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Computational modeling of fracture in encapsulation-based self-healing concrete using cohesive elements

Luthfi M. Mauludin[c,d], Xiaoying Zhuang[e], Timon Rabczuk[a,b,*]

[a] Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
[b] Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, Viet Nam
[c] Institute of Structural Mechanics, Bauhaus University of Weimar, Weimar 99425, Germany
[d] Teknik Sipil, Politeknik Negeri Bandung, Gegerkalong Hilir Ds.Ciwaruga, Bandung 40012, Indonesia
[e] Department of Geotechnical Engineering, College of Civil Engineering, Tongji University, Shanghai 200092, China

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ABSTRACT

Fracture behavior of encapsulation-based self-healing concrete (SHC) is investigated numerically. In this paper, we study the influence of capsules including its volume ratio and core-shell thickness on the load carrying capacity and fracture likelihood of the capsules. In order to randomly create the mesoscale structure of self-healing concrete, an efficient packing algorithm is employed. For a given number of circular capsules with particular diameter and shell thickness, the aggregates are generated from prescribed distributions of their size and volume fraction. The capsules are made of Poly Methyl Methacrylate and potential cracks are represented by pre-inserted cohesive elements with tension and shear softening laws along all element boundaries including the interfaces between different phases. The effects of the volume fraction of capsules and core-shell thickness ratio on the load carrying capacity and fracture probability of the capsules are analyzed. It is found that the load-carrying capacity of self-healing concrete decreases as the capsules volume fraction increases. The capsule core-shell thickness ratio has no significant influence on the specimen strength but a very significant impact on the breakage of capsule shell. Given a fixed volume fraction of capsules, the higher core-shell thickness ratio, the higher is the number of capsules which fracture. Assuming the core-shell ratio thickness is fixed, increasing the volume fraction of capsules will increase the probability of capsules which break.

1. Introduction

The development of self-healing concrete (SHC) has attracted a lot of attention due to its inherent ability of automatic crack detection and crack repairing with the goal of significantly reducing the costs for infrastructure maintenance. Compared to standard concrete, SHC allows the early and timely repairing of deep cracks which are not accessible otherwise. Cracks might endanger the overall durability and integrity of structures as they allow aggressive substances to flow inside the matrix through fluids. Consequently, it seems apparent that investigation, maintenance and repairing activities of concrete cracks are essential. SHC has great perspectives for infrastructures exposed to water and corrosion such as tunnels and bridges. It has been estimated that costs related to the repair works contribute around 50% of the annual construction budget in Europe [1]. SHC promises to reduce the life-cycle cost while maintaining the integrity of structures. With about 2.5 tons per person per year, concrete is the most used building material in the world. In the US, the first self-healing cement was produced by Prof. Dry during the 1990s [2]. More recently, SHC piles have been tested at the construction site of bridges [3]. In general, existing healing methods in cementitious materials can be classified into two categories: firstly intrinsic healing where an autogeneous healing is accomplished by the cement composition itself, and secondly extrinsic (autonomous) healing that requires additives to react with cement. The microscapsule based self-healing method, which is claimed among the most promising techniques, belongs to the latter.

Recent intense research has been drawn to an autonomous type of self-healing method using micro-capsules for more accurate healing location and better healing capabilities [4]. The healing agents are placed inside discrete micro-capsules embedded in the substrate material. Approaching cracks break the capsule shell to release the healing agent and hence the healing occurs in the vicinity of the damaged part, see Fig. 1.

Over the past two decades, both novel and efficient computational techniques for fracture have been developed by researchers including cohesive zone model [6], the extended finite element [7], meshfree

* Corresponding author at: Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam.
E-mail address: timon.rabczuk@tdt.edu.vn (T. Rabczuk).

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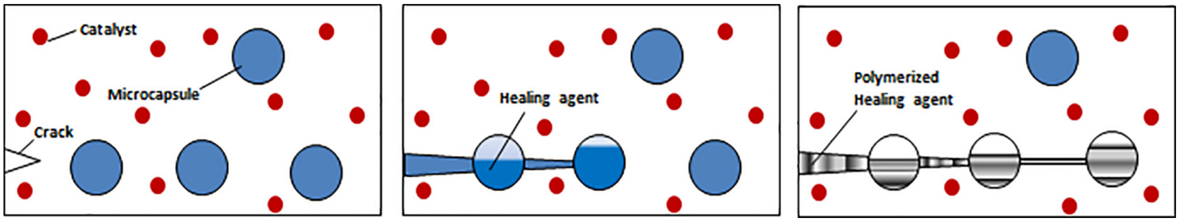

Fig. 1. Autonomous self-healing using micro-capsules (reproduced from [5]).

methods [8], cracking particles methods [9,10], efficient remeshing techniques [11,12], phase field methods [13], screened Poisson models [14], peridynamics [15], dual-horizon peridynamics [16], the extended particle difference method [17–19], and multiscale methods for fracture [20–25], to name a few.

