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A 3D analytical model for the probabilistic characteristics of self-healing model for concrete using spherical microcapsule

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Abstract. In general, cracks significantly deteriorate the in-situ performance of concrete members and structures, especially in urban metro tunnels that have been embedded in saturated soft soils. The microcapsule self-healing method is a newly developed healing method for repairing cracked concrete. To investigate the optimal microcapsule parameters that will have the best healing effect in concrete, a 3D analytical probability healing model is proposed; it is based on the microcapsule self-healing method's healing mechanism, and its purpose is to predict the healing efficiency and healing probability of given cracks. The proposed model comprehensively considers the radius and the volume fraction of microcapsules, the expected healing efficiency, the parameters of cracks, the broken ratio and the healing probability. Furthermore, a simplified probability healing model is proposed to facilitate the calculation. Then, a Monte Carlo test is conducted to verify the proposed 3D analytical probability healing model. Finally, the influences of microcapsules' parameters on the healing efficiency and the healing probability of the microcapsule self-healing method are examined in light of the proposed probability model.

Keywords: self-healing; microcapsule; crack healing; 3D analytical probability healing model

1. Introduction

Cracks typically occur in concrete members and structures due to various external influences; these cracks seriously deteriorate the strength, performance and durability of a structure (Mehta 1997). The degradation of the concrete lining of an urban metro tunnel, which is embedded in saturated soft soils and subjected to underground water, vehicle vibrations and ground pressures, is almost inevitable. Therefore, the challenge of repairing and maintaining urban metro structures regularly confronts engineers. To ensure security, the occurrence and propagation of cracks must be prevented during the extended service life of a metro tunnel structure. Compared with traditional repairing methods in concrete structures, the microcapsule self-healing method, which is one of the newest techniques for repairing concrete structures, has been developed for more than

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10 years by White *et al.* (2001). It will evidently extend the lifetime and improve the security of concrete structures, and it will reduce both the maintenance cost and the rate of occurrence of system failures by incorporating a healing agent into microcapsules. Because it heals autonomously and abundantly and it is adapted to concrete, the microcapsule self-healing method appears to be a promising strategy in urban metro tunnels. The mechanism of the microcapsule self-healing method can be summarized as follows: by incorporating microcapsules that contain a healing agent, self-healing is achieved. A propagating crack randomly makes the microcapsules break, whereupon the healing agent flows out to close this crack; this process is displayed in Fig. 1. Therefore, the cracks embedded in a concrete matrix can be healed by a healing agent.

Many notable studies have been conducted to test this healing method in laboratory conditions. Different types of healing agent have been tested. Mostly, one-compound air-curing healing agents, such as cyanoacrylates (Li *et al*. 1998), epoxy (Nishiwaki *et al*. 2006, Thao *et al*. 2009), silicon (Dry 2001) and polyurethane foam (Van Tittelboom *et al.* 2011, Van Tittelboom *et al*. 2012), perform better than multi-compound healing agents. This performance discrepancy is caused by concerns regarding the potential incomplete mixing of different compounds. However, multi-compound healing agents show more stability. Some authors in fact believe that multi-compound healing agents have greater longevity than one-compound healing agents. Therefore, these authors propose the use of a two-compound epoxy resin and a multi-compound methyl methacrylate (MMA) system. Dry and McMillan propose the use of a three-part methyl methacrylate healing agent, which polymerizes at room temperature (Dry and McMillan 1996). In addition, the shells of microcapsules have been investigated. Yang *et al*. (2011) have found that a silica gel shell can participate in the reactions of cement hydration. Strong bonding between the microcapsules and the cementitious matrix can be expected as a result of the high contact area between the two phases, which will increase the integrity of the structure. Numerous experiments have been performed on the microcapsule self-healing method under different testing conditions, including tests on the fatigue properties, the permeability test (Yang *et al*. 2011, Li *et al*. 2013), microscopic observation of micro-cracks, field emission scanning electron microscopy (FESEM) analyses, studies on the morphologies of the microcapsules and electrochemical impedance spectroscopy measurements (Yang *et al*. 2010).

There are many papers that detail the damage models of materials at the micro and macro levels using continuum damage mechanics(Marigo 1985, Simo and Ju 1987a, b, Ju 1989, Ju *et al.* 1989, Ju 1990, Ju 1991, Ju and Chen 1994a, b, Ju and Lee 1991, Ju and Tseng 1992, Ju and Tseng 1995).

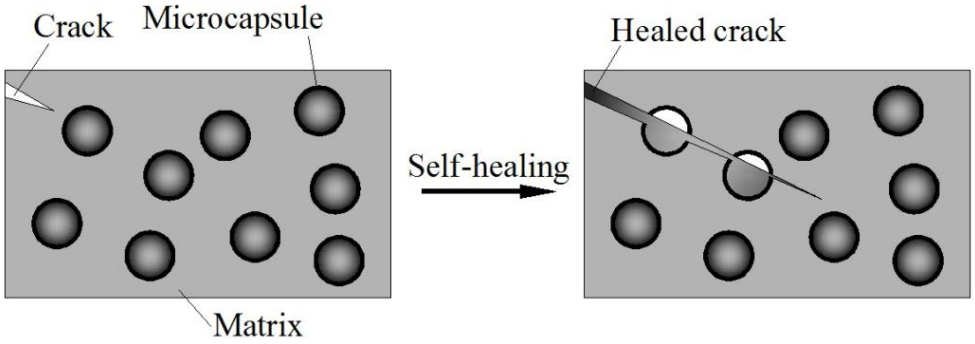


Fig. 1 A schematic illustration of the microcapsule self-healing concept in concrete

However, fewer papers have studied the healing models. Barbero *et al.* (2005) propose a damage-healing constitutive model for self-healing composites based on thermodynamics, which is the starting point of continuum damage-healing mechanics (CDHM). Then, some other healing models based on the framework of CDHM have been developed (Alfredsson and Stigh 2004, Voyiadjis *et al.* 2011, Darabi *et al.* 2012, Ju *et al.* 2012, Yuan and Ju 2013, Ju and Yuan 2012). A discrete element method (DEM) model for local self-healing that allows damage to heal during loading has been proposed, and the relative parameters that the material strength depends on have been examined (Herbst and Luding 2008). However, the inherent healing mechanism of different healing methods at the micro level is ignored in the above healing models, which makes it not appropriate to describe the healing process of the microcapsule self-healing method. Importantly, the randomness of healing is also neglected, even though it must be considered in the microcapsule self-healing method because of the healing mechanism that this method utilizes.

