A study of the effect of crack-induced diffusivity on the service life prediction

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ABSTRACT. *The objective of this paper is to propose a numerical model capable of coupling the transfer of chloride ions and cracking into concrete by developing a meso-macro numerical approach for the determination of macroscopic diffusivity tensors in heterogeneous quasi-brittle materials such as concrete. The strong discontinuity kinematics is added to take into account micro-cracking. The mesoscale coupling with the mass transport part is based on Fick's Law of diffusion with a modified diffusion coefficient accounting for crack opening and aggregates by means of the experimental results of Djerbi et al. [DJE 08]. Then an upscaling process based on the work of Pouya et al. [POU 02] is used to provide a macroscale diffusivity (mean diffusivity tensor). Finally, the obtained mean diffusivity tensor has been employed to predict the corrosion initiation time to study the impact of mechanical cracking on service life of RC structures using Bazant's physical models. The numerical results show an induced-anisotropy of the mean diffusivity tensor and obvious effect of the value of crack opening on the corrosion initiation time.*

KEYWORDS: *Concrete durability; Crack-induced diffusivity alteration; Multiscale modelling; Embedded Discontinuities; Chloride ions transport*

1. Introduction

Despite the fact that concrete is not damaged by the chloride ions itself, a hazardous corrosion can be induced due to the reaction between chloride ions and the reinforcing bars [HAS 12]. When chloride ions penetrate inside the concrete, accumulate in the surroundings of the reinforcing steel and reach a critical value, it may result in a steel corrosion initiation in the presence of oxygen and water, that, in turn, leads to cracking and spalling of concrete cover because of the differential increasing of corrosion products [KWO 09]. The corrosion of the reinforcing steel is the major cause of degradation of reinforced concrete, causing a reduction in the service life and badly affecting the durability of the structure.

Besides, the existence of mechanically-induced cracks might play a very important role in the corrosion kinetics since they facilitate the penetration of aggressive agents.
Many works have been carried out focusing on the study of the transport mechanism and behavior of chloride in sound concrete ([CAS 01] ;[FRI 04] ;[SLE 12],[NGU 14]). Different mechanisms have been considered to represent the chloride transport process, but the main one is diffusion. Diffusion phenomenon occurs when there exist a difference in chloride concentration between two adjacent points. However, the difference in the electrical potential leads to transfer of ions by migration phenomenon if the transport process is conducted by an applied electrical potential. Other mechanisms might provoke the transport of chlorides such as convection and permeation. While chlorides penetrate inside the concrete, a part of them reacts physically or chemically with cement composites (which known as chloride binding) and still noneffective to induce the corrosion initiation process.

Several authors investigated the effects of crack opening factor (as the major crucial factor) on the transport process considering one or more of the aforementioned mechanisms ([JIN] ;[WAN 11] ;[SAV 13] ;[SAV 14] ;[MAR 09], [NIL 15]). While, the crack opening have been simulated by artificial crack in order to simplify the calculations as in the work of Jin et al. (2010) [JIN], Wang and Ueda (2011) [WAN 11] Marsavina et al. (2009) [MAR 09], or by producing a real crack as in Savija et al. (2013, 2014) ([SAV 13] ;[SAV 14]).

Concerning this coupling, researchers link an equivalent diffusion coefficient D_e to a crack width parameter (note that in Gérard et al. [G´ 00], it is related to the crack density and the mean crack aperture). They propose models depending on this coefficient fitted in experimental data. In Jang et al. [JAN 11] and Djerbi et al. [DJE 08], a parallel model (accounting for a crack geometry factor in [JAN 11]) based upon the work of Gérard et al. [G´ 00] is set out. The model is then fitted on experimental results achieved from a migration test in steady-state regime on samples cracked by a tensile splitting test. Djerbi et al. [DJE 08] and Jang et al. [JAN 11] both suggest a linear relationship between the crack width and the equivalent diffusion coefficient D_e. They show that only over a threshold crack width value of 80 μm, the diffusion coefficient starts to increase. In addition, in Djerbi et al. [DJE 08], an important step forward is made : the authors propose a relationship between the crack width and the diffusion coefficient through the crack D_{cr}. This information is of great interest for the mesoscale coupled approach detailed in this paper.

