Finite Elements in Analysis and Design 132 (2017) 42–51

Contents lists available at ScienceDirect

Finite Elements in Analysis and Design

journal homepage: www.elsevier.com/locate/finel

Numerical modelling of the healing process induced by carbonation of a single crack in concrete structures: Theoretical formulation and Embedded Finite Element Method implementation

H. Ranaivomanana, N. Benkemoun*

Université Nantes Angers Le Mans (L'UNAM), GeM, Research Institute of Civil Engineering and Mechanics, CNRS UMR 6183, Nantes University, IUT Saint-Nazaire 58 rue Michel Ange, Saint-Nazaire 44600, France

A R T I C L E I N F O

Keywords:
Embedded Finite Element formulation
EAS method
Weak discontinuity
Healing process
Concrete
Crack
Structure durability

A B S T R A C T

We consider a model for reactive flows which describes the healing process induced by carbonation of a single crack in concrete structures. The aim of this paper is to study the complex interplay between advection-diffusion mechanisms in a crack-matrix system combined with different chemical reactions taking place (dissolution/precipitation). Carbonated water is first injected through a crack. Then, a diffusion process of calcium ions (C_a^{2+}) takes place from the porous matrix to the crack due to the existing calcium ions concentration gradient. Finally, those calcium and carbonates ions (CO_3^{2-}) from the percolating solution react to form a calcite (C_aCO_3) layer responsible for the healing of the crack. The developed model takes the form of transport-reaction partial differential equations for both crack and porous matrix. From numerical point of view these equations are discretized by means of the Embedded Finite Element Method (E-FEM). The E-FEM allows to use meshes not necessarily matching the physical interface, defined herein as the crack, while retaining the accuracy of the classical finite element approach. This is achieved by introducing a weak discontinuity in the calcium ions concentration field for finite elements where the crack is present. A numerical solving strategy is presented to efficiently resolve the FE problem both in terms of calcium and carbonate concentration field variables and weak discontinuity parameters. In addition, an analytical model for the computation of the calcite layer width, resulting in the healing process, is suggested. Finally, considering the dependence of the diffusivity and permeability coefficients on the width of the calcite, a coupled model arises for the numerical modelling of the healing process induced by carbonation in a crack.

1. Introduction

The assessment of concrete structure lifetime is Nowadays necessary for the design of durable structures. As a complementary means to experimental approaches, numerical modelling can be a relevant tool for this lifetime assessment. The development of thorough numerical models requires a comprehension not only of the degradation phenomena but also of the healing process. Indeed, healing process can improve the durability of structures (storage or containment structures for instance). The healing process can occur in both ways (see [1,2] and [3]):

- *naturally* by calcium carbonate formation, expansion of hydrated cementitious matrix, blocking of cracks by impurities present in water (sealing) and further hydration of unreacted cement.
- *artificially* by the use of chemical admixtures, polymers and geo-materials and even microorganism which are able to produce calcium carbonates.

Among the natural healing processes mentioned above, the formation of calcium carbonate is investigated in this study, since it is considered as one of the most promising autogenous healing mechanisms (see [4–6] or [7] for a review and [8] for experimental results concerning microbially-induced calcium carbonate precipitation). Most publications dedicated to the modeling of natural self-healing process mainly concern the process of further hydration of unreacted cement ([1,9,10] and [11]). However concerning the modeling of the natural self-healing process induced by carbonation, there is not so much information in the literature. The authors in [6] have proposed a simplified model for the evolution of the leakage rate through a cracked material versus time, while carbonated water flows through the crack. However, their approach is limited by the fact that two calibration parameters, whose values vary from one material to another, are present in the model. In [12], the authors have developed a multiple phase self-healing-model, that simulates three distinct stages in the healing process: fracture

* Corresponding author.
E-mail address: nathan.benkemoun@univ-nantes.fr (N. Benkemoun).

http://dx.doi.org/10.1016/j.finel.2017.05.003
Received 1 April 2017; Received in revised form 3 May 2017; Accepted 7 May 2017
Available online 19 May 2017
0168-874X/

process, transport of healing agents to the healing location and mechanical strength recovery. The authors introduced a hygro-chemical transportation model (momentum and mass balance equations), in which the active species are transported by advective, diffusive and dispersive fluxes through the pore fluid to damaging and healing sites. More recently, [13] have proposed a finite-element model describing self-healing mechanisms in engineered cementitious composites and based on C_aCO_3 precipitation. The model takes into account the diffusive mechanisms of aqueous species in the material, and the most fundamental chemical equations that take place during the healing phenomenon. The concentration of the three main species (calcium ions C_a^{2+}, carbonate ions CO_3^{2-} and calcite C_aCO_3) acting on the healing process are identified as the main model variables and the modeling results into a reaction-diffusive set of equations. However, the model requires further validations. Indeed simplified assumptions are assumed by the authors such as the fact that the diffusion coefficients are independent from damage and healing variables. In addition no water-flowing through the crack is considered.

In this paper, a numerical approach is presented in the context of the natural healing process. In this sense, we suggest a numerical model for the healing process induced by carbonation of a single crack in concrete structures. Transport equations of C_a^{2+} and CO_3^{2-} written in the crack and transport equation of C_a^{2+} written in the porous media are considered and discretized by means of the Embedded Finite Element Method (E-FEM, see [14] for instance). The E-FEM allows to use meshes not necessarily matching the physical interface, defined herein as the crack, while retaining the accuracy of the classical finite element approach. This is achieved by considering a weak discontinuity [15] in the calcium ions concentration field for finite elements where the crack is present. This enhancement, introduced in the framework of the EAS method [16], allows to have the calcium ions concentration field continuous itself and a jump in the normal direction of the calcium ions concentration gradient, when passing through the crack. This results in a discontinuous leakage flux that flows from the porous matrix toward the crack. This flux represents the mass coupling term between the porous media surrounding the crack and the crack itself. It is important to stress the fact that this coupling term arises naturally in the weak form of the problem, since the crack is directly embedded in the mesh through the E-FEM. This a serious advantage when the FE discretization is performed. Finally, having at hands the calcite and calcium concentration fields values for each time step, the width of the calcite layer in the crack is computed by means of an analytical model, resulting in the healing process in the crack. Finally, considering the fact that diffusivity and permeability coefficients values also depend on this calcite layer width, a coupled model arises for the numerical modelling of the healing process induced by carbonation in a crack.

