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INFLUENCES OF MINERAL COMPOSITION OF CEMENT ON THE MECHANICAL PROPERTIES OF CEMENT PASTE

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Abstract

The hydration processes and products are dependent on the mineral composition of cement, which determine the microstructure of cement paste and eventually its mechanical properties. Hence the mechanical performance of cement paste can be altered by changing the cement mineral composition. The ordinary Portland cement usually consists of C_3S, C_2S, C_3A and C_4AF. In this article four special combinations of constitutes are made to study the effect of C_3S and C_2S on the mechanical properties of cement paste, which include 100%C_3S, 70%C_3S+30%C_2S, 30%C_3S+70%C_2S and 100%C_2S.

The microstructure of cement paste is simulated by the HYMOSTRUC3D model, and then it is evaluated by the 3D lattice fracture model for its global mechanical properties such as Young's modulus, tensile strength and fracture energy, as well as the microcracks propagation and patterns.

The findings in this investigation reveal the relationship between the global mechanical performance of cement paste and the mineral composition of cement. The simulation results suggest that the mineral composition of the ordinary Portland cement is already optimized, as the corresponding cement paste shows the best mechanical performance.

1. INTRODUCTION

The mechanical performance of cement-based materials such as concrete is closely related to the mechanical properties of cement paste. The microstructure of cement paste determines its global properties. During the hydration process a number of factors may influence the microstructure development of cement paste, such as water/cement ratio, cement fineness and the mineral composition of cement. An investigation is carried out to reveal the relationship between the mechanical properties of cement paste and the mineral composition of cement.

The ordinary Portland cement usually consists of four phases, which are C_3S, C_2S, C_3A and C_4AF. The mass percentage of these four phases varies across different types of cement. For example the CEM I 42.5N is normally made up of 64% C_3S, 13% C_2S, 8% C_3A and 9% C_4AF. The investigation in this article focuses on the constituents C_3S and C_2S.

The microstructure of cement paste can be obtained either experimentally or numerically. The micro X-ray computed tomography (CT) [1] offers a non-destructive experimental technique to collect microstructure information of cement paste in terms of digitized voxels. Computer modeling packages are also available to simulate the cement hydration and microstructure formation processes, for instance, the HYMOSTRUC3D model developed by TU Delft [2, 3], the NIST CEMHYD3D toolkit [4] and the Mic model by EPFL [5]. In this investigation the HYMOSTRUC3D model is used to simulate the microstructure of cement paste.

After obtaining the microstructure of cement paste, the 3D lattice fracture model is employed to simulate the fracture behaviors of the cement paste [6, 7]. A uniaxial tensile test is set up and simulated on the cement paste to predict its Young's modulus, tensile strength and fracture energy, as well as the microcracks propagation and cracks pattern in final failure state.

The combined application of the hydration and microstructure formation model (HYMOSTRUC3D model) and the mechanical performance evaluation model (3D lattice fracture model) is sketched in Figure 1.

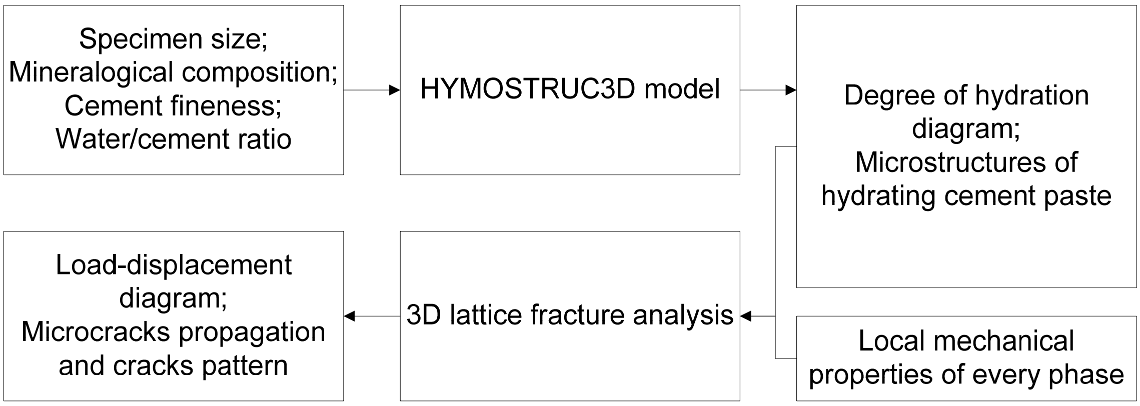


Figure 1 Combined application of the HYMOSTRUC3D model and the 3D lattice fracture model

