SIMULATION OF THE DIFFUSIVITY OF CEMENT PASTE
SUBJECTED TO UNI-AXIAL TENSILE LOAD BY A 3D LATTICE
APPROACH

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Abstract

On the basis of the microstructural change of cement paste during a virtual uni-axial tensile test, the diffusivity of cement paste is predicted by use of a 3D lattice approach in this study. Based on an original microstructure of cement paste generated by the HYMOSTRUC3D model, the fracturing process of cement paste during a virtual uni-axial tensile test is simulated and the creation of micro-cracks are captured by use of 3D lattice fracturing model. A 3D diffusive lattice network is generated from the cracked cement paste where the diffusion coefficient of crack phase is assumed to equal to that of pore phase. By simulation of a virtual steady-state chloride diffusion test on the diffusive lattice network, the diffusion coefficient of cement paste subjected to tensile load can be predicted. Simulations have shown that a sharp increase of diffusivity takes place after the maximum load is reached in the uni-axial tensile test.

1. INTRODUCTION

Diffusivity of cement-based materials is an import factor with regard to the durability issue and the service life prediction of concrete structures. The diffusivity can be significantly increased because of the presence of defects, and in consequence, the service life is reduced. The defects (or in terms of cracks) may be introduced by mechanical loading, freezing/thawing, drying/wetting and so on. In order to study the mechanical loading effects on the transport property of cement-based materials, a number of experimental studies are
carried out [1-2]. In the modeling part, Gérard and Marchand [3] have proposed an analytical model to study the influence of traversing cracks (simple geometry) on the transport of ions in saturated concrete. Bernard et al. [4] have studied the effect of tensile cracking on the diffusivity of mortar by use of finite element method (FEM).

The diffusivity change of cement-based materials when subjected to mechanical loading, in principle, is caused by their microstructural change, i.e., the creation of micro-cracks. The microstructure evolution must be captured during the applying of the external load. The purpose of this paper is to study the influence of external tensile load on the diffusivity of cement paste on the basis of the microstructure evolution of cement paste. Based on a numerical model HYMOSTRUC3D, the original microstructure of cement paste is first generated. Then, micro-cracks are created in the microstructure of cement paste where uni-axial tensile load is applied, which is analyzed by use of 3D lattice fracturing model. Next, the damaged cement paste with micro-cracks is converted into a 3D diffusive lattice network, and from which the diffusivity of cement paste is predicted.

2. METHODOLOGY

The flowchart of numerically modeling the diffusivity of cement paste when subjected to uni-axial tensile load is illustrated in figure 1. The starting point is a microstructure of cement paste, which can be obtained by experiments such as X-ray micro-tomography (micro-CT) and focused ion beam or numerical simulations such as HYMOSTRUC3D, CEMHYD3D and Mic [5]. In this study, the original microstructure of cement paste without any damage is simulated by the HYMOSTRUC3D model [6-7]. From the simulated microstructure of cement paste, the fracturing process during a uni-axial tensile test is configured by a 3D lattice fracture model [8-10]. The creation of micro-cracks in cement paste with the increasing displacement can be obtained at this stage. Next, the damaged microstructure of cement paste with micro-cracks inside is digitized into a voxel-based microstructure. At last, a steady-state diffusion test is simulated on the digitized microstructure, and the diffusion coefficient of cement paste is predicted by a 3D diffusive lattice model.

2.1 HYMOSTRUC3D model

In the numerical model HYMOSTRUC3D, the cement particles are modeled as digitized spheres randomly distributed in a 3D body and the hydrating cement grains are simulated as growing spheres. As cement hydrates, the hydration products, in terms of inner and outer
product, are formed around the grain. Cement utilized in the simulation is CEM I 42.5N with a mineralogical composition of C₃S(64%), C₂S(13%), C₃A(8%) and C₄AF(9%). The minimum particle diameter is 1 µm and the Blaine value is 420 m²/kg. A specimen size of 100×100×100 µm³ is used. For cement paste with 0.4 w/c, the simulated microstructure at 0.93 degree of hydration is shown in Figure 2. In the 3D image of hydrated cement paste, the solid phases are, going from the center of a cement particle in outward direction, unhydrated cement (grey), inner product (red) and outer product (yellow), respectively.

