

A MATHEMATICAL MODEL FOR BACTERIAL SELF-HEALING OF CRACKS IN CONCRETE

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ABSTRACT

Self-healing materials are smart materials with the capability to repair itself autonomously after being damaged. Since cracks commonly occur in structures consisting of materials like concrete, polymers, etc., a self-healing mechanism is crucial for the durability of the material.

In this research, we present a two-dimensional mathematical model of the self-healing process in concrete. This model can help to estimate the influence of various parameters involved on the rate and quality of the crack healing and to find conditions such that healing proceeds in an optimal way, with a minimal influence on other material properties, such as strength, ductility etc.

Bacteria-based self-healing concrete is produced by adding a two-component biochemical self-healing agent to the concrete mixture. The first component, spores of bacteria of a special kind (*Bacillus cohnii*, *Bacillus pseudofirmus*), is incorporated in the concrete matrix at the stage of preparation of the cement paste by mixing the spore suspension with the paste make up water. The second component, the biochemical healing agent, is immobilized in expanded clay capsules prior to addition to the concrete mixture. The homogeneously distributed clay particles will, after setting of the concrete mixture, release the encapsulated healing agent when hit and opened by a crack forming in the concrete matrix. Water entering the crack subsequently disperses the chemicals over the crack surface and activates the bacterial spores which germinate to become metabolically active vegetative cells that are able to convert the organic bio-mineral precursor compound into insoluble inorganic calcium-carbonate-based minerals. Copious production of bacteria-mediated minerals results in sealing off the crack, hence the permeability of concrete and leakage are reduced.

The capsule content is a solid mixture of three components which dissolve in water that fills the crack. About 97% of the mass of the capsule content is calcium lactate ($\text{Ca}(\text{C}_3\text{H}_5\text{O}_3)_2$) which is converted by bacteria on the crack surface into calcium carbonate (limestone) (CaCO_3). Two other components, monosodium glutamate ($\text{C}_5\text{H}_8\text{NNaO}_4$) and monopotassium phosphate (KH_2PO_4), are, respectively, sources of nitrogen and phosphorus which are necessary nutrients for bacteria in order to be able to multiply and to carry out the conversion process.

Since clay capsules with the healing agent have a lower strength than the surrounding concrete matrix, they influence the process of crack propagation. As the crack approaches the capsule close enough, it may change its direction to intersect the weakest material parts, and, therefore, the crack will pass through the capsule. Hence, the capsule “attracts” the crack, and in the most typical case the crack passes through the centre area of the capsule.

Because of this observation, the following geometry of a computational domain for the mathematical model was chosen in order to build a two-dimensional mathematical model of the self-healing process (Fig. 1 (a) and (b)).

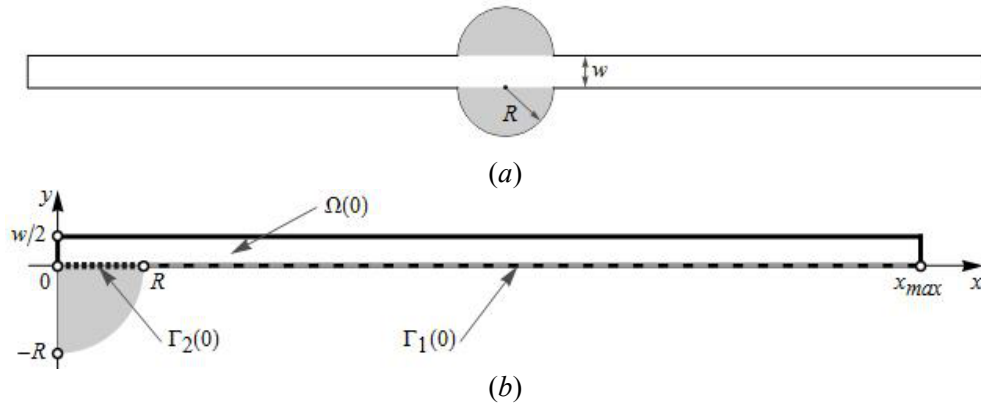


Figure 1: (a) Schematic representation of a crack of width w hitting a capsule section of radius R .
(b) Computational domain for a two-dimensional mathematical model.

A circular capsule section of radius R is broken into two equal parts by a straight streak of width w representing a crack that passes through the centre of the capsule (Fig. 1 (a)). Due to symmetry, we are going to consider only one quarter of this sketch. In Fig. 1 (b), the initial state of the chosen quarter is presented. The domain of computation $\Omega(t)$ corresponds to the area filled with water. Its boundary includes the part $\Gamma_1(t)$ (first interface) which represents at initial time point a fragment of the crack wall, and the part $\Gamma_2(t)$ (second interface) corresponding to a front of the solid capsule content. The processes of limestone precipitation and dissolution of the capsule content will lead to changing of the positions of Γ_1 and Γ_2 in the course of time.

From a computational point of view, the model of the self-healing process represents a kind of moving boundary problem for a system of diffusion equations. In the present study the diffusion equations are solved using a Galerkin Finite Element method on the structured triangular mesh which needs to be modified locally for each time step due to evolution of the computational domain. The boundary of the computational domain contains two moving fragments of different type which are tracked using an implementation of the level set method applied independently on both of them. The level set method allows us to treat topological changes of the dissolving or growing phases.

The results obtained through a computer simulation (Fig.2) on the basis of the above model allow to determine different parameters of the healing process, such as the time needed for the limestone layer to reach the middle of the crack (and stop thereby the penetration of water in the concrete structure), as well as the rate of filling the crack by limestone depending on the crack width and capsule size.

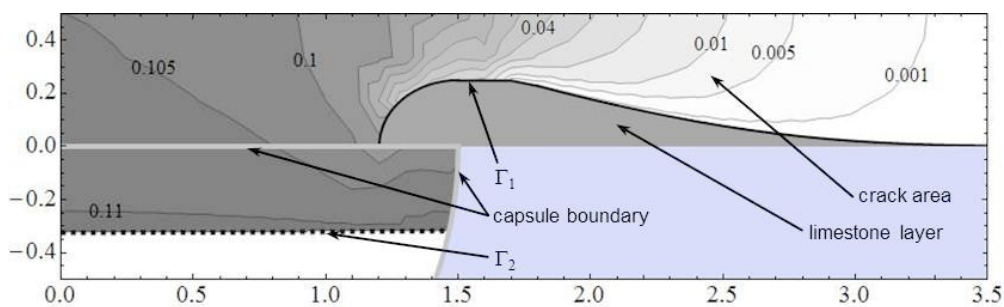


Figure 2: Contour plot of the concentration of calcium lactate in the domain of computation after 250 time steps (corresponding to 20 hours 50 minutes of healing process); $R = 1.5$ mm, $w = 1$ mm.