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Review Paper

Modeling of Self-Healing Concrete: A Review

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Abstract. Self-healing concrete (SHC) has received a tremendous attention due to its advanced ability of automatic crack detection and crack repairing compared to the standard concrete. Two main approaches which considered as to-date self-healing mechanisms are autogenous and autonomous healing. In the past several years, the effort of the research has been focused on experimental works instead of numerical models to simulate the healing process. The purpose of this study is to provide a comprehensive comparison of different self-healing concrete (cement based materials) modeling approaches which are available. In this review, special attention is given to the autonomous healing model and a few of recent works related to the autogenous healing model are also investigated. Moreover, this review covers both analytical and numerical simulation methods of self-healing concrete model.

Keywords: Self-healing concrete; Autogenous healing; Autonomous healing; Numerical models.

1. Introduction

Concrete is the most commonly used material in the construction area due to its high strength and durability relative to its cost. Because of the limited tensile strength, concrete is quite sensitive to the crack formation which can endanger the durability of concrete structures as a whole. Cracks or micro-cracks might appear at any stages of service life of concrete structures because of excessive loadings, harsh environment exposure, shrinkage, etc. Cracks can lead to the deterioration of concrete structures since aggressive liquids and gasses are able to penetrate into the matrix, and therefore, reduce the mechanical performance of concrete structures. Accordingly, the inspection, maintenance, and repair works are obviously needed. According to previous research [1], in Europe, the repair works costs have been estimated to contribute at least around 50% of the annual total construction budget, aside from indirect costs, due to the productivity loss. However, when the appearance of cracks or microcracks are not visible and accessible, the repair activities would become difficult and demand very high costs. Therefore, making self-healing concrete with triggering crack healing mechanism without human intervention would be highly beneficial.

Recently, self-healing concrete has received a tremendous attention from researchers in civil engineering sciences due to their wide range of capabilities; for example, less human intervention in maintenance and increase the service life of structures. In the domain of self-healing concrete, there are a limited number of studies which discuss their work. For example, different strategies of self-healing mechanism in cementitious materials were reviewed by Wu et al.[2]. They covered different possible mechanisms of self-healing approach based on the substantial experimental and practical works. The comparison between different healing techniques and healing agents were also discussed. The capability of self-healing approach in Engineered Cementitious Composite (ECC) was also introduced as summary of their review. Van Tittelboom and De Belie [3] conducted a comprehensive review of self-healing approaches in cementitious materials. They discussed the advantages and disadvantages of different types of healing agents and encapsulation techniques. The different mechanisms which could be triggered to



activate self-healing was also evaluated. The review of self-healing concrete based on the three key taxonomies, i.e. natural self-healing, chemical self-healing, and biological self-healing was presented by Talaiekhazan et al. [4]. They reviewed the unexpected cracking of concrete by focusing on biological processes. Lv and Chen [5] discussed self-healing technologies of both autogenous and autonomous types. They reviewed the improvement of durability and performance of self-healing structures based on the experimental and practical investigation. A brief overview of the analytical and simulation model of self-healing in cementitious materials were also presented. The effectiveness of self-healing with respect to its application in actual structures were evaluated by Ahn et al. [6]. They reviewed all researches on ultrasonic-based nondestructive methods and case studies relating to the self-healing concrete. Both the applicability and the limitation of different nondestructive methods in assessing self-healing performance were also highlighted.

In connection with the aforementioned review papers, the comprehensive review of computational techniques for fracture in brittle and quasi-brittle materials by focusing on continuum models was conducted by Rabczuk [7]. Fracture modeling techniques of quasi-brittle materials such as concrete have been carried out over decades [8, 9, 10, & 11]; for instance, the mesh-free methods [8, 11, 12, 13, 14, 15, & 16], the particle method [9], and the cohesive crack method [10]. Since the computational model is become a valuable resource for the experimentalists to select materials and start the experimental works, the review of self-healing concrete from the computational model point of view is necessarily important. According to the best-knowledge authors, it is difficult to find the references which discussed the computational modeling techniques of self-healing in cement-based materials.

In this study, a review on the modeling of self-healing concrete (cement-based materials) of both autogenous and autonomous healing is provided. First, different approaches of the autogenous healing model are presented. Subsequently, more comprehensive computational techniques of the autonomous healing model are discussed. Finally, future perspectives on the research in modeling techniques for self-healing concrete are highlighted. Since this study focuses on modeling techniques of the self-healing concrete, the other types of materials and sorts of experimental works are out of domain of this research.

2. Modeling of self-healing concrete

2.1 Autogenous healing model

The autogenous healing is one of the classic types of self-healing in concrete. The healing mechanism attributed to the microcracks is due to re-hydration of unhydrated cement particles in the concrete matrix [17]. Some researchers have investigated and concluded that the main contributions of self-healing in cement-based materials were further hydration of unhydrated cement particles and the nucleation of calcite [18, 19, 20, 21]. In terms of the numerical model, recently, some of researchers have developed a novel computational model to investigate the behavior of autogenous healing in self-healing concrete. Lv and Chen [22] investigated the efficiency of self-healing with hydration reaction of unhydrated cement nuclei. They used splitting crack and dome-like crack modes to model the cracking in the unhydrated nuclei. The self-healing efficiency was presented in terms of geometrical probability. They showed that the degree of self-healing efficiency is characterized based on the crack modes. Moreover, Huang and Ye [23] proposed a model of self-healing by providing extra water on unhydrated cement for further hydration. They assumed that there exists an amount of water stored in capsules and can be passed by cracks and unhydrated cement particles as well. These unhydrated particles were exposed on both of crack surfaces and embedded inside the cement paste as shown in Fig. 1.