2.2 Configuration of a virtual uni-axial tensile test

The 3D fracturing process of cement paste under uni-axial tensile load is performed by use of 3D lattice analysis through the following procedure: Generation of 3D lattice structure → Property determination of each element → Applying boundary conditions → 3D fracturing process. The output from the lattice analysis include the displacement-load diagram and the creation of micro-cracks (in terms of fractured elements).

2.2.1 Generation of 3D lattice structure

According to the microstructure of cement paste obtained from the HTMOSTRUC3D model, every hydrated cement particle is considered as a node and every two connected hydrated cement particles are considered as one beam element. The 3D lattice mesh generated from the hydrated cement paste with 0.4 w/c and 0.93 degree of hydration is illustrated in figure 3.

![Figure 2: 3D image of the microstructure of cement paste (w/c=0.4, α = 0.93).](image)

![Figure 3: 3D lattice mesh of cement paste (CEMI 42.5N, w/c=0.4, α=0.93).](image)

2.2.2 Property determination of each element

The Young’s modulus and shear modulus (Eₙ, Gₙ) of a node are the weighted averages of those of its component solid phases, and the Young’s modulus and shear modulus (E, G) of an element are the weighted averages of those of its two component nodes [9-10]. The tensile strength of an element is determined as 1/10000 of its Young's modulus. Research is ongoing to determine the true relationship between tensile stress analyzed with the model and tensile...
strength of the local material.

2.2.3 Applying boundary conditions
A prescribed displacement boundary condition is imposed. For the uni-axial tensile test, prescribed displacements are assumed to be imposed on the top and bottom surfaces in the x-direction, and the other surfaces in the y-direction and z-direction are free to expand and/or shrink.

2.2.4 3D fracturing process
The stress analysis is performed at this step. It is assumed that when the tensile stress is larger than the tensile strength of an element, the element fractures. In response to the element fractures, a micro-crack is created in the microstructure of cement paste. The simulated load-displacement diagram is shown in figure 4. At various displacements (point B, C, D in figure 4), the created micro-cracks is illustrated in figure 5.

![Load-displacement diagram](image1)

Figure 4 Load-displacement diagram ((CEMI 42.5N cement paste, \(w/c=0.4, \alpha = 0.93\))

![Micro-crack illustrations](image2)

Figure 5: Illustration of the creation of micro-cracks at different fracturing steps.

2.3 Microstructure digitalization
The microstructure of cement paste obtained from the HYMOSTRUC3D model is
represented by spherical particles (vector-presented), which can be digitized into voxel-presented microstructure, represented by pore, unhydrated cement, inner product and outer product. For cement paste with micro-cracks introduced by mechanical loading, cracked voxels are taken into account. Figure 6 illustrates the digitalization of micro-cracks into cracked voxels. The voxel-based microstructure (200×200×200 voxels) of cement paste after fractured by uni-axial tensile test is shown in figure 7.

![Figure 6: Illustration of the micro-crack is digitized as cracked voxels.](image)

Figure 6: Illustration of the micro-crack is digitized as cracked voxels.

![Figure 7: 3D image of voxel-based cement paste (w/c=0.4, α=0.93).](image)

Figure 7: 3D image of voxel-based cement paste (w/c=0.4, α=0.93).

### 2.4 Configuration of a virtual steady-state diffusion test

From the voxel-based microstructure of cement paste, a 3D diffusive lattice network can be constructed. Figure 8 illustrates how to determine a diffusive lattice element. A virtual steady-state chloride diffusion test is simulated in this part. The following assumptions are addressed in the simulation: (1) Both the non-damaged and damaged cement pastes are water saturated. (2) No ions’ fixation happens during the diffusion process. (3) The diffusive phase of cement paste is pore, cracked voxels, inner product and outer product. For the diffusive lattice element $ij$ relating voxel $i$ and voxel $j$, its diffusion coefficient $D_{ij}$ is [4]:

$$D_{ij} = \frac{2}{\frac{1}{D_i} + \frac{1}{D_j}}$$

(1)

