3D Simulation of micromechanical behavior of cement paste

Z. Qian, G. Ye, E. Schlangen & K. van Breugel
Microlab, Delft University of Technology, the Netherlands

ABSTRACT: Numerical modeling of fracture processes of brittle materials, such as cement paste, mortar, concrete and rocks, started in the late 1960s when the discrete and smeared cracking models were introduced. In the 1990s, Schlangen and van Mier proposed another numerical model to compensate the drawbacks of the discrete and smeared cracking models, which is called lattice fracture model. From then on, plenty of investigations were conducted to exploit various applications of lattice fracture analysis, and this contribution is one of them. This paper studies the fracture process of cement paste at microscale, especially the tensile strength, elastic modulus and cracking due to external mechanical loads. The study is based on the microstructure of hardening cement paste and attempts to reveal the relationship between the microstructure and its global performance. Moreover, the crack propagation during the fracture process is also investigated in detail. In this paper, the microstructure of hydrating cement paste is simulated by HYMOSTRUC3D first, and then it is converted into a voxel based image. In the next step, a lattice network is created and the local mechanical properties are mapped from the simulated microstructure. After that, the fracture process is simulated using lattice analysis to obtain the load-displacement diagram and crack propagation. A series of numerical experiments are carried out to illustrate the influences of various input parameters, for instance, the degree of hydration, the Blaine value of cement and the water/cement ratio.

1 INTRODUCTION

Numerical modeling of fracture processes of brittle materials, such as cement paste, mortar, concrete and rocks, started in the late 1960s when the discrete and smeared cracking models were introduced. In the 1990s, Schlangen and van Mier proposed another model to compensate the drawbacks of the discrete and smeared cracking models, which is called lattice model (Schlangen 1993, Lilliu 2007). From then on, plenty of investigations were conducted to exploit various applications of lattice analysis, and this contribution is one of them.

This paper studies the fracture process of cement paste at microscale (Qian et al. 2009b), especially the tensile strength, elastic modulus and cracking due to external mechanical loads. The study is based on the microstructure of hydrating cement paste and attempts to reveal the relationship between the microstructure and its global performance. Moreover, the microcracks propagation during the fracture process is also investigated in detail [Qian et al. 2008].

In this paper, the microstructure of cement paste is simulated by HYMOSTRUC3D [van Breugel 1997, Ye 2003] first, and then it is converted into a voxel based image. In the next step, a lattice network is created and the local mechanical properties are mapped from the simulated microstructure. After

that, the fracture process is simulated using lattice analysis to obtain the load-displacement diagram and microcracks propagation. A series of numerical experiments are carried out to illustrate the influences of various input parameters, for instance, the degree of hydration, the fineness of cement and the water/cement ratio.

2 SIMULATION OF MICROSTRUCTURE

The hydration and microstructure formation process of cement paste is simulated using the HYMOSTRUC3D model. The required inputs for this model consist of specimen size, mineralogical composition of the cement, cement fineness represented by Blaine value and water/cement ratio. The outputs include the degree of hydration diagram and the corresponding microstructure information of the hydrating cement paste system at every specified time point. The input and output of the HYMOSTRUC3D model are summarized in Figure 1.
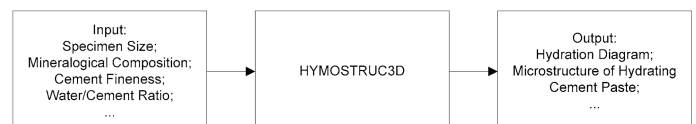

Figure 1. Input and Output of the HYMOSTRUC3D Model.

In the HYMOSTRUC3D model, it is assumed that only CSH (Calcium Silicate Hydrates) gel and CH (Calcium Hydroxides) gel are produced during the hydration process, furthermore the CH product is transferred to volume equivalent CSH product for simplicity. The CSH product is divided into inner product and outer product. Hence, the hydrating cement particle may consist of three layers in general, namely unhydrated cement, inner product and outer product. As the hydrating cement particle is assumed to be in the shape of sphere, the location of which is represented by sphere center coordinates and the size by diameters.