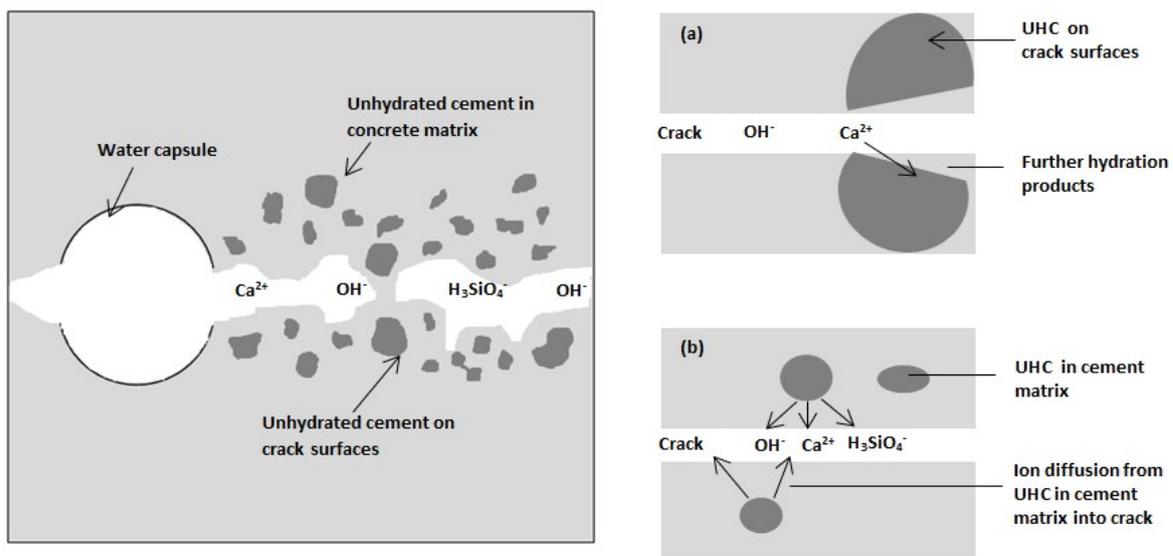


Fig. 1. Schematic mechanism of further hydration (a) On crack surfaces (b) On cement matrix (UHC represents unhydrated cement particles) (reproduced from [23]).

HYMOSTRUC3D was used to simulate the distribution of unhydrated cement particles. A micro-crack with the dimensions of 40 mm (length)x 40 mm (depth) x 10 μ m (width) was assumed to pass through a water capsule due to the hydration

formed in the cement paste. The ion diffusion model based on Ficks second law was used to calculate the concentration of ions in each micro pixel. A water-filled section with the size of $100 \mu\text{m} \times 100 \mu\text{m}$ was modelled to simulate further hydration processes using the thermodynamics model. The schematic of simulation model is illustrated in Fig. 2. The result of their simulations showed that the amount of unhydrated cement and extra water on further hydration processes can be optimized quantitatively based on the self-healing efficiency.

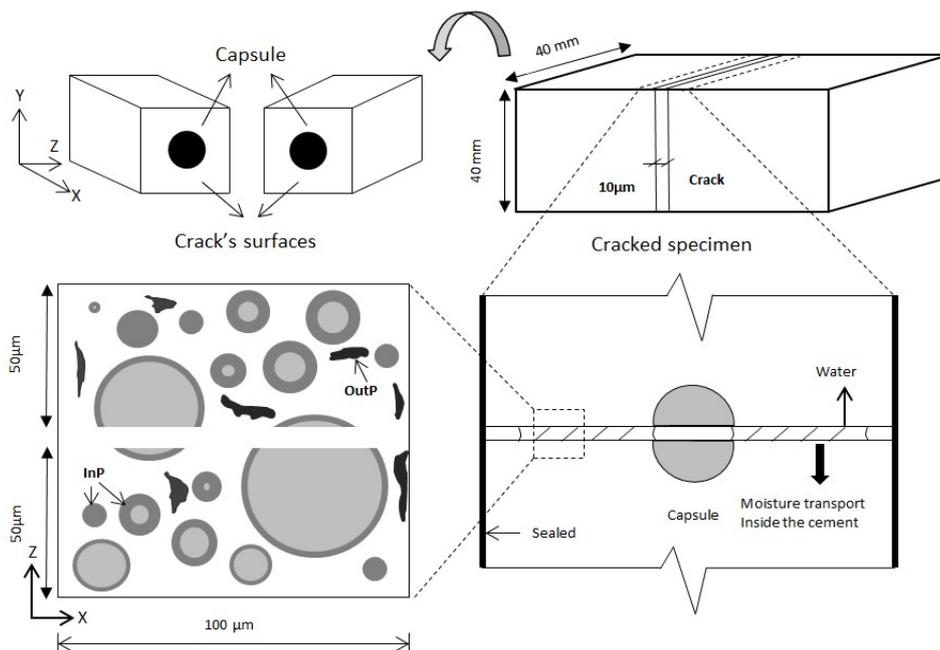


Fig. 2. Schematic of computational model (InP = inner product, UHC = unhydrated cement particles) (reproduced from [23]).

Numerical modeling of self-healing capacity in cement-based materials was conducted by Ferrara et al. [24 & 25] using the micro-plane model M4 and the solidification-micro-prestress theory. The hygro-thermal-chemical problem was used to reproduce the moisture, heat fields, and the hydration degree as well. They incorporated self-healing effects on some internal variables in the model which characterize the process, diffusivity, and the repairing effects. The self-healing recovery degree λ_{sh} was introduced to describe the effects of self-healing in the model in terms of regain the strength after its damage or cracking (strength recovery). When $\lambda_{sh} = 1$, it means that the strength of materials has completely recovered to its origin state, from damage or deterioration. Moreover, a good agreement was shown between experimental and numerical results in all simulated experimental cases. They also showed that the mix composition and the duration of exposure significantly influence the recovery of the load carrying capacity.