Regarding the numerical simulation of this coupling, some studies are particularly relevant, taking into account artificial cracks (see Jin et al. [JIN] and Wang and Ueda [WAN 11]), or by performing a mechanical simulation to lead to real cracks (see Šavija et al., [SAV 13] and [SAV 14]) . In Šavija et al. ([SAV 13] and [SAV 14]), the authors propose a numerical coupling between two models : for mechanical and diffusion simulations respectively, the Delft lattice model (see [SCH 93] for details) and the transport lattice model (see [SAV 13] for details). Contrary to the prior numerical works, mechanical simulations are performed to produce realisitic cracks. In Šavija et al. [SAV 14], according to findings of Yoon et al. [YOO 07], the authors impose a chloride concentration only on cracks wider than 12 μm obtained after the numerical simulation of a splitting test. In Šavija et al. [SAV 13], the authors assess their numerical model with (1) the experimental results of Sahmaran [SAH 07] and Ismail et al. [ISM 08] for cracked mortar samples by considering D_{cr} of Djerbi et al. [DJE 08], (2) with the experimental results of Ismail et al. [ISM 04] for cracked bricks samples – trial and error method to obtain the equivalent diffusion coefficient – in the context of artificial cracks.
However, regarding this numerical simulation literature, the computation of macroscopic diffusivity tensors depending on the cracked state of concrete and more globally on its heterogeneous aspect is rarely performed.

From a civil engineering point of view, these macroscopic tensors are crucial regarding durability and service-life problems of civil engineering facilities. We propose in this paper a method based on an upscaling process in order to provide macroscopic diffusivity tensors accounting for the heterogeneous mesoscale structure of concrete, and correlate to the crack pattern and to the crack width values of numerically-induced cracks. In this context, important features of the cracking process are taken into account in the macroscopic diffusivity : (1) the evolution from diffuse cracks in the bulk to localized macro-crack(s), (2) the tortuosity of the crack pattern and (3) the

induced-anisotropy. To the author's knowledge, only the work of Nilenius et al. [NIL 15] provides such macroscopic information.

The effect of crack-induced diffusivity evolution on the service life prediction is assessed by figuring out the initiation period of corrosion as an indication adopted by some of previous study as (Zhang et al. [ZHA 06] ; Liu [LIU 96], Kwon et al. [KWO 09]). Different models were used to investigate the corrosion initiation time, while Fick's Law-based model is still broadly used by transforming of Crank's solution into a deterministic model ([KWO 09] [ZHA 06], [AUD 09]).

In this paper, we model concrete at the mesoscale as an heterogeneous quasi-brittle two-phase material based upon the previous work of Benkemoun et al. [BEN 10]. The main features of this work are presented in Section 2. In Section 3, we introduce a simple chloride ions transport model relying on Fick's Law in fully saturated conditions. The mesoscale coupling is then examined. In Section 4, the upscaling method for the determination of macroscopic diffusivity tensors is presented, based upon the work of Pouya et al. [POU 02]. In Section 5, we show the capability of the approach to determine macroscopic diffusivity tensors in the context of concrete-like materials. Finally, in Section 6, we present the effect of crack opening on the service life represented by prediction of corrosion initiation period (t_i).

2. Mechanical model : enriched finite element method

In this section, a brief review of the mechanical model used for modeling of quasi-brittle heterogeneous materials is presented. For more details, see Nathan et al. ([BEN 10], [BEN 12])

2.1. *Meso-scale model of heterogeneous quasi-brittle materials*

The proposed numerical model is based on a fine representation of cracking phenomena in the fracture process of a two-phase (stiff aggregates embedded into a mortar matrix) quasi-brittle cement-based materials. In this direction, the relevant scale considered is the mesoscopic scale ([WRI 06] and [BOR 06]) in order to take into account the influence of the shape, the size, the distribution and the mechanical properties of aggregates on the mechanical behavior of concrete. Moreover, because of the diversity of cracking phenomena for the quasi-brittle materials such as concrete, it is necessary to establish a model that explicitly represent cracks at the interface between aggregates and mortar, and/or at any of the two phases (aggregate and mortar).