Besides the advances in modeling fracturing, computational modeling of self-healing concrete is still in its infancy. Research on this topic incorporates both the research on the modelling of self-healing material in general and the modelling of fracture in concrete. One of the first simulations of cracking and healing of self-healing material was undertaken by the group of Prof. White [4]. They studied how the compliance ratio between the substrate material and the capsule affects the crack propagation path. Mathematical models quantifying the healing efficiency are often based on geometric information. Zemskov et al. [26] for instance developed a statistical model to determine the probability of cracks hitting spherical capsules. Several studies provide useful insight on the probability of cracks hitting the micro-capsules but they do not account for the physical cracking process such as the mechanical properties of the matrix material and the micro-capsules [27,26].

Lv et al.[28] investigated the dosage required for the long capsule in cementitious matrix using combined geometrical probability theory with binomial probability distribution. The probability of cracks hitting capsules with particular volume fraction in 2D and 3D model was also developed by Lv and Chen [29]. Maiti et al. [30] analyzed the curing process of fatigue crack based on cohesive model. To revoke the stress level and retard the propagation of crack, they inserted a wedge at the crack tip. The possibility of using different capsules thickness and the interaction between capsule and the matrix was studied by Gilabert et al. [31].

Recently, experimental work proved that the interfacial bonding between the capsule shell, the healing agent and the cement is not perfect [32]. The voids and interfacial cohesion around the constituents affect the healing process. The strong adhesive between capsule and matrix will forced the capsule to break [33].

In order to achieve the efficiency of the self-healing mechanism, the understanding of the behavior of different constituents and their interactions plays an important role of this area. In this study, 2D numerical models with randomly packed aggregates and capsules are developed to analyze fracture mechanism that play a significant role in the fracture probability of capsules and consequently the self-healing process. This work focuses on the computational modeling of fracture in encapsulated-based self-healing concrete at the mesoscale. The capsules embedded in self-healing concrete should be able not only to break when the crack appears, but also to resist during mixing process. According to recent experimental work, polymeric capsules made of Poly Methyl Methacrylate-PMMA are among the most efficient healing agents. They are not only brittle enough to break when they are subjected to relatively small deformations but also strong enough to resist during the mixing process compared to glass capsule, poly lactic acid (PLA) and polystyrene (PS) [34]. Hence, we focus on these polymeric capsules (Poly Methyl Methacrylate-PMMA) which are uniformly distributed in the mortar matrix. The healing agent (methyl methacrylate) is modelled as 'solid'. Hence, the flow process and the associated polymerization of the healing agent into the crack surface and the associated healing efficiency in the vicinity of the damage is not addressed here but will be the focus of future studies. In order to model the complicated fracture processes in this multi-phases specimen, cohesive elements were inserted in the mortar-matrix, core shell and at the mortar-capsule and mortar-aggregate interface. The scope of this study is twofold: (i) to understand the effects of the volume fraction of capsules on the load carrying capacity and the probability of capsule fracture, which is important for healing efficiency and (ii) to understand the effects of capsule shell thickness on the fracture of the capsule shell which might help the design/improvement of encapsulation-based self-healing concrete materials.

2. Generation of mesostructures and finite element models

2.1. Aggregates and capsules distribution

Concrete is comprised of cement (10–15%), coarse and fine aggregates (60–75%) and water (15–20%). For normal strength concrete, coarse aggregates usually represent about 30–50% of the concrete volume. In order to describe the distribution of the aggregates, the Fuller curve is often used, categorizing the aggregates into a certain number of segments based on the sieve analysis. The aggregate size distributions found in Hirsch [35] and summarized in Table 1 are employed in this study. The sieve size of 2.36 mm is taken as the cut-off size of coarse aggregates. Concrete is treated as a four-phase material consisting of aggregates, mortar, capsule cores and capsule shells.

According to X-ray tomographic images, the coarse aggregates are often of circular and elliptical shape [36]. It was also found that the influence of other shapes barely influence the macroscopic behavior of concrete [37]. Therefore, for the sake of simplicity, circular capsules and aggregates are generated and used in our studies. The size and thickness of capsules can vary according to the agitation rate of experiments. Recent experiments showed that the range of diameter size of capsules is between 1.1–7.2 mm [34] and 1.7 mm–2.3 mm [38]. In this study, the preliminary model will use 2.0 mm as diameter of the capsules and the capsule shell thickness is considered as diameter/27 (from real capsule thickness/diameter ratio [39]). In our studies, we test the influence of the volume fraction of capsules ranging from 1.57% to 9.42% as summarized in Table 2.

2.2. Aggregates and capsules generation

We employ the commercial finite element package ABAQUS in all our studies. In order to randomly disperse the aggregates and capsules in the matrix, we employ a packing algorithm which has been developed in our previous studies [40]. The basic idea of the algorithm is to

Table 1
Aggregate size distribution[35].

Sieve size (mm)	Total percentage retained (%)	Total percentage passing (%)
12.70	0	100
9.50	39	61
4.75	90	10
2.36	98.6	1.4