Hilloulin et al. [26] investigated self-healing phenomenon on Ultra High Performance Concrete (UHPC). The autogenous healing process by further hydration in the material was simulated using hydro-chemo-mechanical model which was implemented in the finite element code Cast3M. This model calculated the self-healing potential by comparing the mechanical properties between virgin and healed models. The comparison took place at different stages during 1 to 40 weeks. The damage occurred after cracking were calculated by the modified-microplane model, while the Fick's law was applied to simulate the ingress of water. The mechanical properties of healed model was obtained by decreasing the damage value assuming that the empty space was filled up with new hydrates. The simulation results revealed that the predicted corresponding load to the end of the first slope are overestimated. This phenomenon is due to the discontinuity of mechanical properties around two-phases modes. The assesment of cracking and healing in changing modal parameters of concrete beams was evaluated by Savija and Schlangen [27]. They used natural frequency changes to identify the damage, and therefore, the indication of healing could also be taken from the recovery of natural frequencies. Dynamic behavior of concrete beams was modelled using spectral element method (SEM) combined with Delft lattice model to investigate the effects of cracking and healing on modal properties of concrete beams. The 2D simulation showed that the appearing microcracks prior to the peak load caused a slight decrease in the first natural frequency. The natural frequency of healing events were recovered (except for the first one), but still it was lower than the first one. On the other hand, the capability of cohesive zone model to simulate self-healing materials was investigated by Abu Al-Rub and Alshegri [28]. They developed the cohesive zone damage-healing model (CZDHM) based on thermodynamics law. The healing mechanism was thermally stimulated through molecular interdiffusion. Damage and healing was described by the damage/healed fraction of the cohesive bonds and its value ranged from 0 to 1. The internal degradation variable D and h are dimensionless such that $D = 0$ means no damage occurred and $D = 1$ demonstrates a complete damage, whereas $h = 0$ means no healing occurred and $h = 1$ indicates the complete healing of the damage. They demonstrated the healing model of mode I fracture using single 2D cohesive element COH2D4 (1 mm x 1 mm). The results showed that increasing temperature and resting time will eventually increase the healing variable of materials. Aliko-Bentez et al. [29]

developed a numerical uncoupled healing model for concrete-based materials by incorporating the physicochemical approach. They proposed a healing mechanism which was activated through the precipitation of calcium carbonate inside the cracks. The mechanical variables were extended simultaneously for both damage and healing processes. Their preliminary models revealed that using different model parameters significantly influenced not only the results but also the qualitative trend derived from the experimental results. Hazelwood et al. [30] presented a numerical model to compare the long-term behavior of a new self-healing concrete system (LatConX) with the standard reinforced concrete. They composed the model from a set of sub-models which combined transient thermo-mechanical behaviors. The self-healing was incorporated in the form of mortar/concrete constitutive model either due to the healing additive or the autogenous healing which could determine the degree of healing. They assumed that the healing process was instantaneously occurred in terms of the healing time and its degree instead of following the healing function. Moreover, the coupled model of a layered beam and thermo-mechanical transient was validated with experimental data. The results showed that LatConX succeeded to reduce 65% of shrinkage stress and also half of the damage was healed. The effects of healing due to ongoing hydration on mechanical recovery were investigated by Hilloulin et al. [31] both experimentally and numerically. They conducted experimental works on cracked specimens at early stage to investigate various parameters, such as age, at cracking, initial crack width, and healing time. Self-healing in cementitious materials was modelled using the micro-mechanical technique. A modified version of CEMHYD3D called CemPP was used to simulate healing due to further hydration for different crack widths, age at cracking and healing time. A microstructure at the age of cracking with discretization of $1 \mu\text{m}$ over a volume of $100 \mu\text{m}$ was generated using CemPP. The hydration process inside specimens were modelled based on the cycles of dissolution, diffusion and reaction. The healed specimens of microstructure from CemPP roled as the input to the finite element code Cast3M to observe the mechanical recovery after healing. They showed that numerical model was in agreement with the experimental results. The numerical model built with Cast3M was based on the map of hydration model of CEMHYD3D. These models revealed that healing process occurred in the first 12 hours for small cracks, but it took longer for larger cracks or cracks created after 72 hours. The decrease of self-healing process was due to the lack of remaining unhydrated cements.

The autogenous healing mathematical model of an early-age cement-based materials was proposed by Chitez and Jefferson [32]. They applied a coupled thermo-hygro-chemical (THC) concept which incorporated the reactive water transport equation to estimate the healing motion. The influence of the crack width and the quantity of unhydrated cement on material behavior was also studied. The microstructural model STOICH_HC2 was used to characterize the porous network and hydration of the materials (defined as porosity curves and the initial concentration of unreacted clinker) and served as the input for the autogenous model. They considered the mean values of crack width as $62.5 \mu\text{m}$ and $187.5 \mu\text{m}$ in the model. The numerical results of $62.5 \mu\text{m}$ crack were in a good agreement with the experimental data reported in the literature. The STOICH_HC2 model proved that before occurring self-healing process, a number of hydration reactions had occurred (around 91%). Caggiano et al. [33] presented a coupled damage-plasticity zero-thickness interface theory to simulate concrete cracking and behavior with the self-healing consideration. The flow theory of plasticity and the continuum damage theory were formulated for the interface model and the fracture energy-based method was employed to control the post-peak response of both failure modes, I and II. The constitutive law of interface was extended to take the self-healing mechanism on strength, stiffness, and post-peak behavior for all fracture modes into account. The self-healing process was introduced as parameter $SH[\psi]$ which defines the evolution of concrete porosity at the post-peak regime. While ψ is the porosity factor of self-healing which depends on the current porosity of the interface during re-hydration and self-healing periods. The numerical results of load-displacement curves and corresponding experimental results were compared. A good agreement between numerical and experimental was achieved especially in the post-cracking response which was highlighting the effectiveness of discontinues approach based on the non-linear interfaces. The proposed model was able to capture softening response not only in the pre-cracking step, but also in the self-healing recovery stage.

A new method using two-phased micro-mechanical model to simulate the self-healing mechanism in cementitious materials was developed by Davies and Jefferson [34]. They used Mori-Tanaka homogenisation along with an Eshelby solution to calculate stress concentration neighbouring on inclusions. On the pther hand, the circular cracks were employed to mimic the microcracks, while solidification formulation was used to incorporate self-healing into the model. The idealised components in cementitious materials along with microcracks can be seen in Fig.3.

The healing process in the model was inserted by restoring stiffness of the damaged component along with 'solidification strain'. The proportion of healing was defined by parameter h ranging from 0 to 1 and the 'solidification strain' (ε_s) was also incorporated to ensure stress free condition in the solidification process of self-healing materials. The healing of microcracks in cementitious material is illustrated in Fig.4 and the current local stress is given by

$$s_{Lh} = (1-\omega)D_L : \varepsilon_{Lh} + h\omega_{th}D_{Lh} : (\varepsilon_{Lh} - \varepsilon_s) \quad (1)$$

where s_{Lh} and ε_{Lh} are the equivalent local stress and strain tensor after healing, respectively. D_{Lh} is the local stiffness of the healed material and ω_{th} is the micro-cracking parameter at the time of healing. They compared the proposed micromechanical model with the experimental results of standard concrete and ultra high performance concrete of both pre-healing and post-healing models. The comparison showed that the proposed micromechanical model is closely match with the experimental results. The results also revealed that the strength and stiffness at time of loading should be measured appropriately since these parameters affect the post-healing response significantly.

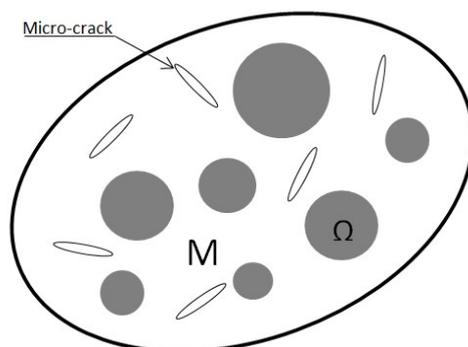


Fig. 3. Idealised micro-mechanical model of cementitious materials (reproduced from [34]).

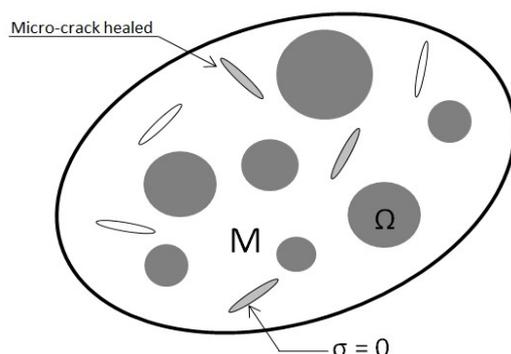


Fig. 4. Microcracks healed in cementitious materials (reproduced from [34]).

Ranaivomanana and Benkemoun [35] studied the complex interaction between the advection-diffusion mechanism to describe the healing process induced by carbonation in concrete structures. Partial differential equations in the form of transport-reaction for both crack and matrix were used. These equations were discretized using Embedded Finite Element Method (E-FEM) along with applying a weak discontinuity in the concentration of calcium ions (Ca^{2+}) where the crack exists. In addition, the calcite layer width, which resulted from healing process, was analytically solved. It was shown that the proposed interaction model dealt with only transport process in the system. The recovery of mechanical properties in the system was not considered though this is an important issue in the self-healing phenomenon. The softening-healing law based on the time-dependent technique was introduced by Zhang and Zhuang [36] to study self-healing phenomenon in concrete. A mixed-mode traction-separation law was used to consider the relationship between crack opening and traction of two surfaces of crack. They considered crack opening of mode I and II for 2D simulation. The back analysis from self-healing experimental works (three point bending test) was applied to obtain some healing parameters of healing agents. In order to evaluate the reliability of the model, the strong discontinuity approach (SDA) based on the standard Statically Optimal Symmetric (SOS) was adopted in their study. Moreover, in order to validate the proposed numerical model, they simulated the gravity dam model with the notch which was investigated experimentally. The concentrated load at 4 heights was applied in the numerical model similar to the experimental work. The result of load-CMOD curves showed a satisfactory agreement between the numerical model and the experimental result for the non-healing model.

Suleiman and Nehdi [37] developed a hybrid approach of genetic algorithm-artificial neural network (GA-ANN) to predict the autogenous self-healing phenomenon in concrete. They implemented genetic algorithm in the network as an optimizing tool to assist in reaching global optimum, and at the same time, the local optima could be avoided. The artificial neural network (ANN) was implemented to capture the multi-difficulty interdependent parameters since self-healing concrete contains high complex processes. The architecture of network consisted of 11 input neurons representing the main parameters influencing the self-healing of concrete for example the cement content, water-to-cement ratio (w/c), supplementary materials in matrix, healing materials, crystalline additives, along with 14 neurons as a hidden layer. The model output with a single neuron representing the crack width as an efficiency of self-healing process. The schematic view of genetic algorithm-artificial neural network (GA-ANN) is illustrated in Fig. 5. The proposed GA-ANN model was validated based on the built database from various experimental studies. The accurate prediction between the proposed algorithm and the experimental results was achieved since the results of both of values was close together.

2.2 Autonomous healing model

The autonomous healing in concrete-based material can be achieved by releasing encapsulated healing agents caused by some trigger mechanisms. The mechanisms to obtain healing action, which have been found in the literature, are triggered by ingress of liquids or gasses, exertion of heat or by crack formation [3]. This review focused on modeling of encapsulation-based self-healing concrete by embedding capsules or microcapsules in the mortar matrix. Zemskov et al. [38] developed a

mathematical model for bacterial self-healing of cracks in concrete structures. They embedded spherical clay capsules along with nutrients for bacteria in the concrete structures. The type of healing agent was calcium lactate which was stored inside the clay capsules. The appearance of crack initiated the breakage of capsule, released its content, combined with the entering water activated the bacteria, and converted calcium lactate into calcium carbonate (limestone). Releasing healing agents from the capsule and the calcium carbonate conversion were modelled with a moving boundary problem. A level set method was used to track the moving boundaries, while the diffusion equations were solved using Galerkin finite element method. The proposed mathematical model considered the combination of some important parameters, such as crack width and capsule size. The results showed that the crack healed completely. The concentration of calcium lactate dissolved around 60% before healing was finished. The mathematical model for bacterial self-healing of crack could be easily extended to 3D model because of symmetry considerations.