Hereby an example is given to illustrate the necessary input parameters for the HYMOSTRUC3D model and the corresponding outputs which indicate the microstructure of cement paste at a certain degree of hydration.

In this example, the hydrating cement paste is in the shape of a cube with the dimension of $100\times100\times100$ μm^3. The Blaine value of cement is $420 m^2/kg$ and the water/cement ratio is 0.4. The environment temperature is 20°C. The mineralogical composition of the Portland cement used in this study is given in percentage of weight content in Table 1.

Table 1. Mineralogical Composition of the Portland Cement CEM I 42.5N after [Ye 2003].

C_3S	C_2S	C_3A	C_4AF
64%	13%	8%	9%

Figure 2. shows one of the outputs from the HYMOSTRUC3D model, which is the degree of hydration diagram.
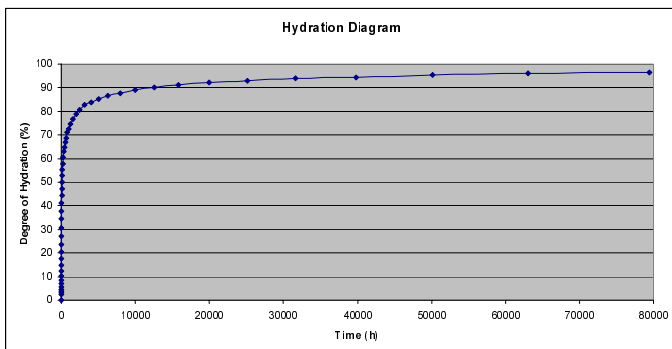

Figure 2. Relationship between the Degree of Hydration and Hydration Time.

At every time point in the above diagram, a microstructure of the hydrating cement paste system is obtained. Figure 3 shows the image of the microstructure of the cement paste at the hydration time 635 hours, and the corresponding degree of hydration is 69%.

The above microstructure is described analytically by the sphere particle center coordinates and the diameters. In order to facilitate the following lattice construction, it is necessary to digitize the above microstructure into a voxel-based image as shown in Figure 4, the resolution of which is 1 μm/voxel. In total, five different phases can be identified, including one void phase and four solid phases which are unhydrated cement, inner product, outer product and mixed phase. The mixed phase is a combination of the unhydrated cement, the inner product and the outer product.
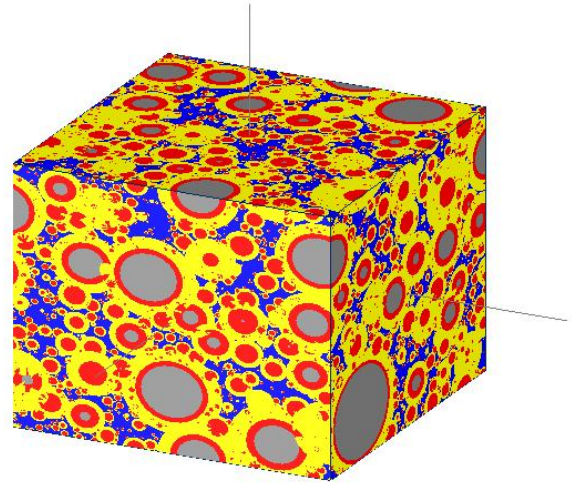

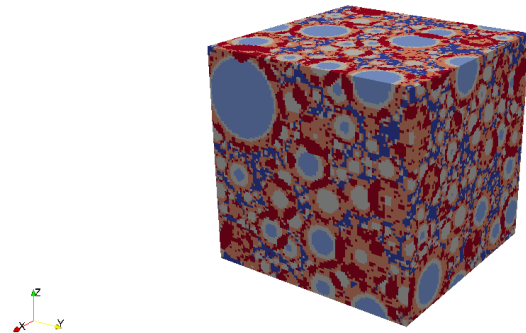Figure 3. The Microstructure of Cement Paste (Blaine Value=420 m^2/kg, Water/Cement=0.4, Degree of Hydration=69%, Size=100×100×100 μm^3).

Figure 4. The Voxel-based Microstructure of Cement Paste (Blaine Value=420 m^2/kg, Water/Cement=0.4, Degree of Hydration=69%, Size=100×100×100 μm^3, 1μm/voxel).