Some healing models consider the healing mechanism of the capsule self-healing method and the randomness of healing. The healing situation of cylindrical capsules has been considered (Yuan and Chen 2013). But the method does not apply to the spherical capsules' situation. Two 2D probability healing models of the capsule self-healing method that use geometry probability have been proposed (Zemskov *et al.* 2010, Zemskov *et al.* 2011). However, these two probability models cannot present the practical situation effectively. The first 2D analytical probability healing model defines the computation cross-section and assumes that all of capsule sections in this cross-section are equal, which is not a valid assumption. The second analytical probability healing model concentrates on the random placement of capsules in a layered structure that is different from the microcapsule self-healing method in concrete. In addition, a 3D numerical probability healing model that can calculate the collision probability of a crack and a particle has been developed (Mookhoek *et al.* 2009). However, these three probabilistic healing model all focus on the capsule self-healing method, whose healing mechanism is different from the mechanism of the microcapsule self-healing method. For example, whereas one crack can be entirely healed by one capsule, it cannot be entirely healed by one microcapsule because of the small volume of a microcapsule. Thus, the healing efficiency and the number of broken microcapsules must be considered. In the capsule self-healing method, the opening value of a crack is quite small compared to the size of the RVE and the radius of a capsule. Hence, the crack opening value can be treated as zero. However, the radius of a microcapsule is as small as the opening value of a crack and as a result, the opening value and volume of a crack should be considered in the microcapsule self-healing method. Practically speaking, the microcapsules may separate from the matrix rather than break due to bad bonding. Consequently, the broken ratio of the microcapsules should be considered.

In this paper, a 3D analytical probability healing model is proposed to describe the healing process of the microcapsule self-healing method. This model can quantitatively characterize the healing efficiency and healing probability of cracked concrete by considering both the geometry probability and the healing method's healing mechanism at the micro level. Subsequently, in view of the sizes of the microcapsules and cracks, a simplified 3D analytical probability healing model is developed to facilitate the calculation. The obtained 3D probability healing model is then verified by means of Monte Carlo tests. Finally, the influence of the microcapsules' parameters is discussed on the basis of the proposed simplified probability healing model to optimize the healing system. Compared with other probabilistic models, our model can consider the healing probability, healing efficiency and relative geometric parameters of microcapsule-enabled self-healing systems comprehensively in 3D situation. Based on practical parameters acquired from engineering, suitable microcapsule-enabled self-healing systems can be designed.

2. Basic Model

The microcapsule-enabled self-healing system involves the healing agent (repairing the microcracks), catalyst (speeding up the polymerization) and shell (encapsulating the healing agent). The healing agents are supposed to be epoxy resin or DCPD in this paper, and the catalyst is distributed uniformly in concrete matrix. Upon further loading, the crack will open up and propagate. The surrounding microcapsules will break. When the healing agents flow into crack, they will be solidified and connect two faces of the crack (Brown *et al*. 2005a, b). The shells studied in this paper are soft enough and easy to break. All healing agents in one microcapsule are assumed to flow into the crack. Ignoring all other aspects, the amount of healing agents released into the crack is essential to obtain a good healing (Mookhoek *et al*. 2009).

To investigate the healing efficiency and healing probability of the microcapsule self-healing concrete, the microcapsules and cracks employed in this paper are described at the micro level. A generalized RVE is considered here and the concrete matrix is treated as one phase to simplify the model (Zhu *et al*. 2014). We assume that there are many microcapsules with a radius r and a total volume V_n in the representative volume element (RVE), as exhibited in Fig. 2. Every RVE contains only one microcrack. So the crack density and total volume determine the dimensions of RVE. Actual crack is idealized as planar crack to simplify the configuration and the opening value of a microcrack is averaged to l_2 (Jang *et al*. 2004). The healing efficiency h is defined as the volume fraction of the crack being filled with healing agents from microcapsules in this paper, which is different from previous research (Brown *et al*. 2002, Li *et al*. 2013).

Every RVE contains one crack and numerous microcapsules. The volume of each RVE is V, and the volume fraction of microcapsules is:

$$V_f = \frac{V_n}{V} \tag{1}$$

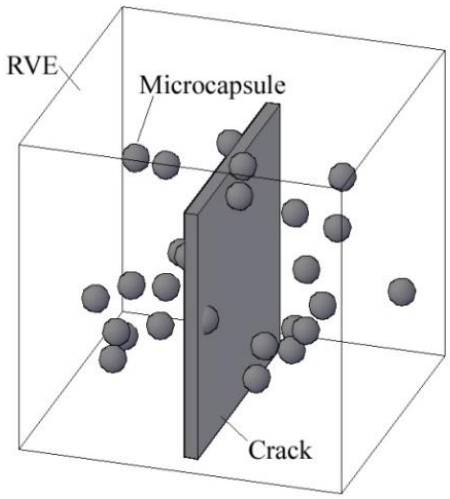
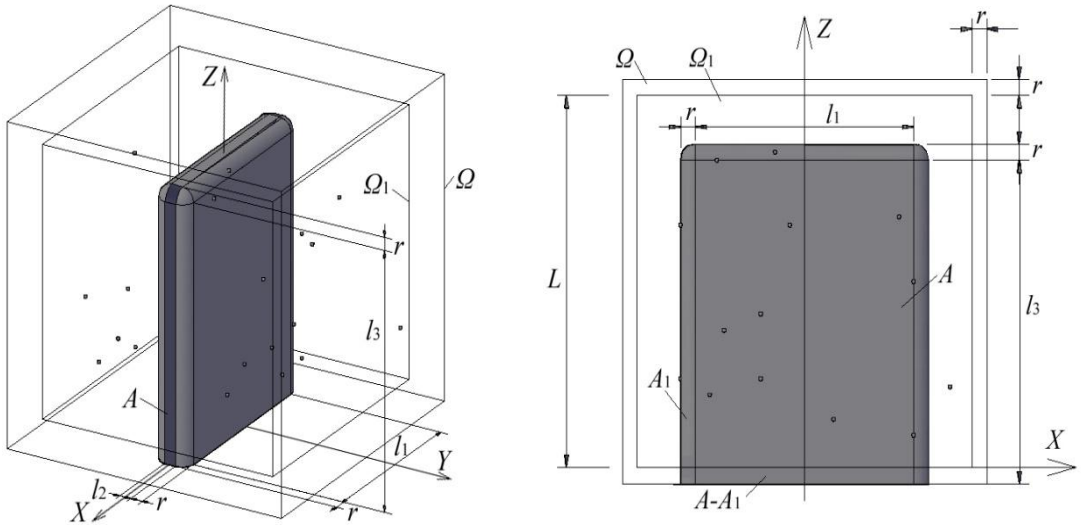


Fig. 2 The dispersed microcapsules and a crack in a representative volume element



(a) (b)

Fig. 3 The domain A_1 in the RVE of the 3D probability healing model

Additionally, the volume of one microcapsule is

$$V_m = \frac{4}{3}\pi r^3 \tag{2}$$

and the total number of microcapsules is

$$n = \frac{V_n}{V_m} = \frac{3V_n}{4\pi r^3} \tag{3}$$

To obtain a three-dimensional analytical probability healing model of the microcapsule self-healing method, we make the following assumptions:

-all of the microcapsules are uniformly distributed within each RVE;

-the crack in the RVE has a length of l_1, an opening value of l_2 and a height of l_3; furthermore, it is perpendicular to the element's surface. This crack is located at $y = 0$ in the local coordinate system, as illustrated in Fig. 3;

-for the three-dimensional model, the microcapsules locate in the cube Ω

$$\Omega = [-\frac{V^{1/3}}{2}, \frac{V^{1/3}}{2}] \times [-\frac{V^{1/3}}{2}, \frac{V^{1/3}}{2}] \times [-r, V^{1/3} - r] \tag{4}$$

The above variables can be obtained from experimental tests, such as from the scanning electron microscopy (SEM). Under these assumptions, all centers of the microcapsules should be in the cube Ω_1

$$\Omega_1=[-\frac{V^{1/3}}{2}+r,\frac{V^{1/3}}{2}-r]\times[-\frac{V^{1/3}}{2}+r,\frac{V^{1/3}}{2}-r]\times[0,V^{1/3}-2r] \tag{5}$$

In this paper, it is assumed that if the center of any microcapsule is in zone *A*, the microcapsule will break or separate from the matrix, and furthermore, the intersection of *A* and $\Omega_1$is denoted by A_1, as illustrated in Fig. 3.

The probability that a single crack hits one microcapsule can be expressed by Eq. (6)

$$p=\frac{V_{A1}}{V_{\Omega 1}}=\frac{\begin{array}{l}l_1\times(l_2+2\times r)\times(l_3-r)+r\times l_2\times(l_3-r)\times 2+\pi\times r^2\times(l_3-r)+\\ r\times l_2\times l_1+\pi\times r^2\times l_1/2+\pi\times r^2\times l_2/2+2/3\times\pi\times r^3\end{array}}{(V^{1/3}-2r)^3} \tag{6}$$

There are *n* microcapsules in a RVE and their centers can be expressed as

$$\mathrm{x}_i=(x_i,y_i,z_i),i=1,...,n. \tag{7}$$

The stochastic event that the i-th microcapsule hits the crack can be expressed as (Zemskov *et al*. 2010)

$$\Lambda_i^n=\Lambda_i^n(\mathrm{x}_1,...,\mathrm{x}_n) \tag{8}$$

The event that Λ_i^n happens means:

- $\mathrm{x}_i=(x_i,y_i,z_i)\in A_1$
- $\mathrm{x}_j=(x_j,y_j,z_j)\in\Omega_1$ for $j\neq i$
- $d(\mathrm{x}_j,\mathrm{x}_k)=\sqrt{(x_j-x_k)^2+(y_j-y_k)^2+(z_j-z_k)^2}\in[2r,\sqrt{3}L]$ for $j,k=1,...,n$
- $L=V^{1/3}-2r$

Based on the fact, the microcapsules are not allowed to overlap each other. Thus, the distance between the centers of any two microcapsules must be larger than 2*r*. Furthermore, because all microcapsules have the same radius, we write

$$P(\Lambda_i^n)=P(\Lambda_j^n)\ \textit{for}\ i,j=1,...,n \tag{9}$$

The healing mechanism of the microcapsule self-healing method is different from the healing mechanism of the capsule self-healing method (Zemskov *et al*. 2010). Whereas one crack can be totally healed by one capsule, it cannot be totally healed by one microcapsule due to the small volume of each microcapsule. Thus, the healing efficiency *h* and the required number of broken microcapsules n' must be considered. In the capsule self-healing method, the opening value of a crack is quite small relative to the RVE and the radius of each capsule. Consequently, the opening value can be treated as zero. However, the radius of each microcapsule is as small as the opening value of a crack, so the opening value of crack l_2 and the volume of crack V_c should be considered in the microcapsule self-healing method, as illustrated in Fig. 4.

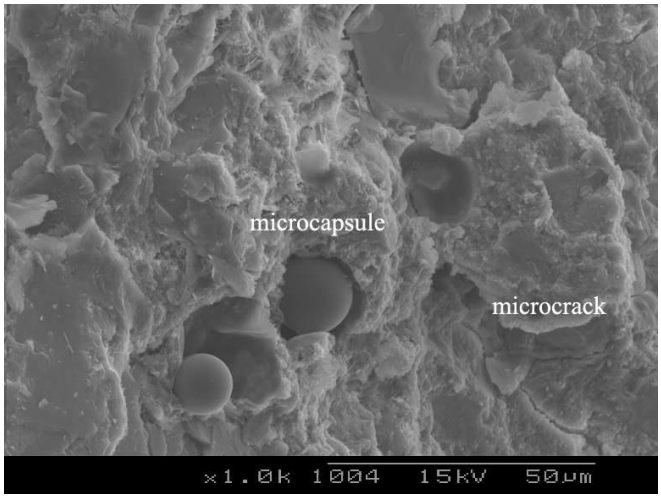


Fig. 4 The microcapsule and the microcrack

In this paper, it is assumed that if the expected healing efficiency of a crack is more than *h*, the number of broken microcapsules must be equal to or greater than n'. In microcapsule-enabled cementitious materials, the microcapsules may separate from the matrix rather than break because of bad bonding, as shown in Fig. 4. The interfacial bonding is weak between inorganic matrix and organic shells by experimental observation. Hence, the broken ratio α of the microcapsules in zone A_1, ranging from 0 to 1, should be introduced to calculate the effective volume fraction of microcapsules. It is defined that if α =0 then all microcapsules separate from the matrix and no microcapsule breaks. Similarly, if α =1 then all of the microcapsules in A_1 are broken. Therefore, the volume of the crack and the number of broken microcapsules can be determined by Eqs. (10)-(11), respectively