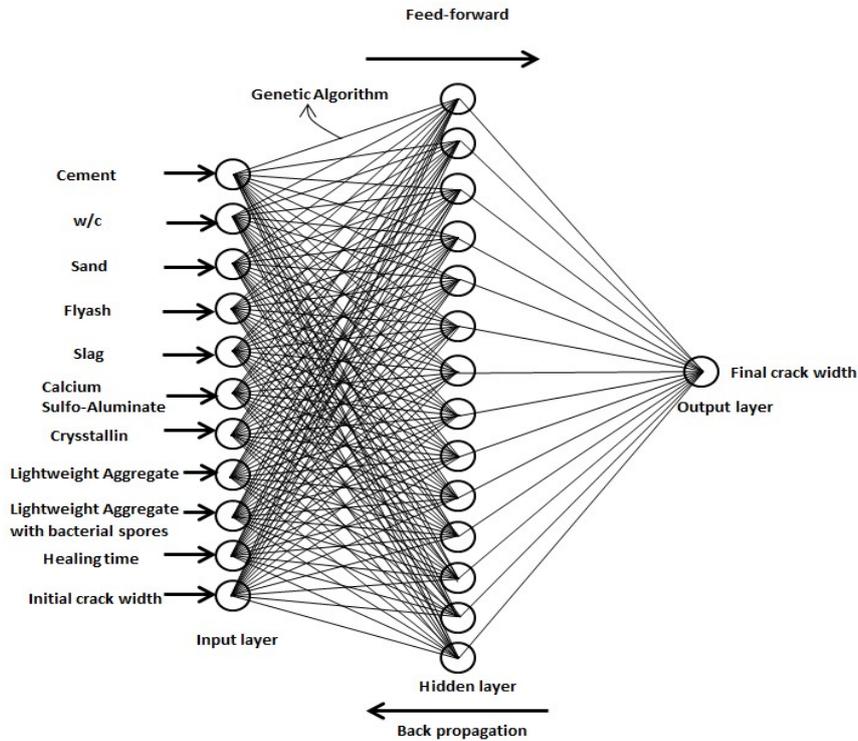


Fig. 5. The diagram of genetic algorithm-artificial neural network (GA-ANN) model (reproduced from [37]).

The probability model of penny-shaped cracks hitting the capsules in 2D and 3D model were presented by Lv and Chen [39]. They developed analytical models on determining capsules dosage embedded in self-healing materials with some target healing levels. The risk-based probabilistic approach was employed to predict the amount of capsules required to fulfill the particular degree of healing as given by

$$P = 1 - \exp[-\sigma(\pi R^2 + 2Rl)] \tag{2}$$

or expressed in terms of fraction area of capsules A_A

$$P = 1 - \exp[-A_A(1 + \frac{2l}{\pi R})] \tag{3}$$

where $A_A = \pi R^2 \sigma$. It means that if the expected healing probability P is determined (in this case it was intersecting probability), the required dosage of capsules can be calculated as follows:

$$A_A = \frac{\pi R}{\pi R + 2l} \ln \frac{1}{1 - P} \tag{4}$$

They also investigated the hitting probability of both spherical and cylindrical capsules with a particular aspect ratio as illustrated in Figs. 6 and 7. The proposed probability model was then compared to the analytical solutions based on the different dosage of capsules and the ratio of crack length to capsule radius. The results showed a good agreement between simulation and analytical results. The stable value of simulated results were achieved when increasing the number of executions.

In addition, Lv et al. [40] developed the simplification of complex crack patterns due to various mechanisms in cementitious materials into linear crack and planar crack patterns in 2D and 3D models, respectively. They assumed that the average spacing between adjoining cracks is less than the length of the embedded capsules. With this assumption, the analytical solutions of predicted dosage of capsules required in each type of crack pattern models were determined using

geometrical probability. Some of the crack pattern models in 2D and 3D can be seen in Figs. 8 and 9. The reliability of simulation results of both probability and dosage models closely matched to the analytical solutions. on the other hand, the intersecting probability of crack hitting capsules tended to be more stable as the number of capsules increased. Moreover, the probability of healing ratio reached a stable value, 1, as the size of sampling increase.

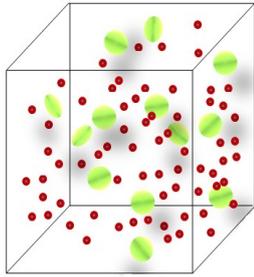


Fig. 6. 3D self-healing model with spherical capsules and penny-shaped cracks (reproduced from [39]).

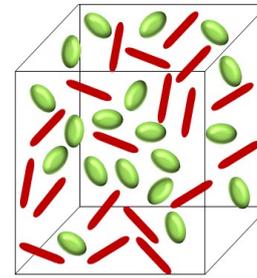


Fig. 7. 3D self-healing model with cylindrical capsules and penny-shaped cracks (reproduced from [39]).

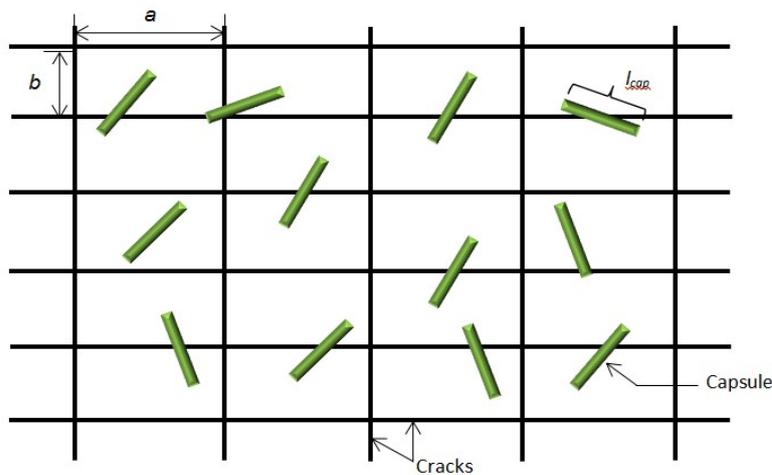


Fig. 8. 2D simplified cell-like crack model pattern (reproduced from [40]).

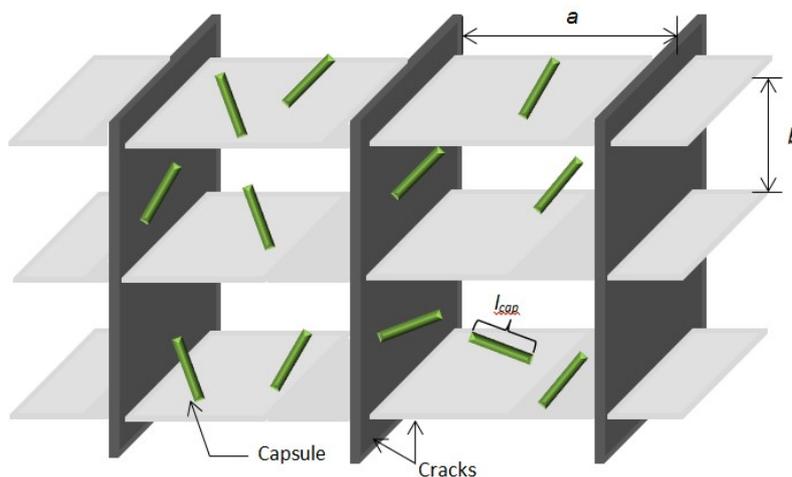


Fig. 9. 3D simplified orthogonal planar crack model pattern (reproduced from [40]).