The elastic properties of the solid phases can be measured or simulated as presented in [Sanahuja et al. 2007, Manzano et al. 2007, 2009], the values of which are scattered due to different measurement techniques applied. Table 2 shows the elastic properties of solid phases employed in this paper.

Table 2. Elastic Properties of Solid Phases.

Phase	Solid Phase	Young's Modulus E (GPa)	Shear Modulus G (GPa)
1	Unhydrated Cement	130	50
2	Inner Product	30	12.1
3	Outer Product	22	8.87
4	Mixed Phase	60.7	23.7

3 MECHANICAL PERFORMANCE EVALUATION OF MICROSTRUCTURE

The lattice fracture model was applied a lot in the last two decades to simulate the fracture process of cement-based materials [Schlangen et al. 2009]. In this paper, a quadrangular lattice structure is constructed first, and then the local mechanical properties of lattice elements are mapped on the basis of the microstructure of cement paste. A pre-processing package called ImgLat (Image to Lattice) is developed to create the lattice system. The next step is to apply a prescribed displacement on the top and bottom surfaces of the cubic specimen. The fracture process simulation starts and the broken lattice elements are removed from the system gradually until the system cannot sustain any load. The package GLAK (Generalized Lattice Analysis Kernel) is built to complete the task. The outputs of fracture process simulation are the load-displacement diagram and microcracks propagation. The load-displacement diagram reveals the tensile behavior of cement paste at microscale, from which the elastic modulus and tensile strength can be obtained. The procedures are elaborated in the following subsections.

3.1 Lattice Mesh

In every voxel a sub-voxel is generated first, the length ratio of the sub-voxel and the voxel is defined as randomness. The randomness represents the heterogeneity of the materials. In this paper, the randomness is set to 0 for all the boundary voxels and 0.5 for all the other voxels. This configuration would yield to a realistic crack pattern and a regular specimen shape. After all the voxels and sub-voxels are meshed, a lattice node is positioned within every sub-voxel randomly, and then all these lattice nodes are connected by lattice beam elements. However, if the voxel represents void phase, then no lattice node is generated in that voxel. The result of 3D lattice construction is given in Figure 5.
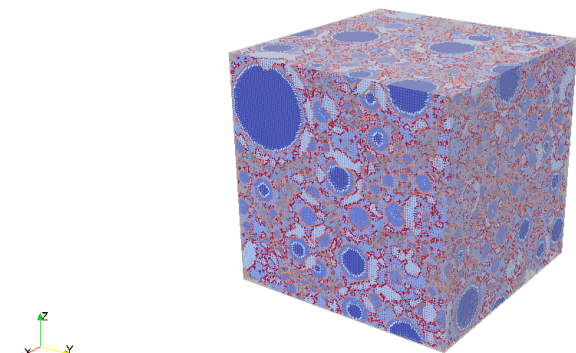

Figure 5. 3D Lattice Construction on top of the Voxel-based Microstructure of Cement Paste.

The cross-section of lattice element is assumed to be circular, and its area is equal to the perpendicular voxel surface area, which is 1 μm^2 in this paper. An alternative approach to determine the cross-section area of lattice element is proposed by Bolander in [Bolander & Sukumar 2005]. The elastic modulus of lattice element is the simple average of the modulus of its node phases.

For the fracture analysis, it is also required to specify the local strength for every lattice element. This parameter should be obtained from lab experiment, however, there is insufficient information about the local strength of each phase at microscale currently, hence, it is assumed that the local tensile strength of each lattice element is proportional to its Young's modulus and the proportional coefficient is 0.0001 [Schlangen & Garboczi 1997], the local compressive strength is infinite which means the lattice element can never fail if it is in compression.