From a numerical point of view, the mesoscale model developed is based upon a 3D lattice finite element model ([SCH 92], [SCH 97], [YIP 05] and [LAC 05]) whose truss elements kinematics is enhanced by two discontinuities embedded in the elements. We chose to work with a spatial truss models, whose geometry is built using Delaunay triangulation.

The first discontinuity is a weak discontinuity – continuous displacement field and discontinuous strain field, [ORT 87] – introduced because of the non-adaptated meshing process [MOË 03]. This process consists in a unique homogeneous mesh whose nodes are placed independently from the morphology of the aggregates, and herein, some elements are cut into two parts, each having different elastic properties.

Cracking and softening behavior observed for quasi-brittle materials such as concrete are introduced by the second discontinuity -strong discontinuity- (discontinuous displacement field and unbounded strain field, [SIM 93]) within each element. These discontinuities represent the micro-cracking which may occur in any phase (aggregates or mortar) and the debonding at the interface between the two phases.

2.2. *Finite element resolution framework*

Among all the methods ([MOË 99], [STR 00]) to introduce the two existing discontinuities in the element, the total strain is written in the context of the EAS (Enhanced Assumed Strain, [SIM 90]) method such as :

$$\boldsymbol{\varepsilon} = \underbrace{\nabla^{\mathrm{s}}\bar{\boldsymbol{u}}}_{\text{regular}} + \underbrace{\tilde{\boldsymbol{\varepsilon}}}_{\text{weak}} + \underbrace{\hat{\boldsymbol{\varepsilon}}}_{\text{strong}}, \tag{1}$$

where $\nabla^{\mathrm{s}}\bar{\boldsymbol{u}}$ is the symmetric gradient of the displacement field. As in [SIM 90], we refer to $\tilde{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\varepsilon}}$ as the enhanced parts of the strain field. The notation $\tilde{\bullet}$ (resp. $\hat{\bullet}$) refers to weak (resp. strong) discontinuity.

In the context of a truss element, $\tilde{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\varepsilon}}$ have the following form :

$$\tilde{\boldsymbol{\varepsilon}} = \boldsymbol{G}_{\mathrm{w}}^{\oplus/\ominus}[|\epsilon|] \quad \text{and} \quad \hat{\boldsymbol{\varepsilon}} = \boldsymbol{G}_{\mathrm{s}}[|u|], \tag{2}$$

where $\boldsymbol{G}_{\mathrm{w}}^{\oplus/\ominus}$ and $\boldsymbol{G}_{\mathrm{s}}$ are enhanced functions. $[|\epsilon|]$ and $[|u|]$ are the enhanced interpolation parameters and belong to the set of unknowns.

This strain field (equation (1)) is then introduced in the Hu-Washizu variational formulation [WAS 82] leading to the Finite Element problem to be solved in terms of the displacement field $\boldsymbol{d}$ and the parameters $[|\epsilon|]$ and $[|u|]$. It is important to indicate that the solving procedure of the finite element system is done at two levels : (1) the local level where parameters $[|\epsilon|]$ and $[|u|]$ are obtained by "operator split" method ([SIM 97] and [BEL 03]) the global level where the displacement field $\boldsymbol{d}$ is calculated after statically condensed $[|\epsilon|]$ and $[|u|]$.

The fundamental parameter (for each finite element) $[|u|]$ which is representing the value of the crack opening for each time step, is an output of the mechanical problem. As we will see later, it will be reused as input data for the diffusion transfer problem leading to weak coupling in mesoscopic scale.

3. Mesoscale mechanical-transport coupled model

As presented in Section 2, the mechanical model is based upon the Strong Discontinuity Approach (SDA). This approach leads to the representation in terms of displacement jump of the fine scale cracks and to the computation of this jump as the crack width $[|u|]$. Thus the crack width values for each finite element are given by the mechanical model at the end of each time step. These crack width values are then used as input data in the chloride ions transport problem leading to a weak coupling at the mesoscale with the mechanical problem. In this Section, we first present the chloride ions transport model selected for this work and then show how the aforementioned weak coupling is performed.