$$V_c = l_1 \times l_2 \times l_3 \tag{10}$$

$$n' = \frac{V_c \times h}{V_m} \times \frac{1}{\alpha} \tag{11}$$

Furthermore, the probability that a crack hits at least n' microcapsules is

$$P(H_n^{n'}) = n \times C_{n-1}^{n'-1} \sum_{j=0}^{n-n'} (-1)^j C_{n-n'}^{j} \times k_{j+n'}^{n} / (j+n') \tag{12}$$

where

$$k_{j+n'}^{n} = P(\Lambda_1^n \bigcap \ldots \bigcap \Lambda_{j+n'}^n) \tag{13}$$

In order to explain the above functions, it is assumed that there are three microcapsules in the RVE. When n' =1, the probability function becomes

$$P(H_3^1)=3\times C_2^0\sum_{j=0}^{2}(-1)^j C_2^j\times\ k_{j+1}^3/(j+1)=3P(\Lambda_1^3)-3P(\Lambda_1^3\bigcap\Lambda_2^3)+P(\Lambda_1^3\bigcap\Lambda_2^3\bigcap\Lambda_3^3)$$

When n'=2, the probability function reads

$$P(H_3^2)=3\times C_2^1\sum_{j=0}^{1}(-1)^j C_1^j\times\ k_{j+2}^3/(j+2)=3P(\Lambda_1^3\bigcap\Lambda_2^3)-2P(\Lambda_1^3\bigcap\Lambda_2^3\bigcap\Lambda_3^3)$$

Similarly, when n'=3, the probability function is

$$P(H_3^3)=P(\Lambda_1^3\bigcap\Lambda_2^3\bigcap\Lambda_3^3)$$

According to previous work (Zemskov *et al.* 2010), any $k_{j+n'}^n$ can be theoretically expressed by the probability of event Λ_1^2. When the probability of Λ_1^2 is obtained, the probability of $H_n^{n'}$ can be evaluated.

3. The analytic framework to calculate the probability

The purpose of this section is to obtain the probability of Λ_1^2, which can be expressed with the following function (Zemskov *et al.* 2010)

$$P(\Lambda_1^2(\mathrm{x}_1,\mathrm{x}_2))=P((\mathrm{x}_1\in A_1)\bigcap(d(\mathrm{x}_1,\mathrm{x}_2)\geq 2r))=P(d(\mathrm{x}_1,\mathrm{x}_2)\geq 2r\,|\mathrm{x}_1\in A_1)\times P(\mathrm{x}_1\in A_1)\qquad(14)$$

It is easy to determine $P(\mathrm{x}_1\in A_1)$, as it can be obtained by Eq.(6). Hence, attention should be paid to the conditional probability. To calculate the conditional probability, new stochastic variables *X*,*Y* and *Z* are introduced as

$$\begin{aligned}X&=x_1-x_2\in[-\frac{L+l_1}{2}-r,\frac{L+l_1}{2}+r]\\ Y&=y_1-y_2\in[-\frac{L+l_2}{2}-r,\frac{L+l_2}{2}+r]\\ Z&=z_1-z_2\in[-L,l_3]\end{aligned}\qquad(15)$$

for $\mathrm{x}_1=(x_1,y_1,z_1)\in A_1$, $\mathrm{x}_2=(x_2,y_2,z_2)\in\Omega_1$.

The locus of *X*,*Y* and *Z* must be in the rectangular region *D*, which can be classified as being inside of a sphere with a radius of 2*r* or outside of the sphere, as shown in Fig. 5.

The former space represents that two microcapsules overlap each other, which is physically impossible, and the latter space signifies two microcapsules that are separate from each other. The conditional probability can be rendered as

$$P(d(\mathrm{x}_1,\mathrm{x}_2)\geq 2r\,|\,\mathrm{x}_1\in A_1)=\iiint\limits_{\substack{X,Y,Z\in D\\ X^2+Y^2+Z^2>4r^2}} f_X(X)\,f_Y(Y)\,f_Z(Z)dXdYdZ \tag{16}$$

In the above equation, $f_X(X)$ is the distribution density of X, $f_Y(Y)$ denotes the distribution density of Y and $f_Z(Z)$ signifies the distribution density of Z. These distribution density functions can be expressed as follows

$$\begin{cases} f_X(t)=\int_{-\infty}^{\infty} f_{x_1}(u)\,f_{-x_2}(t-u)du \\ f_Y(t)=\int_{-\infty}^{\infty} f_{y_1}(u)\,f_{-y_2}(t-u)du \\ f_Z(t)=\int_{-\infty}^{\infty} f_{z_1}(u)\,f_{-z_2}(t-u)du \end{cases} \tag{17}$$

Where f_{x_1}, f_{x_2}, f_{y_1}, f_{y_2}, f_{z_1} and f_{z_2} are the distribution densities of x_1, x_2, y_1, y_2, z_1 and z_2, respectively. After obtaining these distribution density functions, the conditional probability can be calculated. Therefore, attention should be paid to these functions.