3.2 Uni-axial Tensile Test

A uni-axial test is carried out on the lattice system, the external load is imposed on the top and bottom surfaces in the z-direction and all the other four surfaces are free to expand and/or shrink as shown in Figure 6.
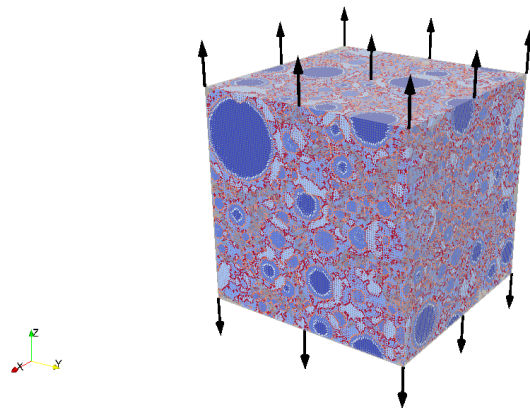

Figure 6. Applied Load and Boundary Conditions.

3.3 Fracture Process Simulation

The kernel part of lattice fracture analysis is the simulation of fracture process, the results of which are the load-displacement diagram and the microcracks propagation. The load-displacement diagram reveals the tensile behavior of cement paste at microscale, from which the elastic modulus and tensile strength can be obtained.

The basic idea of lattice analysis is that imposing a prescribed displacement on the lattice structure, finding the critical lattice element that has the highest stress/strength ratio, removing it from the system, recomputing the stress distribution. This procedure is repeated until the system fails.

Roughly speaking, lattice analysis is a set of linear analysis on the lattice structure using Finite Element Method. This implies that the fundamental of lattice analysis is nothing else but the conventional structural analysis. As a result, the steps required for lattice analysis are quite similar to the standard finite element analysis for frame structure, except that the critical element is removed and the analysis is repeated until the system fails as shown in Figure 7.
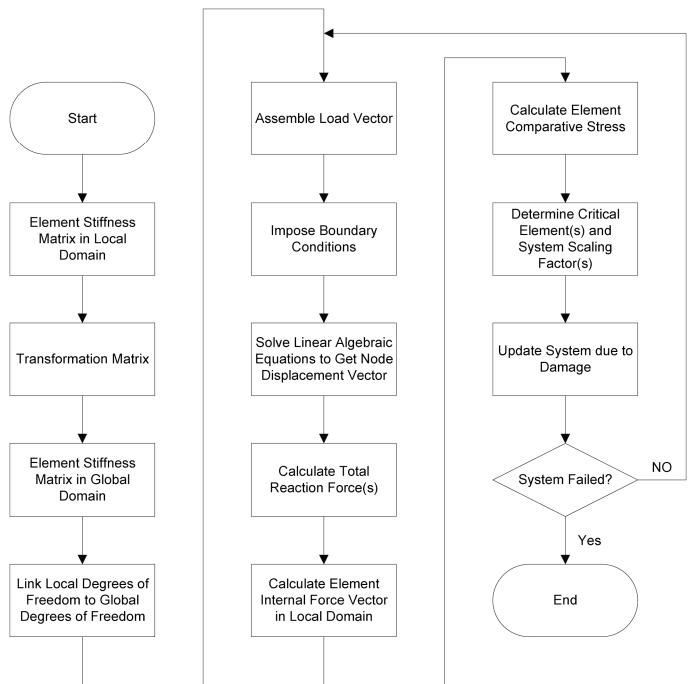

Figure 7. The Flowchart of GLAK (Generalized Lattice Analysis Kernel).

The fracture process simulation by GLAK is the most time consuming part through the entire numerical analysis. An attempt is made to parallelize the GLAK implementation in [Qian et al. 2009a] to reduce computational time.

4 MICROMECHANICAL BEHAVIOR OF CEMENT PASTE

The fracture process in cement paste is influenced by some physical factors. In this paper, the influences of the degree of hydration, the fineness of cement and the water/cement ratio are investigated through a set of numerical experiments at micro scale. The microstructures of cement paste are simulated by the computer model HYMOSTRUC3D. The reference case is defined in Table 3.

Table 3. Reference Input Parameters.

Degree of Hydration	Blaine Value of Cement	Water/Cement Ratio
69%	420 m^2/kg	0.4

4.1 Influence of Degree of Hydration

The degree of hydration is varied at 44%, 69% and 90% respectively, the corresponding load-displacement diagram for uni-axial micro tensile test is given in Figure 8. It is observed that the hydrating cement paste system with higher degree of hydration always has higher tensile strength and higher elastic modulus, furthermore it also behaves more brittle.
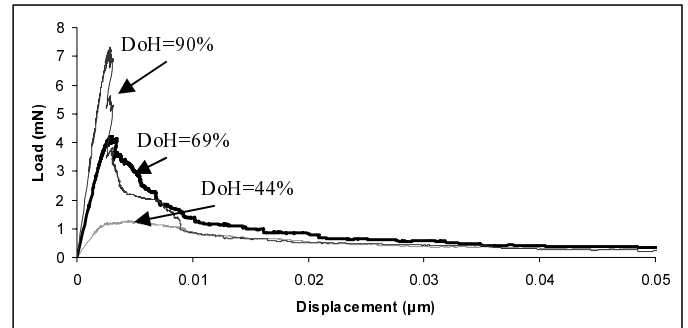

Figure 8. Load-displacement Diagrams at Different Degrees of Hydration (Blaine Value=420 m^2/kg, Water/Cement=0.4).

To study the influence of degree of hydration on the micro-crack propagation, it is necessary to compare the micro-crack patterns of damaged cement paste in final failure state as shown in Figure 9a~c. The results reveal that the micro-cracks are more localized for the damaged cement paste system with higher degree of hydration.
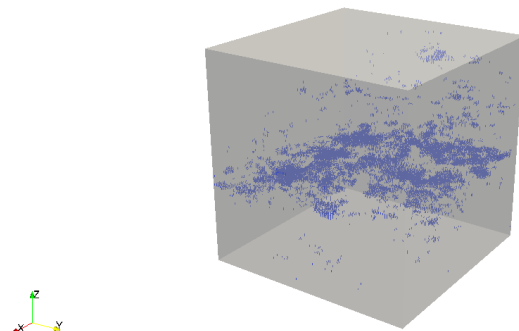

Figure 9a. 3D Micro-crack Pattern in Final Failure State with Degree of Hydration 44%.
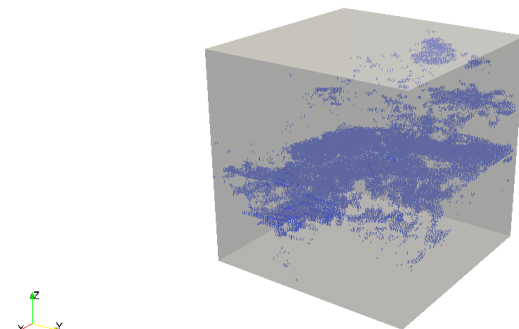

Figure 9b. 3D Micro-crack Pattern in Final Failure State with Degree of Hydration 69%.
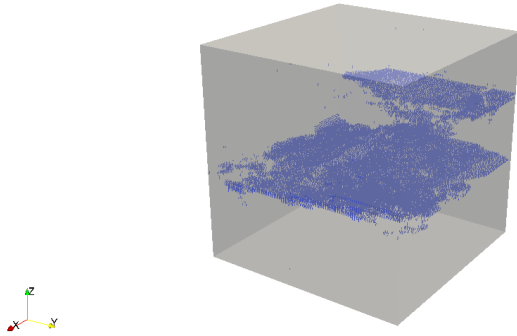
Figure 9c. 3D Micro-crack Pattern in Final Failure State with Degree of Hydration 90%.

4.2 Influence of Cement Fineness

The cement fineness has important influence on the mechanical properties of hardened cement paste and it can be represented by the Blaine value. The higher the Blaine value is, the finer the cement will be. In this study, three different Blaine values are taken which are 210 m^2/kg, 420 m^2/kg and 600 m^2/kg respectively. The load-displacement diagrams for different fineness of cement are presented in the Figure 10. It is obvious and reasonable that finer cement always gives higher tensile strength because of a denser microstructure. It is also interesting to observe that the elastic modulus remains the same, which means it is independent of the fineness of cement.
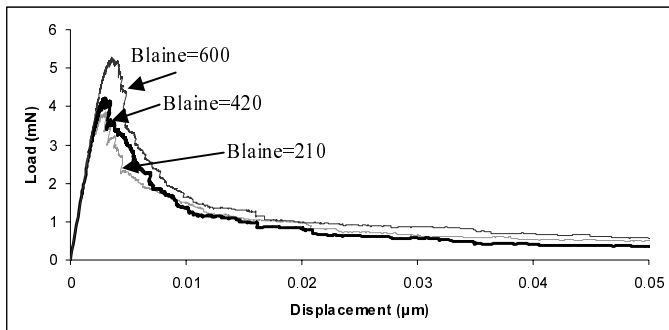

