



# Embedded finite element formulation for the modeling of chloride diffusion accounting for chloride binding in meso-scale concrete



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## ABSTRACT

This paper presents the FE formulation for the numerical modelling of chloride ions diffusion accounting for the chloride binding capacity in meso-scale concrete. The finite element formulation is built through a discrete (lattice) finite element model and the meso-structure is based on a two-phase 3D representation of heterogeneous materials, such as concrete, where stiff aggregates are embedded into a mortar matrix. In order to take into account these heterogeneities in the mesh, we turn to the Embedded Finite Element Method (E-FEM). The E-FEM allows to use meshes not necessarily matching the physical interface (aggregates/mortar matrix) while retaining the accuracy of the classical finite element approach. This is achieved by introducing a weak discontinuity in the chloride concentration field for finite elements where the physical interface is present. A numerical solving strategy is presented to efficiently resolve the FE problem both in terms of chloride concentration field variables and weak discontinuity parameters. We investigate through 1D simulations the influence of the microstructure properties and the chloride binding capacity on the chloride concentration profiles. We show that taking explicitly into account the diffusion coefficients of the microstructure and the chloride binding capacity are important to consider for a better prediction of the time span until corrosion initiation. This is important for accurately estimating the service life of a structure. Numerical homogenization experiments are also performed on 3D meso-structures to compute macroscopic diffusivity tensors accounting for two-phase material. Comparison with Maxwell's equation are performed to show the accuracy of the proposed numerical approach.

## 1. Introduction

Regarding reinforced concrete civil engineering facilities, some corrosive external agents, like dissolved salt from sea water and spray, deicing salt put on roads when winter is coming or even materials making up concrete (sand or additives), are susceptible to penetrate cement materials. The most corrosive penetrating agent as regards concrete is chloride ions. Once the cover concrete is penetrated, chloride ions may reach the reinforcement which may be corroded when the threshold value is reached [1]. Consequently, because of deteriorated mechanical performances, the structure durability and service life are affected. The ingress rate of chloride ions, in turn, is highly dependent of the diffusion properties of concrete. Hence if the diffusion properties of concrete can be modelled and estimated, a better prediction of the time span until corrosion initiation is possible.

On the one hand, interest of the computational mechanics community has significantly increased over the last decades in the use of

Enriched Finite Element Methods such as the Generalized Finite Element Method (G-FEM, [2,3]), the eXtended Finite Element Method (X-FEM, [4–6]), the Nitsche method ([7] and [8]) and the Embedded Finite Element Method (E-FEM, [9–12]). The advantage of these methods is to retain all the advantages of the finite element approach (applicability to different constitutive laws, robustness, compatibility with homogenization techniques,...) while considerably easing the meshing step of physical discontinuities such as cracks, fractures, slip lines and material interfaces. Indeed, the mesh does not necessarily need to match these physical discontinuities. They are taken into account by enriching the finite element approximation space through specific enhancements in the displacement/strain fields for mechanical problems and/or in the pressure/pressure gradient [13] and temperature/temperature gradient [14] for multi-physics problems for instance. Consequently, these physical discontinuities have the representation of their (complex) geometry and its evolution through the time facilitate by means of these methods. In the literature,

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the enhancements are in general sorted into two categories<sup>1</sup>:

- strong enhancements - a jump within the displacement (and/or the pressure, the temperature, the concentration,...) fields is introduced by the means of a so-called strong discontinuity ([15]);
- weak enhancements - a jump within the strain (and/or the pressure gradient, the temperature gradient, the concentration gradient,...) fields is introduced by the means of a so-called weak discontinuity ([16]).

On the other hand, the modeling of a material through meso-scale models where the microstructure of the specimen is explicitly taken into account became more and more popular since the pioneering works of Schlangen and van Mier [17]. These models have demonstrated to be efficient in modeling important features of the behavior of concrete-like materials, not only for mechanical aspects (Benkemoun et al. [12], Roubin et al. [18] and [19]) but also for mass transport aspect (Jourdain et al. [20], Benkemoun et al. [21] and Grassl and Bolander [22]). In the context of chloride ions transport modeling, several mesoscale models have, in this sense, emerged in the literature ([23–27]). Consequently modeling chloride ions transport with a meso-scale model based on the aforementioned Enriched Finite Element Methods might provide yet another efficient and original way to tackle durability issues relative to chloride ingress in concrete. It can be an efficient alternative numerical approach for taking into account the microstructure in the design of mesoscale models for chloride ions transport. In this paper, among the different Enriched Finite Element Methods evoked in the introduction, we turn to the Embedded Finite Element Method (E-FEM)<sup>2</sup> and we also present the enrichment function, based upon a weak discontinuity, for capturing the physical interface in the mesh. This type of function is also retained in [29] in the context of the X-FEM. Regarding the literature, a considerable amount of effort has been devoted to the modelling of chloride ion transport mechanisms (diffusion [30], migration [31], convection) and behaviour (interaction or not with other ions [32]) within cement materials (saturated or unsaturated [33]) at the mesoscale. The key idea being that the adequate knowledge of the significant physical phenomena and interactions between the different phases of the material at the meso-scale are needed to obtain realistic results when homogenizing the behavior to compute effective physical properties. We focus in this paper on transport by diffusion accounting for chloride binding in a saturated media. In this sense, a distinction between chloride ions fixed on the solid matrix (called “bound-chlorides” captured by the hydration products) and the ions contained in the pore solution (called “free-chlorides”) responsible for reinforcement corrosion is made. This choice is relevant for the study of service life of concrete structures. Firstly, it involves a reduction of the free chloride concentration around the reinforcement which will reduce the occurrence of corrosion. Secondly, it removes chloride from the diffusion flux, thus retarding the time span until corrosion initiation. Consequently, the effect of chloride binding must be taken into account when studying the chloride ions diffusion in concrete. It should be noted that other important mechanisms, that are not taken into account in this paper, influence the chloride ions diffusion and consequently the time span until corrosion initiation. Among them, the effect of the electrical double layer (EDL) is important (see [34] and [35] for EDL consideration). In [32], the authors show that the EDL sign has a strong influence on the chloride ingress.