For $(x_2,y_2,z_2)\in\Omega_1$, the distribution density functions are as follows

$$\begin{cases} f_{x_2}(t)=\dfrac{1}{L},\ t\in[-\dfrac{L}{2},\dfrac{L}{2}] \\ f_{y_2}(t)=\dfrac{1}{L},\ t\in[-\dfrac{L}{2},\dfrac{L}{2}] \\ f_{z_2}(t)=\dfrac{1}{L},\ t\in[0,L] \end{cases} \tag{18}$$

In addition, the probability density functions f_{x_1}, f_{y_1}, f_{z_1} are as follows

$$f_{x_1}(t)=\begin{cases} f_{x_1}^{(1)}(t),\ t\in[-r-l_1/2,-l_1/2]\cup[l_1/2,l_1/2+r] \\ f_{x_1}^{(2)}(t),\ t\in(-l_1/2,l_1/2) \end{cases} \tag{19}$$

where

$$\begin{cases} f_{x_1}^{(1)}(t)=\left[(\sqrt{r^2-(|t|-l_1/2)^2}+l_3-r)l_2+2(l_3-r)\sqrt{r^2-(|t|-l_1/2)^2}+\pi(r^2-(|t|-l_1/2)^2)/2\right]/V_{A1} \\ f_{x_1}^{(2)}(t)=\left[l_3l_2+2(l_3-r)r+\pi r^2/2\right]/V_{A1} \end{cases} \tag{20}$$

and

$$f_{y_1}(t)=\begin{cases} f_{y_1}^{(1)}(t),\ t\in[-r-l_2/2,-l_2/2]\cup[l_2/2,l_2/2+r] \\ f_{y_1}^{(2)}(t),\ t\in(-l_2/2,l_2/2) \end{cases} \tag{21}$$

where

$$\begin{cases} f_{y_1}^{(1)}(t)=\left[(\sqrt{r^2-(|t|-l_2/2)^2}+l_3-r)l_1+2(l_3-r)\sqrt{r^2-(|t|-l_2/2)^2}+\pi(r^2-(|t|-l_2/2)^2)/2\right]/V_{A1} \\ f_{y_1}^{(2)}(t)=\left[l_3l_1+2(l_3-r)r+\pi r^2/2\right]/V_{A1} \end{cases} \tag{22}$$

and

$$f_{z_1}(t)=\begin{cases} f_{z_1}^{(1)}(t),\ t\in[0,l_3-r] \\ f_{z_1}^{(2)}(t),\ t\in(l_3-r,l_3] \end{cases} \tag{23}$$

where

$$\begin{cases} f_{z_1}^{(1)}(t)=\left[l_2l_1+2l_2r+2l_1r+\pi r^2\right]/V_{A1} \\ f_{z_1}^{(2)}(t)=\left[(2\sqrt{r^2-(t-(l_3-r))^2}+l_2)l_1+2l_2\sqrt{r^2-(t-(l_3-r))^2}+\pi(r^2-(t-(l_3-r))^2)\right]/V_{A1} \end{cases} \tag{24}$$

After obtaining the f_{x_1}, f_{x_2}, f_{y_1}, f_{y_2}, f_{z_1} and f_{z_2}, $f_X(t)$, $f_Y(t)$ and $f_Z(t)$ become

$$f_X(t)=\begin{cases} 0,\ t\in(-\infty,-\frac{L+l_1}{2}-r) \\ \int_{-\frac{l_1}{2}-r}^{t+\frac{L}{2}} f_{x_1}^{(1)}(u)\frac{1}{L}du,\ t\in[-\frac{L+l_1}{2}-r,-\frac{L+l_1}{2}) \\ \int_{-\frac{l_1}{2}-r}^{-\frac{l_1}{2}} f_{x_1}^{(1)}(u)\frac{1}{L}du+\int_{-\frac{l_1}{2}}^{\frac{L}{2}+t} f_{x_1}^{(2)}(u)\frac{1}{L}du,\ t\in[-\frac{L+l_1}{2},-\frac{L-l_1}{2}) \\ \int_{-\frac{l_1}{2}-r}^{-\frac{l_1}{2}} f_{x_1}^{(1)}(u)\frac{1}{L}du+\int_{-\frac{l_1}{2}}^{\frac{l_1}{2}} f_{x_1}^{(2)}(u)\frac{1}{L}du+\int_{\frac{l_1}{2}}^{\frac{L}{2}+t} f_{x_1}^{(1)}(u)\frac{1}{L}du,\ t\in[-\frac{L-l_1}{2},-\frac{L-l_1}{2}+r) \\ \int_{-\frac{l_1}{2}-r}^{-\frac{l_1}{2}} f_{x_1}^{(1)}(u)\frac{1}{L}du+\int_{-\frac{l_1}{2}}^{\frac{l_1}{2}} f_{x_1}^{(2)}(u)\frac{1}{L}du+\int_{\frac{l_1}{2}}^{\frac{l_1}{2}+r} f_{x_1}^{(1)}(u)\frac{1}{L}du,\ t\in[-\frac{L-l_1}{2}+r,\frac{L-l_1}{2}-r) \\ \int_{t-\frac{L}{2}}^{-\frac{l_1}{2}} f_{x_1}^{(1)}(u)\frac{1}{L}du+\int_{-\frac{l_1}{2}}^{\frac{l_1}{2}} f_{x_1}^{(2)}(u)\frac{1}{L}du+\int_{\frac{l_1}{2}}^{\frac{l_1}{2}+r} f_{x_1}^{(1)}(u)\frac{1}{L}du,\ t\in[\frac{L-l_1}{2}-r,\frac{L-l_1}{2}) \\ \int_{t-\frac{L}{2}}^{\frac{l_1}{2}} f_{x_1}^{(2)}(u)\frac{1}{L}du+\int_{\frac{l_1}{2}}^{\frac{l_1}{2}+r} f_{x_1}^{(1)}(u)\frac{1}{L}du,\ t\in[\frac{L-l_1}{2},\frac{L+l_1}{2}) \\ \int_{t-\frac{L}{2}}^{\frac{l_1}{2}+r} f_{x_1}^{(1)}(u)\frac{1}{L}du,\ t\in[\frac{L+l_1}{2},\frac{L+l_1}{2}+r) \\ 0,\ t\in[\frac{L+l_1}{2}+r,\infty) \end{cases} \tag{25}$$

