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Numerical modeling for crack self-healing concrete by microbial calcium carbonate

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HIGHLIGHTS

- The developed model is able to predict the bioconcrete crack-healing relatively well.
- A crack width of 0.4 mm was healed at 70 days compared to 60 days in the model.
- With the increasing of urea hydrolysis, more calcium carbonate could be formed.
- The hydrolysis of urea induces the diffusive transport mechanism to the boundary.

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ABSTRACT

The inevitable existence of microcracks in concrete matrix can create interconnected flow paths due to external load, which will then provide easy access to harmful substances, and thus yielding to corrosion of reinforcement. Consequently, this affects the durability of the structure. Recent researches are devoted in crack self-healing concrete, which mimics the natural remarkable biological system of wounds healing. Despite that, the issue revolving around the efficiency of crack self-healing technique remains important. Microbial calcium carbonate offers an attractive biotechnique to fill pores volume as well as both micro and macrocracks in the affected cementitious material, resulting in barriers to inhibit water or aggressive chemical flow. However, results of this approach have only been demonstrated at laboratory scale and theoretical information is still limited. The present study describes a theoretical model to simulate the kinetics of calcite precipitation induced in response to the hydrolysis of urea in concrete crack. In addition, a second-order partial differential equation in time and space to model the healing process, rationally based on physic-bio-chemical issues, was developed. Both finite element and finite difference were implemented to solve this equation. SEM images were conducted to verify the predicted crack-healing results through artificial cracked mortar specimens incorporating indigenous *Lysinibacillus sphaericus*. As such, it could be concluded that a prediction of the healing process of the affected cementitious materials can be provided via the developed model.

1. Introduction

Inevitable microcracks remain to be a challenge to civil engineers as they are considered as a threat to the durability of structures. Such microcracks, porosity and interconnectivity of pores volume create an easy pathway for harmful substances to enter and cause reinforcement corrosion [1–6]. However, concrete is capable of plugging these microcracks themselves, which is well known as autogenous healing. Nonetheless, the ability is still limited to crack width that is less than 0.06 mm [7]. Various manual cracks repairing techniques are available to extend the life of structures. However, several drawbacks have been detected such as short period of time (10–15 years), high cost, difficult-to-access locations and the fact that most traditional repair techniques are polymer based that lead to hazards associated with the environment and health [8].

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Therefore, researchers have devoted considerable efforts to mimic natural biohealing by incorporating bacteria in cementitious material in recent years. The direct use of bacteria with their nutrients in fresh concrete mix without human intervention was first proposed by Jonkers and colleagues [9–12]. The potential ability of bacteria to seal cracks through the formation of calcium carbonate was investigated through different mechanisms such as sulfate reduction bacteria [13,14], oxidation of organic acids [15–17], nitrate reduction bacteria [18,19] and ureolytic bacteria [20,21]. 0.46 mm of concrete crack-width was completely healed after 100 days via *Bacillus alkalinitrilicus*, while ureolytic bacterial has proven its ability to heal crack widths of up to 0.97 mm in 8 weeks of water submission [22,23]. In the same context, nitrate reducing bacteria also showed its capability to heal crack widths of 0.46 mm in 56 days [18]. However, most of these studies have only focused primarily on both laboratory and experimental work and they are still suffering from the lack of numerical simulation to accurately predict experimental behaviour, which can result in the decrease of cost. Examples of mathematics researches of polymer self-healing are available in the previous studies [24–30].

On the other hand, computational research into self-healing concrete is still in its infancy stage and there are only a few numerical modelling involving the healing process of affected cementitious material. Autogenous crack-healing in cementitious material through further hydration was mathematically simulated using water transport theory, ion diffusion model and thermodynamics model [31]. The results showed that the rate of healing processing speed increased according to the amount of water available that was assumed to be in a capsule. Further modelling study was focused on the interaction between the crack and embedded micro-capsule in cementitious material [32]. In addition, autogenous self-healing concrete by calcium carbonate due to the carbonation of dissolved calcium hydroxide was also developed byAliko-Benítez, Doblaré [33]. Moving from Autogenous self-healing model to bacteria-based self-healing, a numerical model was developed to describe the healing process of cracks in concrete using bacteria, which relies on the oxidation of organic acids [34]. The diffusion of the healing agent over the crack is governed by diffusion equation which is solved using Galerkin finite element, while the evolution of moving boundary due to calcite precipitation is solved using level set method.