In this investigation the specimen size is fixed at $100 \times 100 \times 100\ \mu m$, the water/cement ratio is 0.4, the Blaine value of the cement is $600\ m^2/kg$, and the microstructure of cement paste at the curing age of 28 days is simulated and evaluated for its mechanical performance. The mineral composition of the cement is varied and listed in Table 1.

Table 1 Mineral compositions of the cements used in this investigation

Combination	C_3S	C_2S
(a)	100%	0
(b)	70%	30%
(c)	30%	70%
(d)	0	100%

2. MICROSTRUCTURE OF CEMENT PASTE

The ordinary Portland cement usually consists of C_3S, C_2S, C_3A and C_4AF. Four special combinations are made to study the effect of C_3S and C_2S on the mechanical properties of cement paste, as given in Table 1. These special cements are produced in laboratory by Italcementi in Italy [8]. The particle size distribution are measured and then hydration tests are carried out by CSIC (Spanish National Research Council) in Spain [9]. Several batches of the special cements are measured and a Rosin-Rammler distribution $F(x) = 1 - e^{-bx^n}$ with $n = 1.014$ and $b = 0.0754$ is fitted, as shown in Figure 2. The corresponding Blaine value is $600\ m^2/kg$. The fitted curve will be used in the HYMOSTRUC3D model to simulate the microstructures of cement paste.

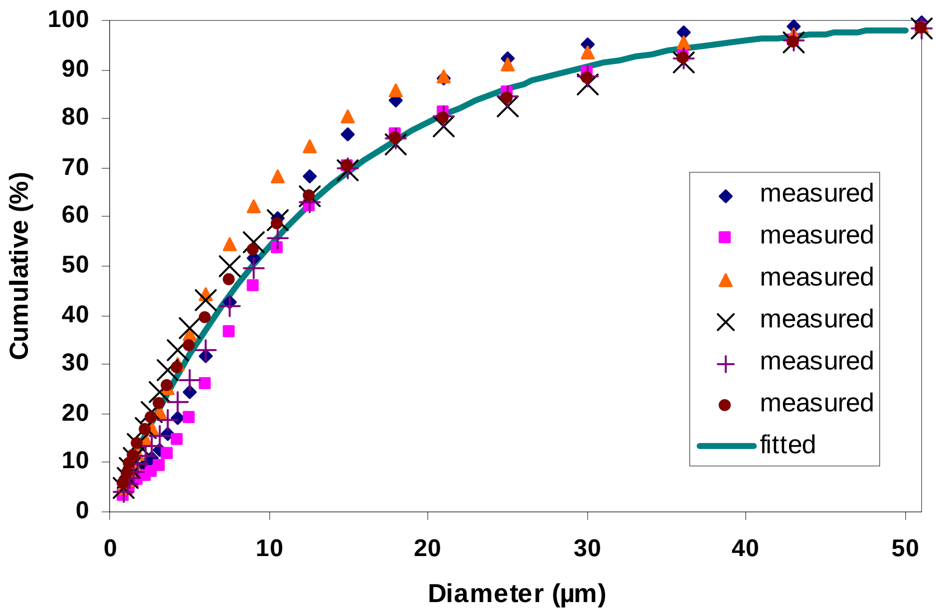


Figure 2 Particle size distribution of the special cements

The water/cement ratio is 0.4 and the specimen size is $100 \times 100 \times 100\ \mu m$ in the numerical experiment. The initial microstructures of cement paste for the four combinations of mineral compositions are the same, because the same particle size distribution and water/cement ratio are applied, as shown in Figure 3.