and

$$f_Y(t)=\begin{cases}0,\ t\in(-\infty,-\dfrac{L+l_2}{2}-r)\\ \int_{-\frac{l_2}{2}-r}^{t+\frac{L}{2}} f_{y_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[-\dfrac{L+l_2}{2}-r,-\dfrac{L+l_2}{2})\\ \int_{-\frac{l_2}{2}-r}^{-\frac{l_2}{2}} f_{y_1}^{(1)}(u)\dfrac{1}{L}du+\int_{-\frac{l_2}{2}}^{\frac{L}{2}+t} f_{y_1}^{(2)}(u)\dfrac{1}{L}du,\ t\in[-\dfrac{L+l_2}{2},-\dfrac{L-l_2}{2})\\ \int_{-\frac{l_2}{2}-r}^{-\frac{l_2}{2}} f_{y_1}^{(1)}(u)\dfrac{1}{L}du+\int_{-\frac{l_2}{2}}^{\frac{l_2}{2}} f_{y_1}^{(2)}(u)\dfrac{1}{L}du+\int_{\frac{l_2}{2}}^{\frac{L}{2}+t} f_{y_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[-\dfrac{L-l_2}{2},-\dfrac{L-l_2}{2}+r)\\ \int_{-\frac{l_2}{2}-r}^{-\frac{l_2}{2}} f_{y_1}^{(1)}(u)\dfrac{1}{L}du+\int_{-\frac{l_2}{2}}^{\frac{l_2}{2}} f_{y_1}^{(2)}(u)\dfrac{1}{L}du+\int_{\frac{l_2}{2}}^{\frac{l_2}{2}+r} f_{y_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[-\dfrac{L-l_2}{2}+r,\dfrac{L-l_2}{2}-r)\\ \int_{t-\frac{L}{2}}^{-\frac{l_2}{2}} f_{y_1}^{(1)}(u)\dfrac{1}{L}du+\int_{-\frac{l_2}{2}}^{\frac{l_2}{2}} f_{y_1}^{(2)}(u)\dfrac{1}{L}du+\int_{\frac{l_2}{2}}^{\frac{l_2}{2}+r} f_{y_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[\dfrac{L-l_2}{2}-r,\dfrac{L-l_2}{2})\\ \int_{t-\frac{L}{2}}^{\frac{l_2}{2}} f_{y_1}^{(2)}(u)\dfrac{1}{L}du+\int_{\frac{l_2}{2}}^{\frac{l_2}{2}+r} f_{y_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[\dfrac{L-l_2}{2},\dfrac{L+l_2}{2})\\ \int_{t-\frac{L}{2}}^{\frac{l_2}{2}+r} f_{y_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[\dfrac{L+l_2}{2},\dfrac{L+l_2}{2}+r)\\ 0,\ t\in[\dfrac{L+l_2}{2}+r,\infty)\end{cases}\tag{26}$$

and

$$f_Z(t)=\begin{cases}0,\ t\in(-\infty,-L)\\ \int_0^{t+L} f_{z_1}^{(1)}(u)\dfrac{1}{L}du,\ t\in[-L,-L+l_3-r)\\ \int_0^{l_3-r} f_{z_1}^{(1)}(u)\dfrac{1}{L}du+\int_{l_3-r}^{t+L} f_{z_1}^{(2)}(u)\dfrac{1}{L}du,\ t\in[-L+l_3-r,-L+l_3)\\ \int_0^{l_3-r} f_{z_1}^{(1)}(u)\dfrac{1}{L}du+\int_{l_3-r}^{l_3} f_{z_1}^{(2)}(u)\dfrac{1}{L}du,\ t\in[-L+l_3,0)\\ \int_t^{l_3-r} f_{z_1}^{(1)}(u)\dfrac{1}{L}du+\int_{l_3-r}^{l_3} f_{z_1}^{(2)}(u)\dfrac{1}{L}du,\ t\in[0,l_3-r)\\ \int_t^{l_3} f_{z_1}^{(2)}(u)\dfrac{1}{L}du,\ t\in[l_3-r,l_3)\\ 0,\ t\in[l_3,\infty)\end{cases}\tag{27}$$

Thus, by substituting Eqs. (25)-(27) into Eq. (16), the probability of Λ_1^2 can be obtained

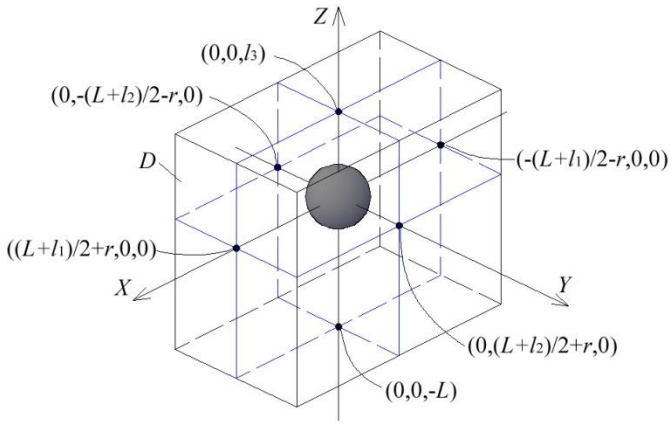


Fig. 5 The rectangle domain D outside of a sphere with a radius of 2r

numerically with given values for α, V, h, r, V_f, l_1, l_2, and l_3. From the engineering point of view, the practical parameters in our model should be obtained from experimental tests, such as from the scanning electron microscopy (SEM). Then by using our model, the healing probability and efficiency can be used to design suitable radius and volume fraction of microcapsules. However, the exact solution of $P(H_n^{n'})$ is difficult to achieve when both n and n' are very large. For example, when r=0.15 mm, l_1 = 4 mm, l_2 = 0.1 mm, l_3 = 4 mm, V_f = 0.1, h = 0.5, α = 1 and V = 125 mm^3, the total number of microcapsules in RVE is 885 and the number of broken microcapsules is 57. It is difficult to calculate the probability by using the above 3D model. Therefore, it is necessary to find a simplified method to obtain an approximate answer for the microcapsule self-healing method.