In this study, indigenous ureolytic bacteria was utilised to induce microbial calcium carbonate by releasing urease enzyme, which in turn stimulated the urea degradation to carbonate and ammonium under appropriate condition as expressed in Eq. (1) [35]. At the same time, the formation of calcite would develop due to the reaction between the carbonate and calcium ions on the cell wall of the bacteria since it is negatively charged, which was specifically considered as bacterial aggregate as shown in Eq. (2).

$$CO(NH_2)_2 + 2H_2O \xrightarrow{urease} 2NH_4^+ + CO_3^{-2} \quad (1)$$

$$Ca + CO_3^{-2} \rightarrow CaCO_3 \quad (2)$$

The evolution of bacterial aggregate was predicted by developing a numerical model. In the said model, urea, calcium, nutrient and bacteria were pre-mixed in the concrete matrix and distributed homogeneously. In addition, urea was assumed to be stored in capsules, which would break if they were intersected by a crack. On the contrary, bacteria, nutrient and calcium were assumed to exist in the crack domain. Consequently, with water and nutrients, the spores of the bacteria would germinate and reproduce, and thus limestone would develop in the crack as shown in Fig. 1. In other words, both the urea and calcium (artificial blood platelet) would be recruited to the damage area to block the water filled crack. This mechanism was inspired by the idea of blood clotting in skin wounds via platelet, which exists in the blood, and ultimately, stops the bleeding. Specifically, the said process was mathematically simulated using a system of equations including first-order ordinary differential equation and second order partial differential equation, in which both finite difference and finite element methods were used to solve the said form of bio-chemical-diffusive model.

2. Mathematical development of the model

2.1. Model description

In this study, the model is schematically shown in Fig. 2. A macro-crack with the size of 20 mm (length) × 0.4 mm (width) × 20 mm (depth) was supposed to pass through a capsule. In addition, the crack domain was also assumed to be filled with water instantaneously. The model was developed rationally, relying on the physics, biology and chemistry of the healing process respectively.

Firstly, urea was recruited to the damage area due to the flux (F). In our model, flux denoted that the ion species are allowed to diffuse as a consequence of a natural movement from a high concentration area to a low concentration area inside the cracks developed in the concrete cover. The mechanism of diffusive was governed by Fick's first law for ion species as shown in Eq. (3), where c is the concentration of species in mol/m^3, D is the diffusion coefficient in unit of m^2/day and flux F is in units of mol/m^2 day.

$$F = -D\frac{\partial c}{\partial x} \quad (3)$$

Secondly, calcium ions would stick and gather on the bacteria cells that release urease enzyme to catalyse the decomposition of urea to carbonate ions. These bacteria cells exist in all boundaries of the crack with different numbers since cell growth cannot repro-

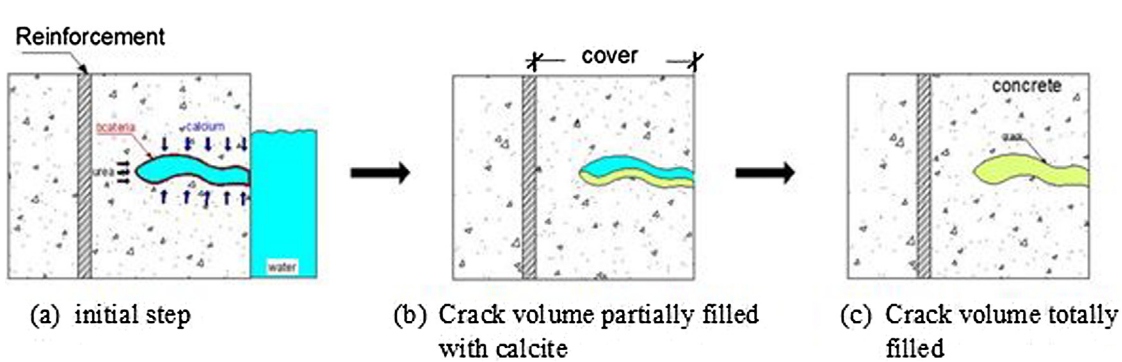

Fig. 1. The evolution of a crack closing in different stages.