The outline of this paper is as follows. In Section 2, the governing equations of the problem are introduced. They consist in the transport equation of C_a^{2+} in the porous media and in the crack, and the transport equation of CO_3^{2-} in the crack. In Section 3, the weak form of the problem is suggested. It is obtained by means of the Galerkin approximation, leading to the FE to be solved. In Section 4, the method to compute the coupling term is shown. Also we present the analytical model to evaluate the width of the calcite layer, resulting in the healing process. In Section 5, the FE discretization of the concentration fields, based upon the E-FEM, and the solving strategy are presented.

2. Governing equations

In this section a model for reactive flows which describes the healing process induced by carbonation of a single crack in concrete structures is considered. In this sense, the strong form of the model governing equations is presented. We consider the transport equations of C_a^{2+} and CO_3^{2-} written in the crack and the transport equation of C_a^{2+} written in the porous media. Also chemical reactions (dissolution/precipitation) in the porous matrix and the crack are regarded.

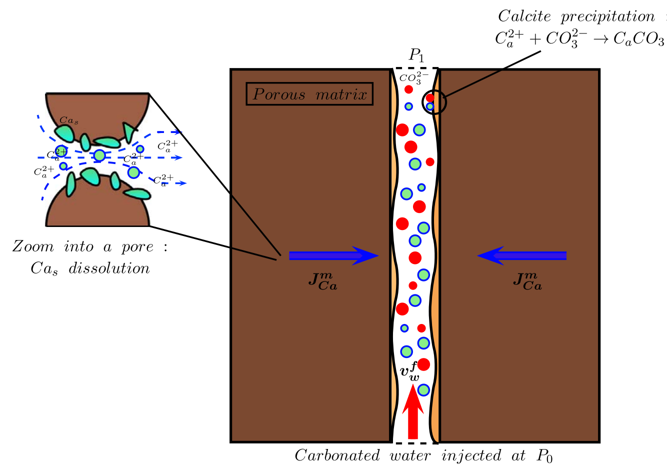

Fig. 1. Schematic of the mechanisms taking place during the healing process induced by carbonation into a single crack.

Technically speaking, carbonated water is first injected through the crack. Then, a diffusion process of calcium ions (C_a^{2+}) takes place from the porous matrix to the crack due to the existing calcium ions concentration gradient. Finally, those calcium and carbonates ions (CO_3^{2-}) from the percolating solution react to form a calcite (C_aCO_3) layer responsible for the healing of the crack. Those mechanisms are illustrated in Fig. 1 and are described hereafter for each transport equation.

2.1. Transport equation of C_a^{2+} in the porous media

We note C_{Ca} the calcium ions concentration in the pore solution of the matrix, Φ^m the matrix porosity and φ_{Ca_s} a source term taking into account the dissolution of the calcium in the solid phase Ca_s. Transport by diffusion, resulting from the existing calcium ions concentration gradient between the crack and the porous matrix, is considered through the flux $\boldsymbol{J}^m_{Ca}$. Consequently, the transport equation (diffusion equation) of C_a^{2+} in the porous media is such as:

$$\frac{\partial \Phi^m C_{Ca}}{\partial t} + \nabla \cdot (\boldsymbol{J}^m_{Ca}) = \Phi^m \varphi_{Ca_s} \tag{1}$$

2.2. Transport equation of C_a^{2+} in the crack

Transport by diffusion and permeation is considered through the fluxes $\boldsymbol{J}^f_{Ca}$ and $\Phi^f C_{Ca} \boldsymbol{v}^f_w$, respectively. Again transport by diffusion, resulting from the existing calcium ions concentration gradient between the crack and the porous matrix, is considered through the flux $\boldsymbol{J}^m_{Ca}$. Transport by permeation takes place because of the pressure gradient in between the bottom and the top side of the crack (see Fig. 1: $\nabla p_w = P_1 - P_0$). We note $\boldsymbol{v}^f_w$ the fluid velocity and Φ^f the crack porosity. Last but not least, considering the fact that the C_a^{2+} and CO_3^{2-} ions react together all over the time to form calcite C_aCO_3 into the crack, the evolution of calcite formation has to be also taken into account. This is achieved by means of the source term $-\frac{\partial \xi}{\partial t}$ where ξ is the amount of calcite formed in the crack. This formation of calcite results in the healing process taking place into the crack.

This leads to the following transport equation (diffusion-permeation equation) of C_a^{2+} in the crack:

$$\frac{\partial \Phi^f C_{Ca}}{\partial t} + \nabla \cdot (\boldsymbol{J}^f_{Ca}) + \nabla \cdot (\Phi^f C_{Ca} \boldsymbol{v}^f_w) = -\frac{\partial \xi}{\partial t} \tag{2}$$

2.3. Transport equation of CO_3^{2-} in the crack

We note C_{CO_3} the carbonate ions concentration in the crack. Transport by permeation is considered through the flux $\Phi^f C_{CO_3} \boldsymbol{v}^f_w$. It takes place also because of the pressure gradient in between the bottom and the top side of the crack.

The transport equation of CO_3^{2-} in the crack is such as: