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Experimental and numerical evaluation of mechanical properties of interface between filler and hydration products

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HIGHLIGHTS

- The mechanical properties of interface between filler and hydrates are evaluated.
- Limestone exhibits superior bond characteristics with hydrates compared with quartz.
- Limestone-hydrates interface appears superior in strength compared with matrix.
- Adhesion mechanisms between filler and hydrates are proposed.

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ABSTRACT

The interface between filler and hydration products can have a significant effect on the mechanical properties of the cement paste system. Surface analysis techniques and mechanical model can be used to study the mechanical properties of the interface. These studies can provide insight into the adhesion mechanisms between filler and hydration products. In this paper, cement pastes blended with fillers (micronized sand and limestone powder) are discussed. Crack paths and fracture surfaces of loaded cement pastes were investigated by scanning electron microscopy (SEM) observation. Parallel with the SEM observations, the influence of interface properties on crack propagation, tensile strength and fracture energy was studied numerically by using a lattice model. With these SEM observations and simulation results the mechanical properties of the interface between filler and hydration products were evaluated. Limestone powder exhibited superior bond characteristics with hydration products compared with micronized sand. Furthermore, it suggests that the limestone-hydration products interface is even stronger than hydration products. This is likely due to the strong electrostatic interactions or the iono-covalent forces between limestone particles and C-S-H particles.

1. Introduction

Portland cement is a basic component of concrete with a high environmental impact because of high CO_2 emission and energy consumption during production. Fillers such as limestone or quartz powder are used as a replacement for Portland cement to make concrete cheaper and more environment friendly [1–3]. Additions of limestone or quartz powder have a small chemical effect on cement hydration [4,5]. The main quasi-chemical effect of added limestone and quartz powder is that they accelerate cement hydration by facilitating nucleation of hydrates at their surfaces [1,5]. Finer fillers in cement paste can result in improvements in strength because of a denser packing [6]. However, the use of fillers results in dilution of Portland cement particles in the paste. Above a critical amount of fillers, this 'dilution' effect will lead to a lower strength of the hardened paste or concrete [1,7]. Besides, the mechanical properties of the interface between filler and hydration products have a significant influence on the development of the fracture process in blended cement paste under compressive loading, and thus the strength of the cement paste blended with fillers.

Improvement of the effect of fillers in cementitious materials, especially on the mechanical properties of the interface between filler and hydration products, is a big issue and a challenge today. So far not many attempts are known to quantify the mechanical properties of the interface between filler and hydration products in cement paste. To evaluate the mechanical properties of the interface between filler and hydration products, a surface analysis technique of scanning electron microscopy (SEM) observation was used in this study. Scanning electron microscopy is known as an

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appropriate method to characterize the crack paths and the fracture surfaces in cementitious materials [8–12]. The mechanical properties of the interface have a strong relationship with the crack propagation, and the cracks will preferentially propagate along the weak interfaces [12]. Therefore, in order to evaluate the mechanical properties of the interface between filler and hydration products, the crack paths and the fracture surfaces between fillers and hydration products of the loaded blended cement pastes were investigated by SEM observations.

In order to predict the effect of the micromechanical properties of the interface on the fracture process in the cement paste blended with fillers, a numerical model was applied. This model, called lattice fracture model, was proposed by Schangen and Van Mier in the 1990s and has been further developed by many others [13–15]. In the lattice fracture model, the material is represented by a lattice of beam elements. Subsequently, the microstructure of the material can be mapped onto these beam elements by assigning them different properties, depending on whether the beam element represents a grain, interface or matrix. Various conventional laboratory experiments can be simulated by the lattice fracture model and the model can be applied to cement-based materials [15,16]. This approach has been extensively used in the past decade both for mesoscale and microscale modelling of concrete and cement paste. Van Vliet investigated the size effect on tensile fracture of concrete using this model [17]. The effect of the strength of the interface transition zone and the particle density on the crack formation and propagation in concrete was investigated by Lilliu using lattice fracture model [18]. The numerical results showed that the model can reproduce the fracture processes observed in real physical experiments. This model was also used to study the interface fracture in cement-based materials [19,20]. In this study, the lattice fracture model was used to study the influence of interface properties on crack propagation, tensile strength and fracture energy. The output from the simulated direct tension test will be compared to experimental results and will then be used to predict the micromechanical properties of the interface.

As mentioned previously, the mechanical properties of the interface in cement paste systems have a direct relationship with interfacial bonds between hydration products and the filler particles. To understand the development of the strength of the interface between filler and hydration products, interfacial bonds between filler particles and hydration products were discussed in more detail at the end of this paper.

2. Materials and experimental methods

2.1. Materials

The cement used in this study is ordinary Portland cement (OPC) CEM I 42.5 N, produced by ENCI, The Netherlands. Fillers are limestone powder (LP) and micronized sand (M6). The chemical composition and physical characteristics of these materials are listed in Table 1. The mineral composition of OPC was calculated by the Bogue equation [21] and is reported in Table 2. Particle size distribution (PSD) data of the materials is shown in Fig. 1. Details about the measurement method are described in section 2.2.1. Two series of specimens were prepared denoted as M01 and L01. The percentage of different filler and the w/b are given in Table 3.

2.2. Methods

2.2.1. Particle size distribution analysis

The particle size distribution (PSD) of cement powder and fillers is an important factor influencing the rate of hydration and microstructure development of cement paste. To determine the PSD of the cement and fillers, laser diffraction method (DIPA 2000) was applied. Three measurements were made, and the average value was used.

Table 1
Chemical composition (% by mass) and physical characteristics of cement and fillers.

Name	OPC	LP	M6
Chemical composition			
CaO	64.40	–	0.02
SiO_2	20.36	0.34	99.5
Al_2O_3	4.96	0.2	0.20
Fe_2O_3	3.17	0.07	0.03
K_2O	0.64	0.01	0.04
Na_2O	0.14	0.02	–
SO_3	2.57	0.05	–
MgO	2.09	0.27	–
$CaCO_3$	–	97.46	–
Physical properties			
Density (g/cm^3)	3.15	2.67	2.65
D_{50} (μm)	44.5	34.6	62.3

Table 2
Mineral composition of cement (% by weight).

Phase	C_3S	C_2S	C_3A	C_4AF
Weight (%)	67.1	5.9	7.8	9.6

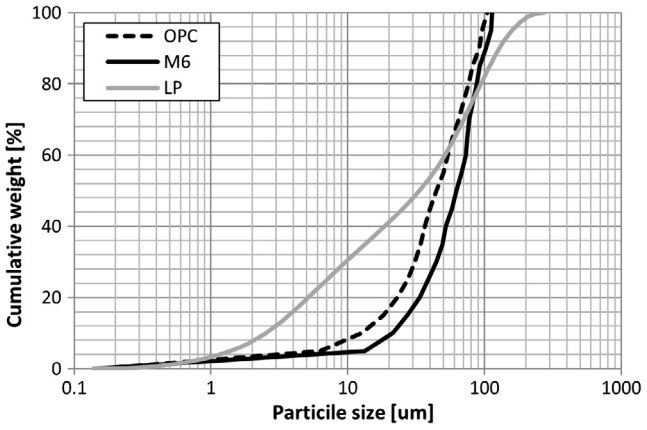

Fig. 1. Particle size distribution of cement and fillers.

Table 3
Mixture compositions of cement pastes.

Mixtures	OPC*(%)	M6*(%)	LP*(%)	w/b
M01	70	30	–	0.4
L01	70	–	30	0.4

* Percentage of the total mass of binder by weight.

2.2.2. Experimental procedures

The mixtures were prepared in a Hobart mixer according to the standard procedure described in ASTM C305 [22]. After mixing and casting, cement pastes were covered with a plastic sheet and stored in the laboratory at 20 ± 2 °C. After 24 h, all the specimens were demolded and then stored in the curing room with a constant temperature of 20 ± 2 °C and a relative humidity of 95 ± 5% until the designated testing age.

2.2.3. SEM analysis

Scanning electron microscopy equipped with energy dispersive spectroscopy (SEM/EDS) under a working voltage of 20 kV was