The degrees of hydration are measured and simulated for the four combinations respectively, and the resulting hydration diagrams are shown in Figure 4. The microstructures at the curing age of 28 days are taken for further analysis, as shown in Figure 5. The corresponding degree of hydration and phase segmentation are given in Table 2. It is observed that C_3S hydrates faster than C_2S by comparing the combination (a) and (d). However the combination (b) hydrates faster than pure C_3S even though it consists of some C_2S. This phenomenon can be explained by separating the hydrations of C_3S and C_2S. The combination (b) can be obtained by replacing 30% C_3S with C_2S based on the combination (a). At 28 days the 30% C_2S consumes less water than C_3S as C_2S hydrates slower, the effect is the 70% C_3S

could attract more water, thus its hydration process speeds up. The 30% C_2S hydrates slower while the 70% C_3S hydrates faster, the net effect is determined by the amount portions of C_3S and C_2S. When the weight of C_2S is increased to 70%, as shown in the combination (c), the hydration rate is decreased.

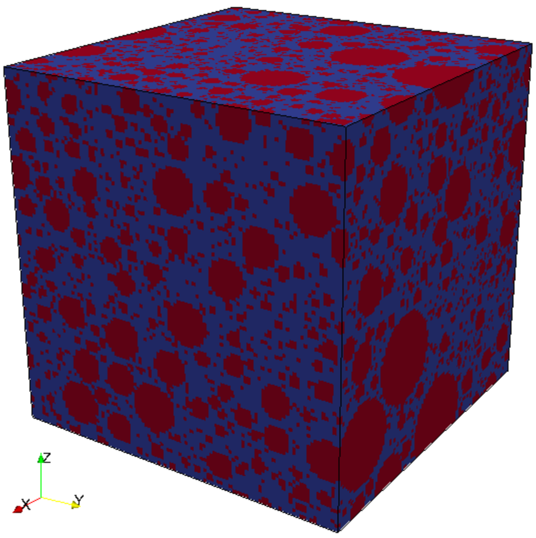
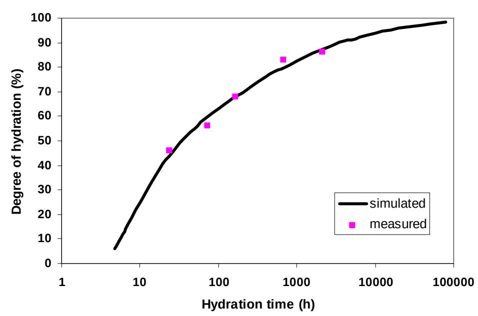
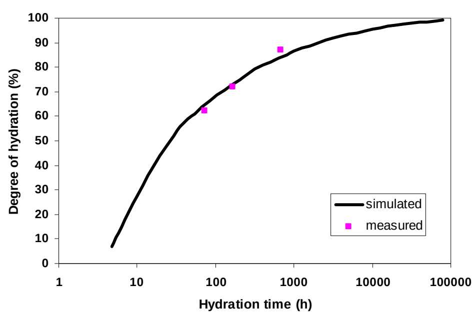


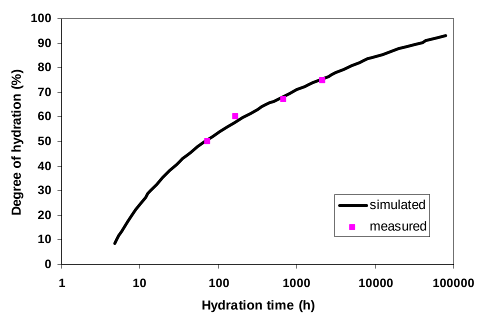
Figure 3 Initial microstructure of the special cement paste (porosity=56%)