The remainder of this paper is organized as follows. The homogenization method retained to compute effective diffusivity tensor at the macroscale is described in Section 2. The mesoscale model based on the Embedded finite element formulation is detailed in Section 3.

The method to solve this formulation in terms of concentration field and enriched concentration field is presented. In Section 4, 1D numerical results are presented to demonstrate the accuracy and simplicity of the E-FEM. Finally computational homogenization is used to determine effective diffusivity tensor in RVE containing microstructure embedded through the E-FEM.

## 2. Homogenization method: macroscopic diffusivity tensors computation

In this Section focus is made on the homogenization method retained in this paper to compute macroscopic diffusivity tensors. We consider a heterogeneous diffusive 3D domain  $\Omega$ . In this domain we assume that a fluid flow takes place under effect of imposed concentration<sup>3</sup> on the contour  $\partial\Omega$ . The domain  $\Omega$  is made of materials with different diffusivity values. These values are characterized by a scalar value denoted as  $D$ .

### 2.1. Mean gradient of concentration and mean flux

We define the mean concentration gradient  $\vec{G}$  [ $kg/m^4$ ] and the mean flux  $\vec{Q}$  [ $kg/(m^2 s)$ ] within the domain  $\Omega$  by the following relationship:

$$\vec{G} = \frac{1}{V} \int_{\Omega} \vec{\nabla} c(\vec{x}) d\Omega, \quad (1)$$

$$\vec{Q} = \frac{1}{V} \int_{\Omega} \vec{q}(\vec{x}) d\Omega, \quad (2)$$

where  $V$  is the volume of  $\Omega$ . In the context of transport by diffusion,  $\vec{q}(\vec{x})$  is Fick's velocity at point  $\vec{x}$  and  $\vec{\nabla} c(\vec{x})$  is the concentration gradient at this point such as Fick's Law gives:

$$\vec{q}(\vec{x}) = -D \cdot \vec{\nabla} c(\vec{x}), \quad (3)$$

where  $D$  is the mesoscale diffusion coefficient. In order to compute macroscopic diffusivity tensors within the domain  $\Omega$ , we use the method proposed in [36] and [37] for hydraulic transport problems (permeability problems in rock). Herein we extend the method to chloride ions transport problems in heterogeneous media. In this sense, the mean concentration gradient  $\vec{G}$  and the mean flux  $\vec{Q}$  are computed from the values of concentration and flux on the frontier  $\partial\Omega$  of the domain  $\Omega$  such as:

$$\vec{G} = \frac{1}{V} \int_{\partial\Omega} c(\vec{x}) \vec{n}(\vec{x}) dS, \quad (4)$$

$$\vec{Q} = \frac{1}{V} \int_{\partial\Omega} (\vec{q} \cdot \vec{n}) \vec{x} dS, \quad (5)$$

where  $\vec{n}$  is the outward unit vector from the surface  $S$  and  $dS$  is a surface element of  $\partial\Omega$ .

Eqs. (4) and (5) provide an efficient way to compute macroscopic diffusivity tensors when boundary conditions are applied. These equations respectively represent the concentration gradient and the flux computed from the values of concentration and flux on the contour for any heterogeneous media, any boundary condition – Dirichlet or Neumann-type – and, any frontier shape.

### 2.2. Boundary conditions: linear concentration

With regards of the numerical simulations proposed in [36], Dirichlet-type boundary<sup>4</sup> conditions are assumed in the present work. We consider condition of linear concentration at the contour such as:

<sup>1</sup> Except for the G-FEM where the specific enhancement is quite different.

<sup>2</sup> This method presents several numerical advantages that are sum up in [28].

<sup>3</sup> The case of an imposed flux can also be taken into account, nevertheless it is not regarded in this paper.

<sup>4</sup> Neumann-type boundary conditions are also treated in [36].

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