Figure 10. Load-displacement Diagrams for Different Fineness of Cement (Degree of Hydration=69%, Water/Cement=0.4).
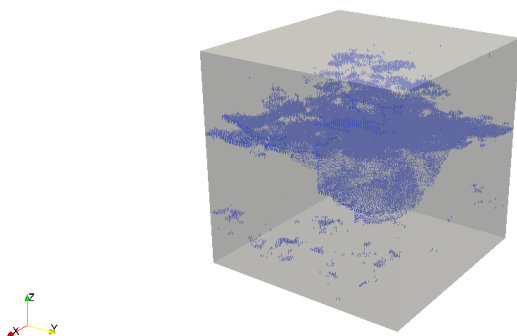

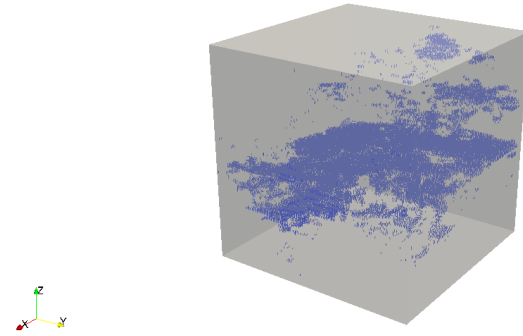Figure 11a. 3D Micro-crack Pattern in Final Failure State with Blaine Value 210 m^2/kg.

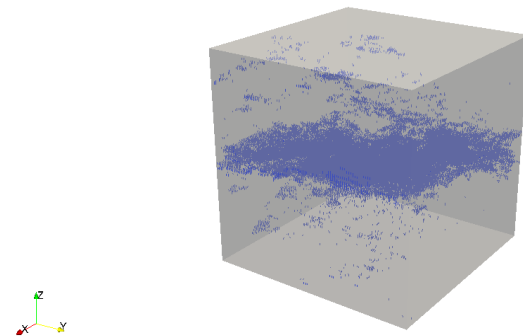Figure 11b. 3D Micro-crack Pattern in Final Failure State with Blaine Value 420 m^2/kg.

Figure 11c. 3D Micro-crack Pattern in Final Failure State with Blaine Value 600 m^2/kg.

For the comparison of micro-crack patterns, three figures are given for the damaged cement paste system with different fineness of cement as shown in Figure 11a~c. For finer cement system, the micro-cracks are more localized

4.3 Influence of Water/Cement Ratio

Water/cement ratio is another import factor which influences the mechanical behavior of cement paste significantly. Three different water/cement ratios are set and studied, all of which are often applied in engineering practice. Figure 12 illustrates the fracture behavior of cement paste with different water/cement ratios at 0.3, 0.4 and 0.5 respectively. From the load-displacement diagram, it is apparent that lower water/cement ratio corresponds with higher tensile strength and larger elastic modulus.

It is worth mentioning that the degree of hydration cannot increase further for the case water/cement ratio 0.3, hence the tensile strength at degree of hydration 69% is almost the ultimate strength. On the other hand, the tensile strength for the other two cases (water/cement ratio 0.4 and 0.5) will increase when the hydration continues, so the ultimate strength will be higher than it is shown in Figure 12, however, it is most likely always smaller than the ultimate strength for the case water/cement ratio 0.3.
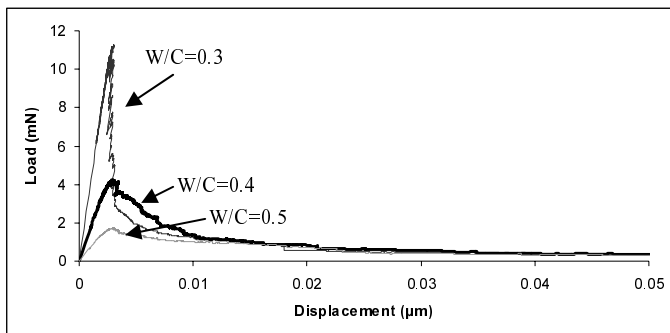
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Figure 12. Load-displacement Diagrams for Different Water/Cement Ratios (Degree of Hydration=69%, Blaine Value=420 m²/kg).