$D_i$ and $D_j$ is the diffusion coefficient of voxel $i$ and voxel $j$, respectively. The flow along the element $ij$ is satisfied with Fick's first law,

$$q_{ij} = -D_{ij} \frac{dc_{ij}}{dx}$$

(2)

where $q_{ij}$ is the flow density through element $ij$. $c_{ij}$ is the concentration gradient. The diffusive lattice network of fractured cement paste is shown in figure 9, where the diffusive lattice elements are colored according to their chloride diffusion coefficient $D_{ij}$ in units of m$^2$/s. The
diffusion coefficient of chlorides in the pore solution/micro-cracks, outer product and inner product are $1.07 \times 10^{-10} \text{ m}^2/\text{s}$, $3.4 \times 10^{-12} \text{ m}^2/\text{s}$ and $8.3 \times 10^{-13} \text{ m}^2/\text{s}$, respectively [11-12].

The concentration boundary conditions are imposed on the 3D diffusive lattice network, as shown in figure 10. The concentration on the inlet surface and the outlet surface are $c_1$ and $c_0$ respectively. In this case, 1.0 mol/m$^3$ for $c_1$ and 0 mol/m$^3$ for $c_0$ are used. The concentration distribution in cement paste at steady-state can be obtained by conjugate gradient method (CG method) [13]. Figure 11 illustrates the chloride concentration distribution in fractured cement paste where the boundary condition is applied in $z$ direction.

![Figure 8 Determination of the diffusive lattice element](image)

![Figure 9: 3D diffusive lattice network of cement paste (w/c=0.4, $\alpha=0.93$).](image)

![Figure 10: Illustration of imposing concentration boundary conditions.](image)

![Figure 11: Concentration distribution in cement paste (w/c=0.4, $\alpha=0.93$).](image)

3. SIMULATION RESULTS

For original cement paste, figure 12 shows a comparison of the effective chloride diffusion coefficient of cement paste by experiments [14-17] and by simulation. Simulations are performed for ordinary Portland cement paste with different $w/c$ after hydration for about 83 days. The simulations are in good agreement with the experiments.
The influence of tensile strain on the diffusivity of cement paste is shown in figure 13. For cement paste which is subjected to tensile load in $x$ direction, in general, its chloride diffusivity in $y$ and $z$ directions increase sharply with the increasing tensile strain, and the chloride diffusivity in $x$ direction is not sensitive to the tensile strain. This might because with the increasing tensile strain in $x$ direction, an increased pore/crack connectivity is obtained in $y$ and $z$ direction. From the simulation results, it is also found that in $y$ and $z$ directions, a slight diffusivity increase is obtained before the peak (point B in figure 4), and the sharp increase of diffusivity takes place after the peak where cement paste is in an elastic-plastic stage.

![Figure 12: Simulated and tested results [14-17] of the effective chloride diffusion coefficient of cement paste.](image1)

![Figure 13: Dependence of chloride diffusivity of cement paste on tensile strain by simulation ($w/c=0.4$, $\alpha=0.93$).](image2)

4 SUMMARY

This paper gives a numerical tool to estimate the diffusivity of cement paste with micro-cracks introduced by uni-axial tensile load. On the basis of the microstructural change, the influence of tensile stress on the diffusivity of cement paste is studied. In this study, the 3D complex microstructure of cement paste is simulated by the numerical model HYMOSTRUC3D. The fracturing process of cement paste during a virtual uni-axial tensile test is simulated and the creation of micro-cracks are captured by use of 3D lattice fracturing model. The diffusion coefficient of cement paste with/without micro-cracks is predicted by use of 3D diffusive lattice model. For cement paste without cracks, simulations are in good agreement with the experiments. The diffusivity of cement paste with micro-cracks introduced by mechanical loading need to be validated further in the future study. Simulations have shown that a sharp increase of diffusivity takes place after the maximum load is reached in the uni-axial tensile test.

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