In order to study the optimum microcapsule parameters with the best effects on self-healing, Zhu et al. [41] proposed the 3D analytical self-healing model based on the probability point of view. They considered some parameters of spherical microcapsules such as radius of microcapsules, volume fraction of microcapsules, targeted healing efficiency, broken ratio, etc. To verify the proposed analytical healing model, they conducted monte carlo test to examine the influence of some key paramaters on healing probability and efficiency. The role of interface and stress concentration around embedded cylindrical capsules in a matrix was investigated by Gilabert et al. [42]. They modelled a matrix as an elastic, homogeneous, and isotropic which subjected to the uniform and uniaxial stress. A model with square plate of length $2L$ consisted a hole with radius R_c and shell thickness t_c was proposed. the quarter specimen with the half-length of square $L = 50$ mm, $R_c = 1.5$ mm and $t_c = 0.1$

75 mm had been performed because of symmetry as shown in Fig. 10.

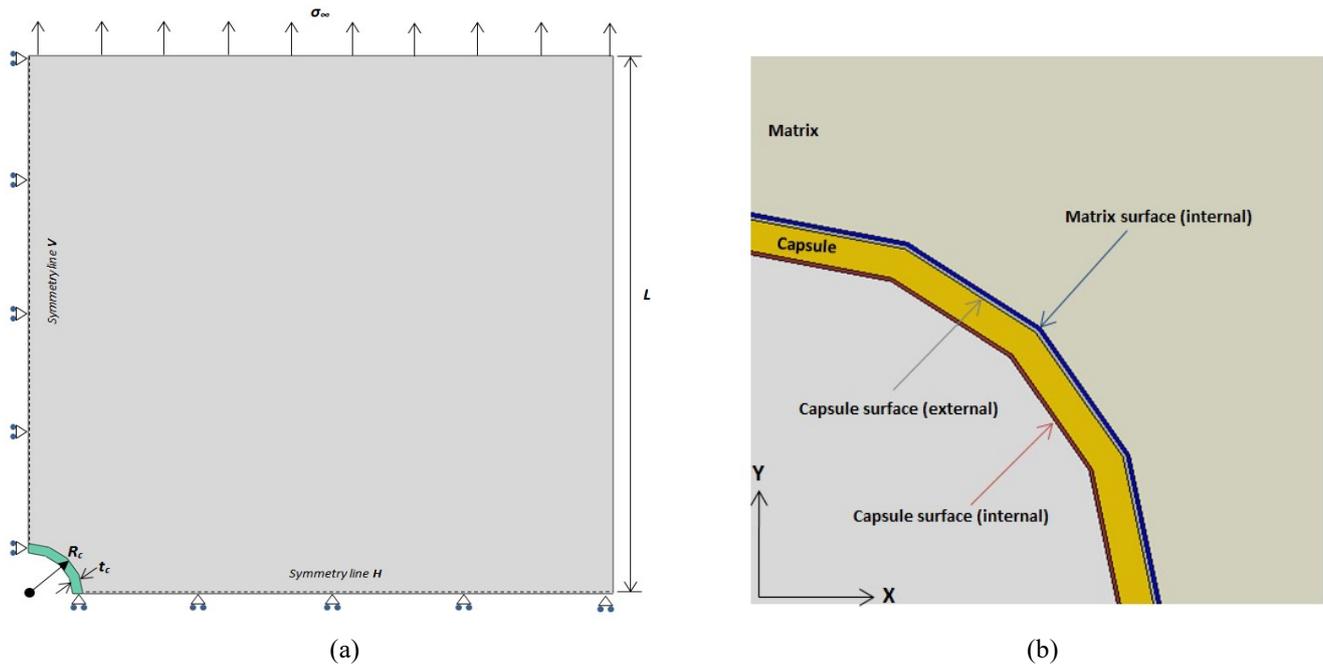


Fig. 10. Schematic of numerical model. (a) Geometry, boundary conditions and uniaxial loads. (b) Detail surfaces between capsule and matrix (reproduced from [42]).

In the above-mentioned research, the optimum combination properties, the effects of variation of elastic properties between matrix and capsule, different thicknesses of capsules, and bonding strength on generation of stress concentration around capsule were studied. The results showed that using a soft capsule ($E_c/E_m < 1/5$) restored the mechanical response governed by Kirsch’s equations for a plate with a hole. Moreover, in order to avoid debonding phenomenon, the required stress depends linearly on the logarithm of the geometric ratio ($t_c/R_c < 0.6$).

Huang and Ye [43] investigated the effects of amount of water supplied to capsules on the healing efficiency due to further hydration of unhydrated cement. The efficiency of the amount of supplied water in capsules determined numerically as a function of capsule dosages and sizes. The probability of crack hitting capsules was simulated with a beam model (40 mm x 40 mm x 160 mm). As shown in Fig. 11, they assumed that all random distribution capsules inside the beam were spherical with identical radius and no overlapping, which can not cross the edge of beam. The cement paste in the model was simplified as homogeneous material and the crack was simplified as planar crack. In their model, the probability of crack hitting capsules is defined as the probability of capsules centered across the influence zone of the crack as illustrated in Fig. 12. To this aim, the statistical analysis of 1000 random samples were conducted. The numerical results shown that the increasing amount of released water were in line with the dosage of capsules at different slopes. From self-healing efficiency point of view, the optimizing size of capsules is 6.5 mm for capsule dosages of 3%, 5%, and 7%, respectively. The mechanical properties of cementitious materials (elastic modulus and tensile strength) decrease as the volume fraction of capsules increase.