4. A simplified three-dimensional analytical probability healing model

When considering the microcapsule self-healing method, the above 3D probability healing model can be simplified due to the particularity of the parameters pertaining to both microcapsules and cracks, which are different from the parameters in the capsule self-healing method (Zemskov *et al*. 2010). To obtain a simplified probability function, we make the following assumptions:

-all of the microcapsules are distributed uniformly within each RVE;

-the crack in the RVE has a length of l_1, an opening value of l_2 and a height of l_3, and furthermore, it is perpendicular to the element's surface. This crack is located at y=0 in the local coordinate system, as displayed in Fig. 6;

-since the microcapsule is very small, it is rational to assume that the radius of a microcapsule is much smaller than the length of the RVE (i.e., $r << \sqrt[3]{V}$), the crack's length (i.e., $r << l_1$) and the crack's height (i.e., $r << l_3$);

-because of practical considerations, it is reasonable to assume that the opening value of the crack is much smaller than the length of the RVE (i.e., $l_2 << \sqrt[3]{V}$), the crack's length (i.e., $l_2 << l_1$) and the crack's height (i.e., $l_2 << l_3$);

-because too many microcapsules will decrease the strength and modulus of concrete, the volume fraction of the microcapsules must be limited. Because of the small radius and small volume fraction of the microcapsules, the probability of the event that the distance between the centers of any two microcapsules is less than 2r can be treated as zero. Additionally, the extended volume around the crack can be neglected, as shown in Fig. 6.

Due to the above assumptions, emanating from Eq. (6), the probability that the crack hits one microcapsule is as follows

$$p = \frac{V_{A1}}{V_{\Omega 1}} = \frac{l_1 \times (l_2 + 2 \times r) \times l_3}{(V^{1/3} - 2r)^3} \tag{28}$$

Furthermore, Eq. (13) can be rephrased as

$$k_{j+n'}^{n} = P(\Lambda_1^n \bigcap ... \bigcap \Lambda_{j+n'}^n) = p^{j+n'} \tag{29}$$

Accordingly, the healing probability in Eq. (12) can be calculated as follows

$$\begin{aligned} P(H_n^{n'}) &= n \times C_n^{n'-1} \sum (-1)^j C_{j+n'}^j / (j+n') \\ &= C_n^{n'} p^{n'} (1-p)^{n-n'} + C_n^{n'+1} p^{n'+1} (1-p)^{n-n'-1} + ... + C_n^n p^n \end{aligned} \tag{30}$$

Moreover, because n is very large and p is very small, the Poisson distribution is employed to estimate $P(H_n^{n'})$. Thus, Eq. (30) can be transformed as

$$P(H_n^{n'}) = \sum_{k=n'}^{n} \frac{\lambda^k e^{-\lambda}}{k!} = 1 - \sum_{k=0}^{n'-1} \frac{\lambda^k e^{-\lambda}}{k!} \tag{31}$$

where

$$\lambda = np \tag{32}$$

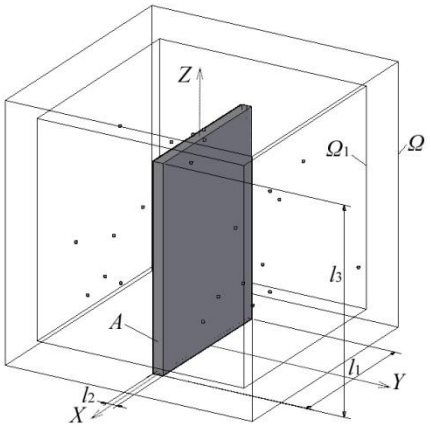
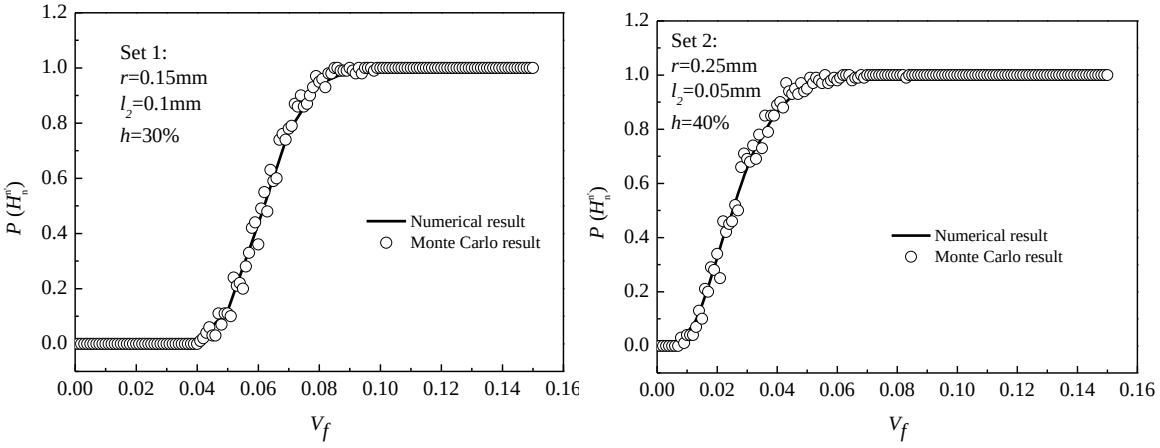


Fig. 6 The calculation diagram of the simplified 3D probability healing model



(a) Set 1 (b) Set 2

Fig. 7 A plot of the probability obtained by Monte Carlo tests and the proposed 3D probability healing model

5. Verification and discussions

5.1. Comparison between the numerical results and the Monte Carlo results

The experimental results are few and hard to validate our model directly. The existing probabilistic models have not considered the healing efficiency or are two-dimensional models and it is difficult to make comparisons. The proposed simplified 3D analytical probability healing model is validated by Monte Carlo tests (Zemskov *et al*. 2010, Zemskov *et al*. 2011). By randomly generating numerous microcapsules in a RVE, the number of broken microcapsules can be counted. Then, 300 experiments for each value of the volume fraction from 0% to 15% with a step of 0.1% are conducted to calculate the practical probability by the Monte Carlo method. The test results with the probability $P(H_n^{n'})$ obtained by the simplified 3D probability healing model are presented in Fig. 7, with two sets of different parameters. The first set of parameters are α = 1, h = 30%, V = 125 mm^3, l_1 = 4 mm, l_2 = 0.1 mm, l_3=4 mm and r = 0.15 mm. The second set of parameters are α = 1, h = 40%, V = 125 mm^3, l_1 = 4 mm, l_2 = 0.05 mm, l_3 = 4 mm and r = 0.25 mm. It is obvious that the results predicted by the proposed 3D probability healing model agree well with the Monte Carlo simulations.

5.2. Discussions on the influence of the microcapsules on the healing efficiency and healing probability by the simplified 3D analytical probability healing model

The above simplified probability healing model $P(H_n^{n'}) = f(r, V_f, h, V, l_1, l_2, l_3, \alpha)$ can be used to calculate the optimal parameters for the microcapsules under given conditions in the microcapsule self-healing system.

