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SIMULATION OF SELF-HEALING BY FURTHER HYDRATION IN CEMENT-BASED MATERIALS

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ABSTRACT

Cracks, caused by shrinkage and external loading, are unavoidable in concrete structures. These cracks facilitate the ingress of aggressive and harmful substances into concrete and reduce the durability of the concrete structures. Fortunately, the cracks can be healed by further hydration when extra water and unhydrated cement are available [1]. It is well known that even after long time service, a big fraction of unhydrated cement remains in the concrete matrixes, especially in high performance concrete. Therefore the main criterion for the self-healing by further hydration is the supply of extra water in the system.

In this research, the extra water was assumed to be stored in capsules which were pre-mixed in the concrete mixture. When the concrete cracks, the cracks could pass through the capsules because of its low strength. In this way the water can be released from the capsules. The released water induces the further hydration of unhydrated cement particles. The efficiency of self-healing by further hydration is significantly influenced by the amount of unhydrated cement, crack width and the amount of extra water. Because of the various influence parameters, it will be importance to predict the efficiency of self-healing by further hydration in certain conditions. In order to provide theoretical guidance for the practice, a model to simulate self-healing of cracks by further hydration was developed based on the chemical thermodynamics theory [2] and diffusion theory [3]. Through the model, the amount of healing products formed in the crack at different time can be determined. Thus the efficiency of self-healing can be predicted as well.

For the application of the model, self-healing of cracks in the cement paste with the water/cement ratio of 0.3 at the age of 28 days was simulated. A microcrack with the width of 10 μm was supposed to propagate and the crack was assumed in the saturation condition.

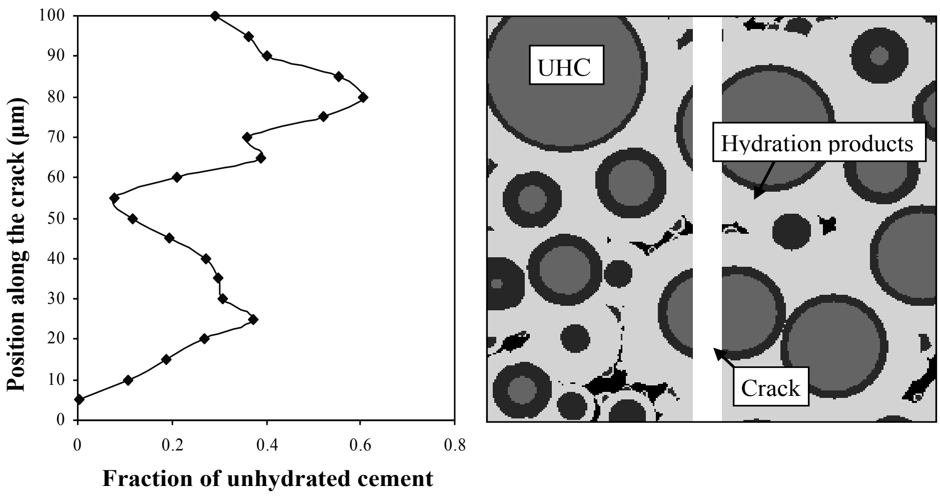

Figure 1: Fraction and distribution of unhydrated cement (2D cement paste slice)

The fraction and distribution of unhydrated cement was figured out by HYMOSTRUC [4, 5], as shown in Figure 1, and input to the model of self-healing. Once the extra water released from the capsules is accessed, the clinker phases of unhydrated cement dissolve and the ions, such as Ca^{2+}, OH^- and $H_3SiO_4^-$, diffuse to the crack due to concentration gradient. The diffusion of ions from unhydrated cement to the cracks was calculated by numerical method. If the concentrations of the ions in the crack solution reach the equilibrium concentration for reaction, the hydration products are formed and the cracks are healed.

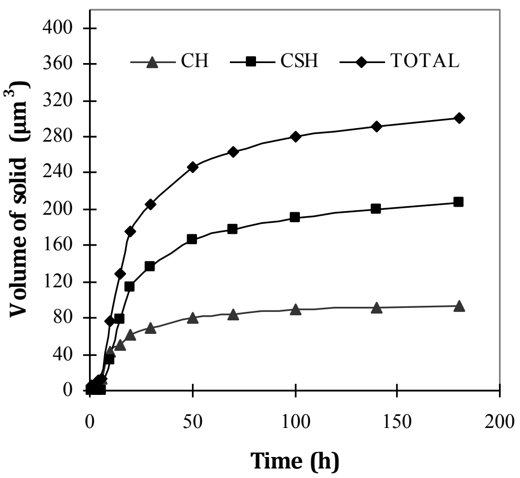

Figure 2: Volume of hydration products in the crack

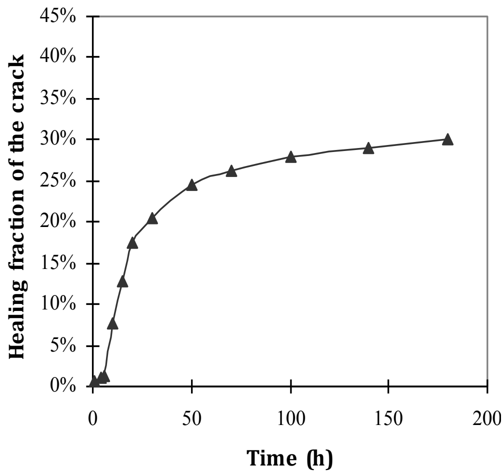

Figure 3: Healing fraction of the crack

The amount of further hydration products can be calculated based on the mass balance, charge balance and chemistry equilibrium, which is shown in Figure 2. The formation of hydration products in the crack mainly took place during the first 50 hours. The speed of self-healing of the crack slowed down apparently after 50 hours. The reason is that the transport of ions to and from the surface of the unhydrated cement particle is getting more and more difficult as the further hydration products are formed around the unhydrated cement. The fraction of the crack as function of time is shown in Figure 3. It can be learned that about 30% of the crack's volume was filled by hydration products after 180 hours of further hydration.

From the simulation it is shown that the model of self-healing based on the chemical thermodynamics theory and diffusion theory can be used to predict the efficiency of self-healing by further hydration. The influence of the fraction of unhydrated cement and the crack width on the efficiency of self-healing can be determined. Future work for the model will be focused on taking the unsaturated condition of cracks into account. Thus the improved model can be used to optimize the amount of capsules (water) for the self-healing by further hydration.

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