Figure 13a~c show the 3D micro-crack pattern for the damaged cement paste with water/cement ratio 0.3, 0.4 and 0.5 respectively. It is found that more localized crack pattern is observed for the cement paste system with lower water/cement ratio.
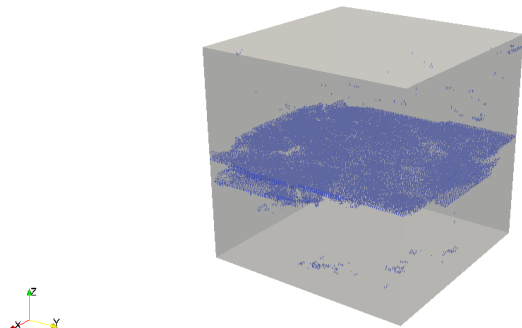

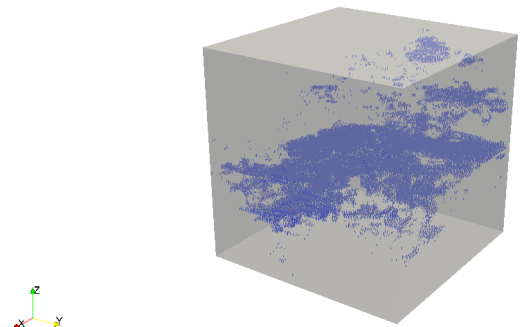Figure 13a. 3D Micro-crack Pattern in Final Failure State with Water/Cement Ratio 0.3.

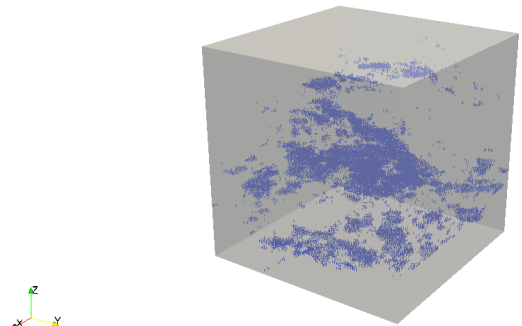Figure 13b. 3D Micro-crack Pattern in Final Failure State with Water/Cement Ratio 0.4.

Figure 13c. 3D Micro-crack Pattern in Final Failure State with Water/Cement Ratio 0.5.

5 CONCLUSIONS

A 3D micromechanical model is built up for the fracture process simulation of cement paste at microscale. The global mechanical properties can be predicted provided that the microstructure and local mechanical properties are known.

In this paper, the microstructure of cement paste is simulated by the hydration and microstructure formation model HYMOSTRUC3D, the output of which is then converted into a voxel-based image. A 3D quadrangular lattice system is constructed based on the microstructure using the package ImgLat (Image to Lattice) and a fracture process is simulated for a uni-axial tensile test using the package GLAK (Generalized Lattice Analysis Kernel). The final simulation results are reported in terms of load-displacement diagram and micro-cracks propagation, from which the elastic modulus and tensile strength can be obtained.

A set of numerical experiments are carried out to investigate the influences of various parameters on the mechanical behavior of cement paste at micro scale, for instance, the degree of hydration, the fineness of cement and the water/cement ratio. The hydrating cement paste with higher degree of hydration, higher Blaine value and lower water/cement ratio always shows higher elastic modulus and tensile strength at microscale, except that the Blaine value has no significant influence on the elastic modulus. Lower water/cement ratio system most likely produces higher ultimate micro tensile strength. More localized microcracks pattern can be observed for the damaged cement paste system with higher degree of hydration, higher Blaine value and lower water/cement ratio.

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