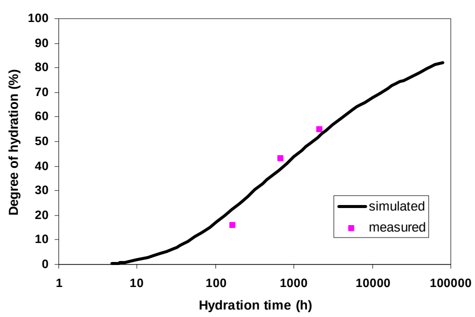
(a) Combination 100%C_3S



(b) Combination 70%C_3S+30%C_2S

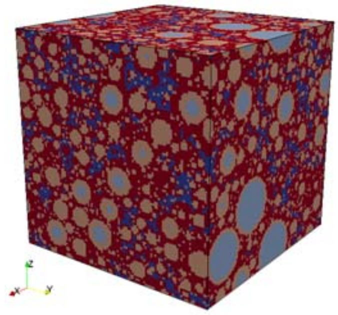


(c) Combination 30%C_3S+70%C_2S

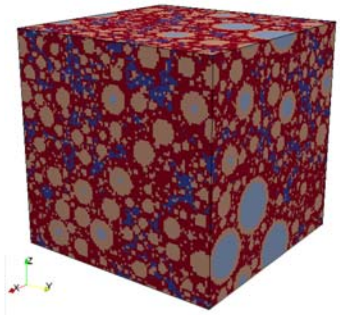


(d) Combination 100%C_2S

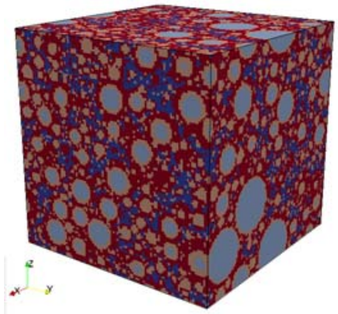
Figure 4 Degree of hydration diagrams for the special cement pastes



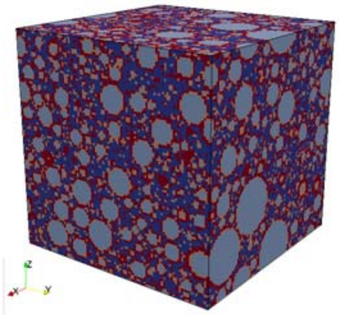
(a) Combination 100%C_3S (porosity=8%)



(b) Combination 70%C_3S+30%C_2S (porosity=6%)



(c) Combination 30%C_3S+70%C_2S (porosity=12%)



(d) Combination 100%C_2S (porosity=30%)

Figure 5 Microstructures of the special cement pastes at the curing age of 28 days

Table 2 Degree of hydration and phase segmentation for the special cement pastes at the curing age of 28 days, corresponding with Figure 5

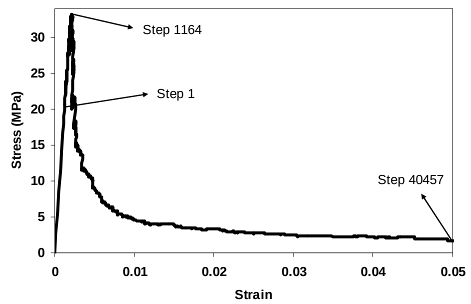
Combination	Degree of hydration	Pore	Unhydrated cement	Inner product	Outer product
(a)	79%	8%	9%	35%	48%
(b)	84%	6%	7%	37%	50%
(c)	68%	12%	14%	30%	44%
(d)	38%	30%	27%	17%	26%

3. MECHANICAL PERFORMANCE EVALUATION

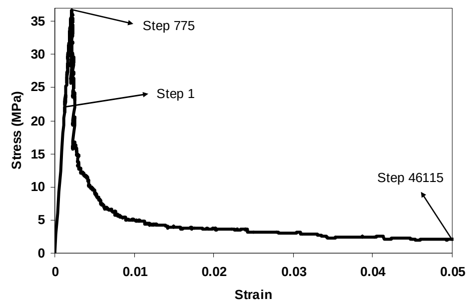
The 3D lattice fracture model is employed to evaluate the mechanical performance of the microstructures in Figure 5 through simulating a uniaxial tensile test. The local mechanical properties for individual solid phases are given in Table 3. More details about the modeling procedures to simulate the test can be found in [10]. The resulting stress-strain response diagrams are shown in Figure 6. Some global mechanical properties are computed and summarized in Table 4 based on Figure 6. The microcracks in final failure state are shown in Figure 7. The combination (b) has the best mechanical performance in terms of Young's modulus and tensile strength, and the most localized cracks pattern, as its degree of hydration is the highest one among the four combinations. This suggests that the mineral composition of the ordinary Portland cement is already optimized, as combination (b) is the most similar one to the ordinary Portland cement.