The breaking mechanism of microcapsules in concrete due to microcracking was studied by Zhou et al. [44]. One circular microcapsule as a void and one microcrack were considered in this model. They simulated the fracture behavior of concrete specimens using two-dimensional particle flow code (PFC2D). The dimension of specimen was 140 mm x 70 mm, and consisted of about 30,000 particles. The radius of particles ranging from 0.25 to 0.415 mm based on the normal particle size distribution. A local high damping coefficient of 0.7 was used in the simulation to ensure the quasi static loading condition. Moreover, Zhou et al. [45] proposed 3D damage-healing of encapsulation-based self-healing system using discrete element method (DEM) under compression load. They investigated the effects of some key parameters on encapsulation-based self-healing materials, such as the strength and stiffness of solidified healing agent, the initial damage, and the partial effect of healing. The specimen was generated using PFC3D with the radius 5.08 cm and height 20.32 cm, and all spheres particles were connected by the parallel bond model as illustrated in Fig. 13.

They proposed scalar healing variable h as a negative damage to take into account in the existing damage model. In the discrete element method, it is assumed that the number of bonds rises after healing, right after the damage occurred, as shown in Fig. 14. Based on the discrete element method, the scalar healing parameter h can be simply determined by

$$h = \frac{N_h - N_d}{N_i - N_d}, 0 \leq h \leq 1 \tag{5}$$

where N_h is the number of bonds after healing, N_d is the number of bonds after damage, and N_i is the number of initial bonds. When $N_h = N_d$, it means that healing is not occurred or $h = 0$. Identically, when $N_h = N_i$, it means that all damaged bonds

are healed or $h = 1$. To obtain the self-healing effect, N_h should be higher than N_d .

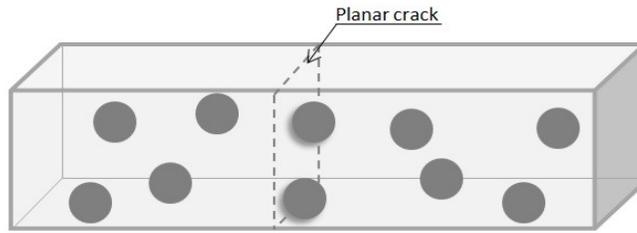


Fig. 11. Diagram of planar crack hitting capsules model (reproduced from [43]).

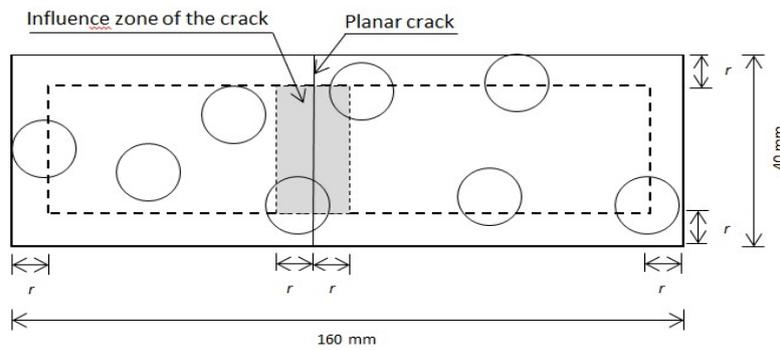


Fig. 12. Schematic distribution of capsules and the influence zone of planar crack (reproduced from [43]).

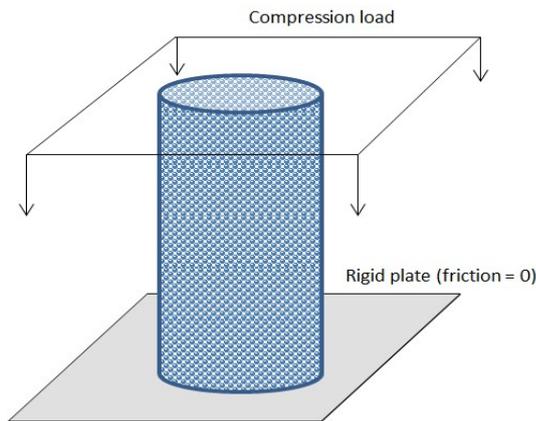


Fig. 13. PFC3D model under compression loading (reproduced from [45]).

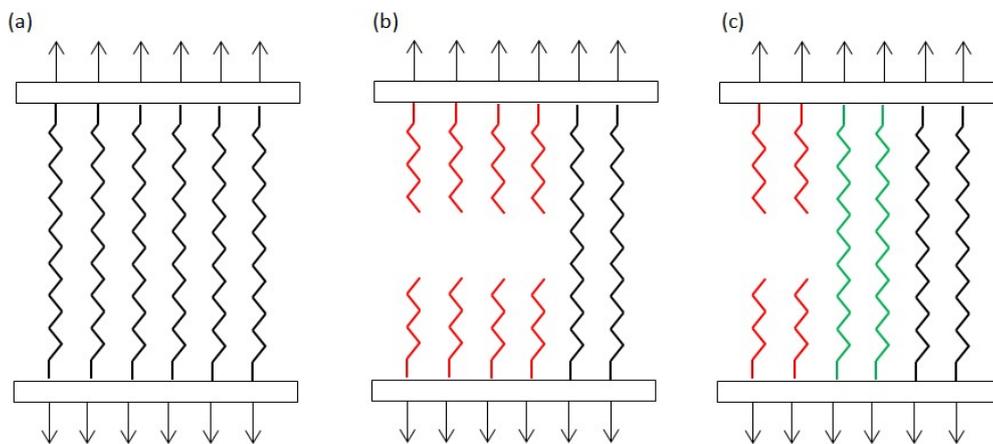


Fig. 14. Discrete element model with number of bonds. (a) The initial number of bonds (N_i), (b) The number of bonds after damage (N_d), and (c) The number of bonds after healing (N_h) (reproduced from [45]).

The DEM under compression load model was calibrated by available experimental results. The numerical results showed that the fluctuation at post-peak regime were observed due to self-healing effects. The compressive strength of the model increases in line with stiffness of solidified healing agent at post-healing. The strength of specimens after healing was influenced by the initial damage and the strength of healing agent.