3.1. *Chloride ions transport model*

In this paper, Fick's law was chosen for modeling of diffusion transfer. This hypothesis, thus, gives the following problem to solve :

$$\frac{\partial c}{\partial t} = -D_m \cdot \frac{\partial^2 c}{\partial x^2}. \tag{3}$$

where D_m the mesoscale diffusion coefficient $[m^2/s]$ and c the mass concentration $[kg/m^3]$. Equation (3) represents the problem to be solved in terms of mass concentration field. The resolution is achieved by means of the Finite Element Method ([LEW 04]) leading to the following discretised form of (3) :

$$\mathrm{A}_{e=1}^{n_{el}}[K^e + \frac{M^e}{\Delta t}]_{n+1}^{(k)} \Delta c_{n+1}^{(k+1)} = -\mathrm{A}_{e=1}^{n_{el}}[R^e]_{n+1}^{(k)}, \tag{4}$$

where A is the assembly operator and n_{el} the number of elements. We note M^e the element mass matrix, K^e the element diffusion matrix and R^e the element residual vector. Euler-backward integration scheme is used for the time dependent term.

3.2. *Mesoscale coupled approach through Djerbi et al. [DJE 08]*

With reference to the literature (see introduction), it was agreed in this work to achieve the diffusion/cracking coupling through the equivalent coefficient of diffusion introduced by Djerbi et al. [DJE 08]. We will then have a diffusion coefficient linked to the crack opening as follows :

$$\begin{cases} D_{cr}(m^2/s) = 1.8 \times 10^{-12} & [|u|] < 30\,\mu m \\ D_{cr}(m^2/s) = 2 \times 10^{-11}[|u|] - 4 \times 10^{-10} & 30\,\mu m \leq [|u|] \leq 80\,\mu m \\ D_{cr}(m^2/s) = 14 \times 10^{-10} & [|u|] > 80\,\mu m \end{cases} \tag{5}$$

Therefore, at each time step of the diffusion problem, the equivalent coefficient of diffusion will change depending on the value of $[|u|]$ for each element to realize a weak coupling at the mesoscopic scale.

By achieving the mesoscale coupling, we now turn to the upscaling method leading to the computation of macroscopic diffusivity tensors.

4. Upscaling method : macroscopic diffusivity tensors computation

In this Section focus is made on a upscaling method leading to the computation of the macroscopic diffusivity tensor. We define the mean concentration gradient $\vec{G}$ $[kg/m^4]$ and the mean flux $\vec{Q}$ $[kg/(m^2 s)]$ within a domain Ω by the following equations :

$$\vec{G} = \frac{1}{V}\int_{\Omega} \vec{\nabla} c(\vec{x}) d\Omega, \tag{6}$$

$$\vec{Q} = \frac{1}{V}\int_{\Omega} \vec{q}(\vec{x}) d\Omega, \tag{7}$$

where V is the volume of Ω. We remind that $\vec{q}(\vec{x})$ 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 :

$$\vec{q}(\vec{x}) = -D_m \cdot \vec{\nabla} c(\vec{x}), \tag{8}$$

where D_m is the mesoscale diffusion coefficient with the form of equation (5).

To determine the mean diffusivity tensor, we propose to follow the method developed by Pouya et al. ([POU 02] and [POU 09]) for permeation transfer problems in heterogeneous media and applied in the context of the Finite Element Method for a cracked concrete by Jourdan et al. [JOU 14] for gas transport problem. In this work, the method is extended to the problems of chloride ions transport problem. 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 Ω such as :

$$\vec{G} = \frac{1}{V}\int_{\partial\Omega} c(\vec{x})\, \vec{n}(\vec{x})\, dS, \tag{9}$$

$$\vec{Q} = \frac{1}{V}\int_{\partial\Omega} (\vec{q}\cdot\vec{n})\, \vec{x}\, dS, \tag{10}$$

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

As we'll see hereafter, equations (9) and (10) are well adaptated for numerical simulations. Their form provides an efficient way to compute the macroscopic diffusivity tensor 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 – presence of cracks and/or inclusions –, any boundary condition – Dirichlet or Neumann-type – and, any frontier shape.

