A three-dimensional numerical research on probability characteristics of a crack hitting capsules for self-healing concrete

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ABSTRACT

In self-healing concrete, healing agents (including the bacteria and nutrients for the bacteria) are often sealed in capsules to survive the mixing of concrete. When the crack occurs, these capsules can be damaged, the healing agents can be released and the chemical actions can be activated. This research mainly focuses on the probability characteristics of a crack hitting the capsules. To conduct the research, the meso-scale models for two kinds of capsules, i.e., spherical and tubular capsules, are established. Statistical analysis is conducted to estimate the hitting probability and the number of capsules damaged by a crack based on the meso-scale models. With the numerical method proposed in this research, it is possible to estimate the efficiency of the self-healing system, as well as optimize the proper usage of the capsules. An application of this numerical method in a bacterial self-healing concrete based on Liapor (a light weight aggregate) is also included.

1. INTRODUCTION

Cracking is a severe problem to almost all the concrete structures. To improve the long-term durability and sustainability performance of the concrete structures, a novel concept of self-healing concrete has been proposed and studied in recent years [1]. The main idea of this concept is to use products of the chemical reactions which autonomously happen inside the concrete to seal the crack. In this way, the concrete can have the capability to repair itself, which is the reason why it is called self-healing concrete. This new material has a potential wide application in the future, not only because it can save a lot of labour work, but also because it can decrease the maintenance cost as well.

To improve the efficiency of self-healing, some bacteria-based healing agents are proposed [2-4]. These healing agents are often sealed in a capsule which can keep them inactive and survive during the mix procedure of concrete. Within this kind of self-healing system, the proper usage of the capsule is a fundamental problem to be solved. Generally, the more capsules exist in the concrete, a better healing efficiency can be expected. However, the introduction of the capsules into the concrete may have some negative effects on the strength of the concrete at the same time, and the cost of the bacteria-based biological material is higher than the normal concrete as well. Thus, there should be an optimized result of the proper usage of the capsule, which will be discussed in this paper.

2. MODELS AND METHODS

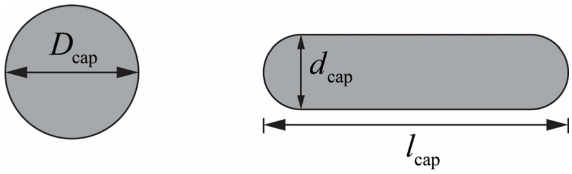


Figure 1: Simplified shapes of spherical and tubular capsules

To obtain the proper usage of the capsules, the numerical study should be conducted at meso-scale. For the mortar, the meso-scale model only contains the capsules as the inclusions, while for the concrete, the coarse aggregates should be also explicitly modelled. In the current research, we only focus our attention on the mortar. But the numerical method can be extended to the concrete. Two major types of capsules, i.e., spherical and tubular capsules, are investigated here. As shown in Figure 1, the spherical capsule is modelled as a sphere, while the tubular capsule is modelled as a cylinder ended with spherical tips. The aspect ratio of the tubular capsule is defined as:

$$\mathrm{AR} = l_{\mathrm{cap}} / d_{\mathrm{cap}} \tag{1}$$

where l_{cap} and d_{cap} are the length and diameter of the tubular capsule, respectively. With this definition, the spherical capsule can be seen as a special tubular capsule with $\mathrm{AR} = 1.0$.

All the capsules are randomly and uniformly placed in a cubic representative volume element (RVE) with the edge length L. The whole procedure of locating the capsules follows the 'take-and-place' method. A separation check is conducted to ensure that no capsules are overlapped with one another. But since the tubular capsule is simplified as a one-dimensional line, the separation check is not needed for this type of the capsule.

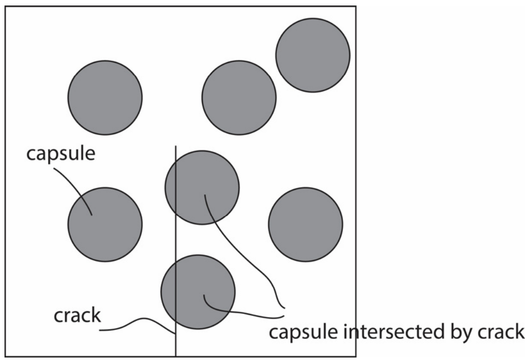


Figure 2: A schematic of identifying capsules intersected by crack

In the current research, we do not consider the influence of the mechanical properties of capsules on the crack pattern. Thus, the crack can be simply taken as a plane perpendicular to the bottom of the cubic model. With a given crack depth, the capsules intersected by the crack can be identified, as shown in Figure 2. The healing agents of these capsules will be released into the crack. Products such as the calcium carbonate which finally seal the crack will be formed during the chemical reactions between these healing agents. Thus, the efficiency of the self-healing system can be defined as:

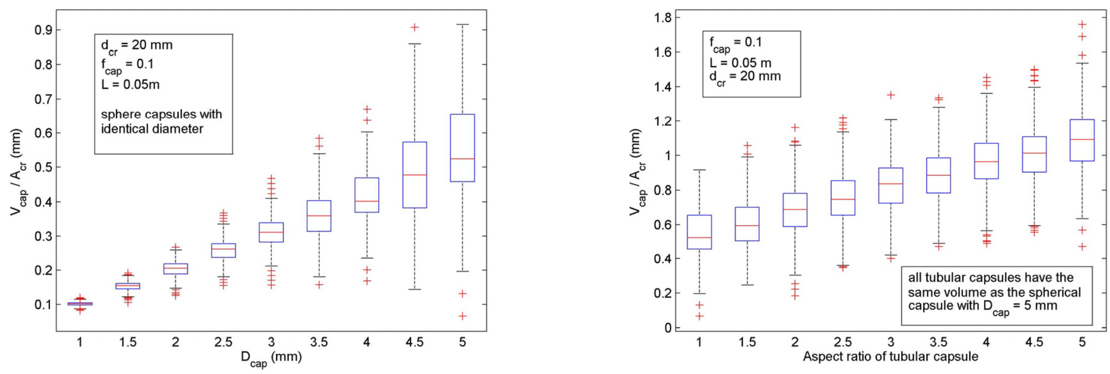
$$\alpha = \frac{V_{\mathrm{prod}}}{V_{\mathrm{cr}}} = \frac{V_{\mathrm{cap}} \cdot \beta_{\mathrm{prod}}}{d_{\mathrm{cr}} \cdot L \cdot w_{\mathrm{cr}} \cdot 0.5} = \frac{V_{\mathrm{cap}}}{A_{\mathrm{cr}}} \cdot \frac{\beta_{\mathrm{prod}}}{0.5 \cdot w_{\mathrm{cr}}} \tag{2}$$

where V_{prod} is the volume of the products which can seal the crack, V_{cr}, d_{cr}, w_{cr} and A_{cr} are the volume, depth, width and area of the crack, respectively. Although the crack initially assumed as a plane, it will gradually open at the bottom of the model under the flexural action. So a V-shaped crack is adopted here. β_{prod} is a nondimensionalized parameter which represents the healing efficiency of per unit volume of the capsule. It is related to the amount of the healing agents sealed in the capsule, and the chemical reactions between the healing agents.

It can be easily figured out that $V_{\text{cap}}/A_{\text{cr}}$ in Equation (2) is only determined by the geometrical aspect of the model, including the shape and position of the capsules. Thus, this parameter is chosen for a general discussion.

3. RESULTS AND DISCUSSION

The most important results of the current study are shown in Figure 3. For the spherical capsules, the result in Figure 3(a) shows that both of the average and the standard deviation of $V_{\text{cap}}/A_{\text{cr}}$ increase with the diameter of the capsule. So if larger capsules are used, a better healing efficieny can be expected from the averaged point of view. But the increase of the standard deviation makes it difficult to predict the exact healing efficiency for a single specimen with enough confidence. The result for the tubular capsule is shown in Figure 3(b). It shows that the average of $V_{\text{cap}}/A_{\text{cr}}$ increases with the aspect ratio of the tubular capsule, while the standard deviation of $V_{\text{cap}}/A_{\text{cr}}$ does not show any obvious change. This result may indicate the potential advantage of tubular capsules in improving the self-healing efficiency. But the other factors from the production of the capsules, etc., should be also considered for the decision-making.



(a) Effect of capsule size on $V_{\text{cap}}/A_{\text{cr}}$ for spherical capsule

(b) Effect of aspect ratio on $V_{\text{cap}}/A_{\text{cr}}$ for tubular capsule

Figure 3: Boxplot of $V_{\text{cap}}/A_{\text{cr}}$ for spherical and tubular capsules, f_{cap} is the volume fraction of capsule, d_{cr} is the crack depth, D_{cap} is the diameter of spherical capsule.

4. APPLICATION

The numerical method in this paper has been applied in a self-healing system by using liapor as the capsule. Liapor is a kind of light weight aggregate (LWA) with a high porosity. Thus, it can provide enough space to hold the healing agents. This case study is to provide advices on the proper usage of the liapor in the mix proportion of the mortar. The result is shown in Figure 4. The parameter β_{prod} in

Equation (2) is determined as $\beta_{\text{prod}} = 0.0805$ based on the detailed healing mechanism. From Figure 4, the proper usage of the liapor can be found according to the permitted maximum crack width and the expected self-healing efficiency. For example, the dashed line in Figure 4 indicates that the crack width of 200 μm and the healing efficiency of 100% will require the volume fraction of about 31%.

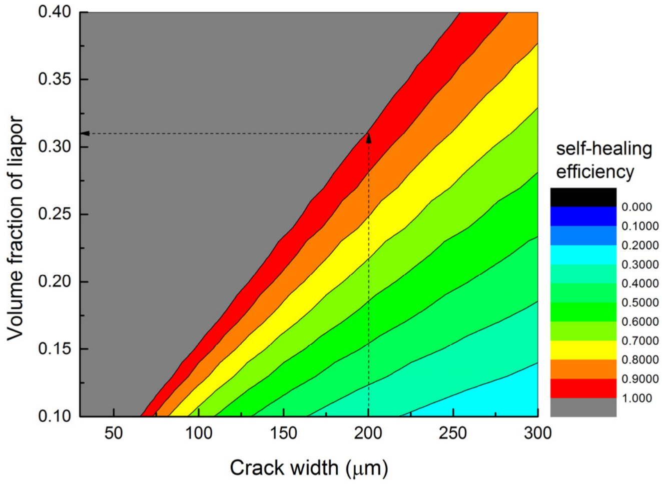


Figure 4: Contour plot of healing efficiency as a function of crack width and volume fraction of liapor in mortar.

5. CONCLUSIONS

A numerical method has been proposed to find the proper usage of the capsule in a self-healing system. Based on the results of several analysis, the following conclusions can be draw.

(1) For the spherical capsules, the self-healing efficiency can be improved by using larger capsules from the average point of view. But the deviation will be also increased;

(2) Theoretically, tubular capsules can have a better healing efficiency than spherical capsules, and the efficiency increases with the aspect ratio of the tubular capsules.

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