Recently, Li et al. [46] investigated the crack propagation process in a matrix and debonding phenomenon of capsules in encapsulation-based self-healing materials. They used the extended finite element method (XFEM) to model crack propagation combined with the cohesive zone model (CZM) to model interface between capsule and matrix. The 2D model consists of an infinite matrix with capsule as a hole and embedded crack. They investigated the effect of geometry, elastic, and fracture properties as parametric studies of the system. The numerical results showed that the effect of capsule wall on fracture behavior was not significant for the small ratio of capsule thickness and its outer radius, while the crack propagation rate was strongly dependent on the ratio of elastic modulus (E_c/E_m). Moreover, the conceptual approach of modelling of concrete as a system not a material was introduced by Breugel [47]. The consequences of adopting changes in the mix design, modelling with different length scales, choosing the evolution of transport properties in cement-based materials, and modelling of self-healing concrete for microcracks were also discussed. The study revealed that sealing a crack was not only filling a crack with the healing agent but also densification of microstructures adjacent to the crack became the main concern in self-healing model.

Apart from the aforementioned review, the development of computer simulation and built-in software to study the self-healing process is still limited. This is due to the complexity of self-healing process in the system of both autogenous and autonomous methods. Some studies are found to discuss this issue concerning the software and open source code that are available to date. He et al. [48,49] studied the self-healing phenomenon due to unhydrated cement nuclei using concurrent algorithm-based computer simulation system SPACE (Software Package for the Assessment of Compositional Evolution). In order to simulate the leakage of healing agent in self-healing materials, Gilabert et al. [50] used free and open source code “OpenFoam” based on C++ library for computational tools in fluid dynamics [51,52] and multiphase flow solver called “interFoam” [53]. The other researchers used simulation aided design to study the self-healing phenomenon in tubular polymeric capsules [54], while the others applied a combination of computer simulation and experimental works using lightweight particles (LWA) to improve the results obtained by both techniques [55]. The overview of all numerical techniques used in self-healing concrete model that were discussed in this review is given in Table 1.

3. Future perspectives

Different analytical and numerical modeling techniques were proposed by some researchers as discussed in this review. There are a lot of interesting modeling methods that were carried out to simulate the healing process in cement-based materials. However, it is quite difficult to determine which technique is better than the other one since each modeling technique has its own standards. In this sense, the authors is only able to give general opinion about the reliability of different modeling techniques.

Among those modeling approaches, some researchers aimed to simulate self-healing process in the autogenous way, while the others tried the autonomous one by incorporating capsules or microcapsules contained healing agents into concrete, so it healed autonomously when the cracks appeared. The autogenous healing model was effectively applied when the composition of constituents inside the matrix (such as hydration of unhydrated particles, dissolution of carbonation, and the presence of water) were suitable enough to trigger reaction mechanism at the appearance of the cracks, and it remained restricted to the limited width of cracks. From this point of view, it seems that the reliability of autogenous healing is still in question. On the other hand, the autonomous healing model based on the reaction with the second component provided by capsules or microcapsules in cementitious matrix is more interesting and reliable since less human intervention is needed and premature curing inside the capsules could be avoided.

Table 1. Summary of numerical techniques used in modeling of self-healing concrete.

| Self-healing method | Techniques | Purposes/Targets | References |
|---------------------|--|--|------------|
| Autogenous | Splitting crack and dome-like crack | Self-healing efficiency | [22] |
| | Further hydration with water stored in capsule | Optimum amount of unhydrated cement and extra water | [23] |
| | Hygro-thermal-chemical model | Self-healing recovery degree | [24,25] |
| | Hydro-chemo-mechanical model | Self-healing potential between virgin and healed material | [26] |
| | Spectral element method with lattice model | Identify the damage using natural frequencies | [27] |
| | Cohesive zone damage-healing model | Healing model with thermally stimulated | [28] |
| | Healing model with physicochemical approach | Healing model which activated through precipitation of calcium carbonate | [29] |



| | | | |
|------------|--|--|------------|
| | Transient thermo-mechanical model | Long-term behavior of self-healing concrete system (LatConX) compared to standard concrete | [30] |
| | Micro-mechanical model | Mechanical recovery due to healing | [31] |
| | Coupled thermo-hygro-chemical model | Estimation of healing motion | [32] |
| | Coupled damage-plasticity model | Concrete cracking behavior with healing | [33] |
| | Two phases micro-mechanical model | Degree of healing | [34] |
| | Embedded finite element method (E-FEM) | Healing process induced by carbonation | [35] |
| | Softening-healing with SDA | Healing model based on time-dependent | [36] |
| | Genetic algorithm-artificial neural network | The crack width | [37] |
| | Mathematical model of bacterial self-healing | Healing efficiency | [38] |
| | Probability model (2D and 3D) | Dosage capsules with healing level | [39] |
| | Geometrical probability (2D and 3D) | Dosage capsules with healing level | [40] |
| | Analytical probability (3D) | Optimum microcapsule parameters | [41] |
| | Combined FEM and cohesive surface | Mechanical performance of interface | [42] |
| | Statistical model of further hydration | Probability of crack hitting capsules | [43] |
| | Particle flow code (PFC2D) | Breaking mechanism of microcapsules | [44] |
| Autonomous | 3D Discrete element method (DEM) | Healing degree | [45] |
| | Combined XFEM-CZM | Crack propagation and debonding | [46] |
| | Conceptual approach | General concept of concrete model | [47] |
| | Concurrent algorithm-based (SPACE) | Healing due to unhydrated cement | [48,49] |
| | OpenFoam | Leakage of healing agent | [50,51,52] |
| | interFoam | Leakage of healing agent | [53] |
| | Delft lattice model | Optimum properties of polymeric capsule | [54] |
| | Lightweight particles (LWA) | Healing degree | [55] |

With regard to the autonomous healing model, there are a lot of physical processes involved in self-healing which are needed to be simulated correctly. To make an autonomous healing model based on capsules or microcapsules effectively applied, it is essential for future research to be allocated to the improvement of a numerical model which covers some key aspects of the self-healing model, i.e., the cracking behavior, breakage of capsules, healing agents transport through discrete cracks, chemical reactions of curing and bonding, and the interaction between constituents inside the matrix as well. However, since the modeling of autonomous healing process is quite complex, it is a difficult task to achieve all those key aspects on a single sophisticated numerical model.

It is obvious in this review that obtaining a complete self-healing concrete model is an interdisciplinary research concerning civil engineering, material science, chemistry, etc. In order to develop such complex coupled mechanism that govern an applicable self-healing approach, it is highly required to communicate and cooperate with researchers of different fields of expertise.

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Conflict of Interest

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