By predicting the healing probability using our probability model, the volume fraction of the microcapsules can be quantitatively assessed. As exhibited in Fig. 8, we can obtain $P(H_n^{n'})$ with

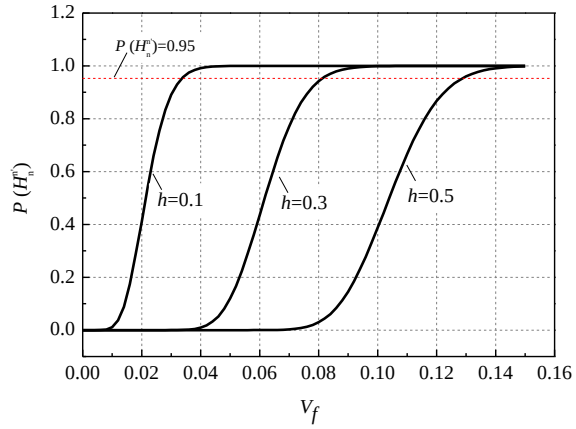


Fig. 8 The influence of the healing efficiency and volume fraction on the healing probability with a volume fraction from 0% to 15%

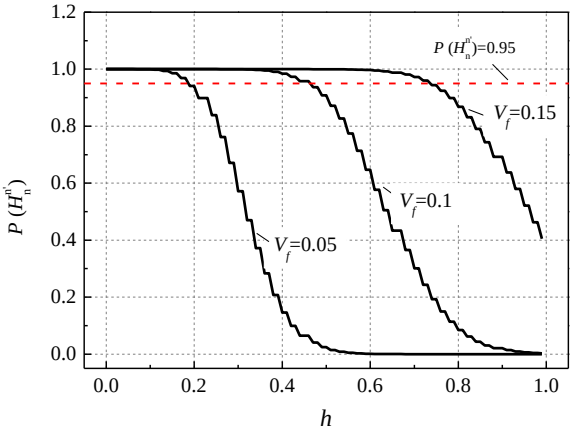


Fig. 9 The influence of the healing efficiency and volume fraction on the healing probability with a healing efficiency from 0% to 100%

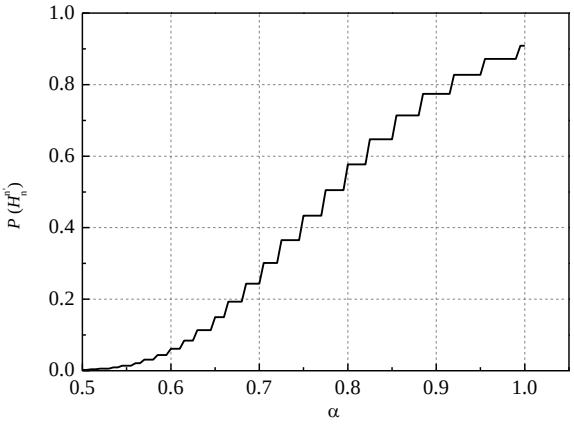


Fig. 10 The influence of the broken ratio on the healing probability with a broken ratio from 50% to 100%

different values for V_f and expected healing efficiencies, with parameters of α = 1, r = 0.15 mm, V = 125 mm^3, l_1 = 4 mm, l_2 = 0.1 mm and l_3 = 4 mm. The result shows that the higher healing efficiency and healing probability we require, the more microcapsules should be added. The middle line in Fig. 8 illustrates the fact that if we want the crack to be healed more than 30% with a probability of 95%, we should add approximately 8% microcapsules into the matrix.

On the basis of the previously proposed 3D analytical probability healing model, the healing efficiency can be quantitatively predicted. As exhibited in Fig. 9, a lower volume fraction and a higher expected healing efficiency will decrease the healing probability. We find that $P(H_n^{n'})$ is a step function. The reason is that, when one more microcapsule needs to be broken, the healing probability will decrease. Here, we assume that when $P(H_n^{n'})$ is greater than 0.95, the healing efficiency will be h. The middle line in Fig. 9 illustrates the fact that the expected healing efficiency is 0.47 if the parameters are α=1, V_f= 0.1, r = 0.2 mm, V = 125 mm^3, l_1 = 4 mm, l_2 = 0.1 mm and l_3=4 mm.

Based on the previously proposed 3D probability healing model, the broken ratio α can seriously influence the healing probability. As exhibited in Fig. 10, a lower broken ratio will cause the healing probability to decrease, given parameters of h = 0.5, V_f= 0.1, r = 0.2 mm, V = 125 mm^3, l_1 = 4 mm, l_2 = 0.1 mm and l_3 = 4 mm. Thus, high-quality interfacial bonding is essential in the microcapsule self-healing method.

6. Conclusion

Cracks significantly deteriorate the in-situ performance of concrete elements and structures, particularly in an urban metro tunnel that has a complicated surrounding environment in terms of underground water, vehicle vibrations and ground pressures. The microcapsule self-healing method, which can automatically heal numerous cracks in concrete, will be a promising strategy for dealing with these problems in the future.

In view of the limited number of healing models that can analytically describe the healing mechanism of this method, a 3D probability healing model is proposed in this paper; it is based on the geometry probability and the healing mechanism of the microcapsule self-healing method. The difference between the healing mechanisms of the microcapsule self-healing method and the capsule self-healing method has been considered. As a result, the healing probability and healing efficiency of the microcapsule self-healing method can now be calculated. Due to the features of the method, a simplified probability healing model is developed on the basis of the 3D analytical probability healing model. The probability framework comprehensively considers the radius and volume fraction of microcapsules, the healing efficiency, the healing probability, the broken ratio and the features of a crack.

The proposed 3D probability healing model is verified by Monte Carlo tests. Furthermore, the properties of microcapsules have been discussed. The parameters of the microcapsules play an important role in the healing probability and healing efficiency, and therefore, they should be properly adjusted to achieve an optimal healing result when using the microcapsule self-healing method.

Further research is warranted to improve the proposed 3D probability healing model. Specifically, other methods that can describe the fractures of microcapsules at the micro level, such as fracture mechanics, can be introduced into the probability healing model.

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