image)
The FEM model is shown in Fig. 3. The triangular elements are used because they are suitable for the shape of aggregate and micro-voids’ boundary. There are about 1.69 million elements in the model.

As shown in Fig. 4, the simulation results of porous mesoscopic model are in agreement with experiment [13], indicating the efficiency of the proposed model. It can be seen that the stress decreases with the increment of displacement gradually because of the decrease of bearing capacity of cement mortar.

The internal damage evolution of cement mortar is shown in Fig. 5, which corresponds to points A to E in Fig. 4. The simulation of crack propagation is realized by deleting the failure elements in the model. As shown in Fig. 5(a) and Fig. 5(b), damage evolution is very slow before peak stress and there are no obvious cracks generated. However, because of the stress concentration near micro-voids, the damage of cement paste increases in this area, which leads to the formation of cracks between micro-voids. According to Fig. 5(c) ~ 5(e), the damage develops locally after peak stress, and cracks connecting a large number of micro-voids are formed. These cracks continue to converge and eventually penetrate the entire cement mortar specimen. The simulation results show that the position of cracks is affected by meso-structure of cement mortar, which leads to the randomness of failure mode of material. It also shows that micro-voids play an important role in promoting the initiation and propagation of cracks. The micro-void belts perpendicular to load direction is finally connected to form a macro-crack, which results in the fracture of material.
Effect of mesoscopic parameters on properties of cement mortar. Based on the established porous mesoscopic model, the effect of mesoscopic parameters such as cement paste strength and porosity on the properties of cement mortar is discussed.

Keep fine aggregate gradation and porosity unchanged, the tensile strength of cement paste is set to 5.0MPa, 5.5MPa, 6.0MPa and 6.5MPa respectively, and the equivalent elastic modulus and peak displacement of cement mortar are shown in Table 1. In order to reduce the influence of meso-structure randomness, the data is averaged. With the increase of cement paste strength, the equivalent elastic modulus and peak displacement of cement mortar are increased.
Table 1 Effect of cement paste strength on cement mortar’s properties

<table>
<thead>
<tr>
<th>Cement paste strength [MPa]</th>
<th>5.0</th>
<th>5.5</th>
<th>6.0</th>
<th>6.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalent elastic modulus [GPa]</td>
<td>21.5</td>
<td>22.8</td>
<td>23.9</td>
<td>25.3</td>
</tr>
<tr>
<td>Peak displacement [μm]</td>
<td>4.35</td>
<td>4.45</td>
<td>4.68</td>
<td>4.79</td>
</tr>
</tbody>
</table>

Table 2 Effect of porosity on cement mortar’s properties

<table>
<thead>
<tr>
<th>Porosity</th>
<th>3%</th>
<th>5%</th>
<th>7%</th>
<th>9%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalent elastic modulus [GPa]</td>
<td>27.4</td>
<td>24.1</td>
<td>21.5</td>
<td>17.2</td>
</tr>
<tr>
<td>Peak displacement [μm]</td>
<td>3.86</td>
<td>4.11</td>
<td>4.36</td>
<td>5.17</td>
</tr>
</tbody>
</table>

The effect of porosity on mechanical properties of cement mortar is shown in Table 2. With the increase of porosity, the equivalent elastic modulus of cement mortar decreases significantly and peak displacement increases. It is because that the integral stiffness is weakened by micro-voids in cement mortar.

Conclusions

In this paper, a porous mesoscopic model is established, which studies damage mechanism and mechanical properties of cement mortar under very fine scale. The main conclusions are as follows.

1. A porous mesoscopic model considering fine aggregates, micro-voids and cement paste is established. This model considers the fact that a large number of micro-voids existing in cement mortar and can simulate the whole process of cracks initiation, propagation and fracture of specimen.
2. The mesoscopic mechanism of cement mortar failure is analyzed. The crack initiation in cement mortar is closely related to the stress concentration near micro-voids. A series of micro-void belts perpendicular to load direction are connected to be cracks which causes the failure of specimen.
3. The influence of mesoscopic parameters on mechanical properties of cement mortar is studied. The increment of cement paste strength increases the equivalent elastic modulus and peak displacement of cement mortar and the increment of porosity reduce its equivalent elastic modulus.

Acknowledgements

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References