Table 3 Assumed local mechanical properties of solid phases of cement paste

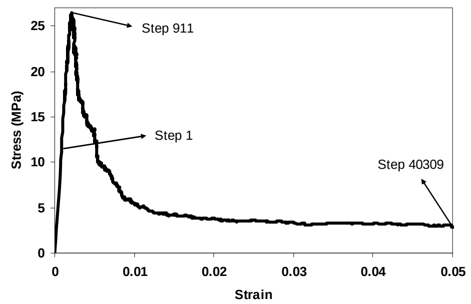
No	Solid phase	Young's modulus E (GPa)	Shear modulus G (GPa)	Tensile strength f_t (GPa)
1	Unhydrated cement	135	52	1.8
2	Inner product	30	12	0.24
3	Outer product	22	8.9	0.15



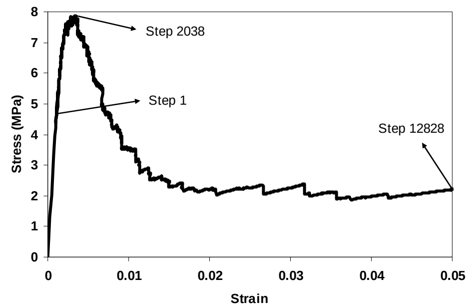
(a) Combination 100%C_3S (degree of hydration=79%)



(b) Combination 70%C_3S+30%C_2S (degree of hydration=84%)



(c) Combination 30%C_3S+70%C_2S (degree of hydration=68%)



(d) Combination 100%C_2S (degree of hydration=38%)

Figure 6 Stress-strain response diagrams for the special cement pastes at the curing age of 28 days

Table 4 Global mechanical properties of the special cement pastes at the curing age of 28 days, corresponding with Figure 6

Combination	Young's modulus E (GPa)	Tensile strength f_t (MPa)	Strain at peak load ε_p	Fracture energy G_F (J/m^2)
(a)	17	33	0.22%	22
(b)	18	37	0.22%	23
(c)	14	26	0.21%	26
(d)	4.2	7.9	0.33%	14

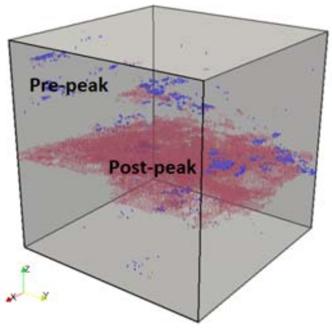
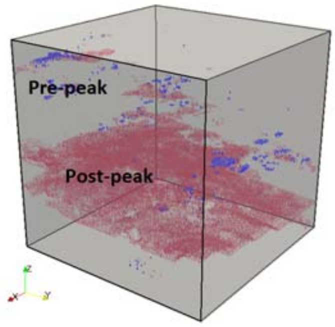
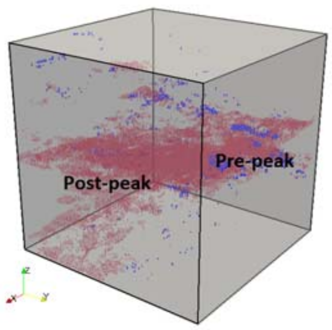
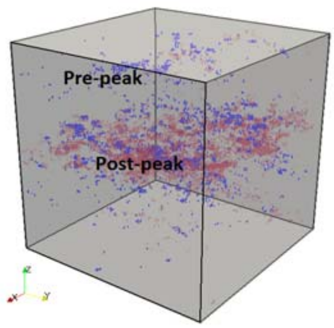
	
(a) Combination 100%C_3S (40457 microcracks)	(b) Combination 70%C_3S+30%C_2S (46115 microcracks)
	
(c) Combination 30%C_3S+70%C_2S (40309 microcracks)	(d) Combination 100%C_2S (12828 microcracks)

Figure 7 Cracks patterns in final failure state for the special cement pastes at the curing age of 28 days, corresponding with Figure 6

4. CONCLUSIONS

The study in this article attempts to reveal the relationship between the mechanical performance of cement paste and the mineral composition of the cement, by employing the HYMOSTRUC3D model and the 3D lattice fracture model. The microstructure of cement paste is simulated by the HYMOSTRUC3D model, and then it is evaluated by the 3D lattice fracture model for its global mechanical behaviors. Four special combinations of constituents are made to study the effect of C_3S and C_2S on the microstructures and the mechanical properties of cement paste. It is found that the combination 70%C_3S+30%C_2S shows the best mechanical performance at the curing age of 28 days, which suggests that the mineral composition of the ordinary Portland cement is already optimized.

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