In this work Dirichlet boundary conditions are chosen. We then consider the linear pressure boundary conditions such as :

$$c(\vec{x}) = \vec{A}\cdot\vec{x} + c_0, \quad \forall \vec{x} \in \partial\Omega, \tag{11}$$

where $\vec{A}$ is a constant vector and c_0 a constant scalar.

Following the development made in Pouya et al. ([POU 02]) for hydraulic transport problem under the condition of linear pressure at the contour, we obtain : the equality $\vec{G} = \vec{A}$ and a direct link between the mean concentration gradient $\vec{G}$ and the mean flux $\vec{Q}$ such as :

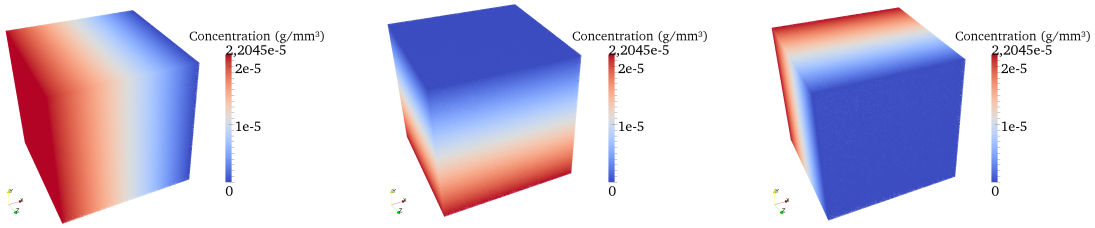
$$\vec{Q} = -\underline{\underline{\boldsymbol{K}}} \cdot \vec{G}, \tag{12}$$

where $\underline{\underline{\boldsymbol{K}}}$ represents the macroscopic permeability tensor of the domain Ω. In our case $\underline{\underline{\boldsymbol{K}}}$ is nothing but the mean diffusivity tensor. We will replace it by $\underline{\underline{\boldsymbol{D}}}$.

Incorporing the equality $\vec{G} = \vec{A}$ in (12) yields :

$$\vec{Q} = -\underline{\underline{\boldsymbol{D}}} \cdot \vec{A}. \tag{13}$$

Equation (13) provides a straightforward way for the numerical computation of the macroscopic diffusivity tensor $\underline{\underline{\boldsymbol{D}}}$. Indeed, the nine components of the tensor $\underline{\underline{\boldsymbol{D}}}$ are obtained by computing $\vec{Q}$ for three distinct directions of the vector $\vec{A}$ present in (11). These directions are shown in Figure 1 for a $100\times100\times100$ mm cubic domain : Figure 1(a) corresponds to X direction, Figure 1(b) to the Y direction and Figure 1(c) to the Z direction of the domain.



(a) $\vec{A}$ in the X direction (b) $\vec{A}$ in the Y direction (c) $\vec{A}$ in the Z direction

Figure 1 – Condition of linear pressure on the contour in the X, Y and Z directions

5. Service life prediction model

The corrosion initiation phase of reinforcement bars is related to the penetration of chloride ions reaching to steel surface. The initiation of corrosion begins when the concentration of chloride around the reinforcement exceeds the threshold chloride concentration (C_{th}). The initiation period ($T_\circ$) can be described mathematically by a simple physical model proposed by Bazant [BAZ 79], as :

$$T_\circ = f(C_s, C_{th}, D, L) = \frac{L^2}{12D\left[1-\sqrt{\frac{C_{th}}{C_s}}\right]^2} \tag{14}$$

Where L concrete cover (mm), D the diffusion coefficient of chloride ions $(mm^/ sec)$, and C_s surface concentration (kg/m^3). Further more, Bazant introduce another model to identify the corrosion propagation time T_p where the concrete cover begins to be deteriorated by cracking and spalling because of the increase of corrosion products ; as in equation (15) :

$$T_{corr} = \rho_{cor}\frac{d_s}{s}\frac{\Delta d_s}{j_r}, \Delta d_s = 4\acute{f}_t\frac{L}{d_s}\delta_{pp} \tag{15}$$

Here, ρ_{cor} corrosion product density, s space of the steel bar, j_r rust production rate, δ_{pp} the bar hole flexibility. Therefore, the critical time at which corrosion starts to induce cracks is ([BAZ 79] :

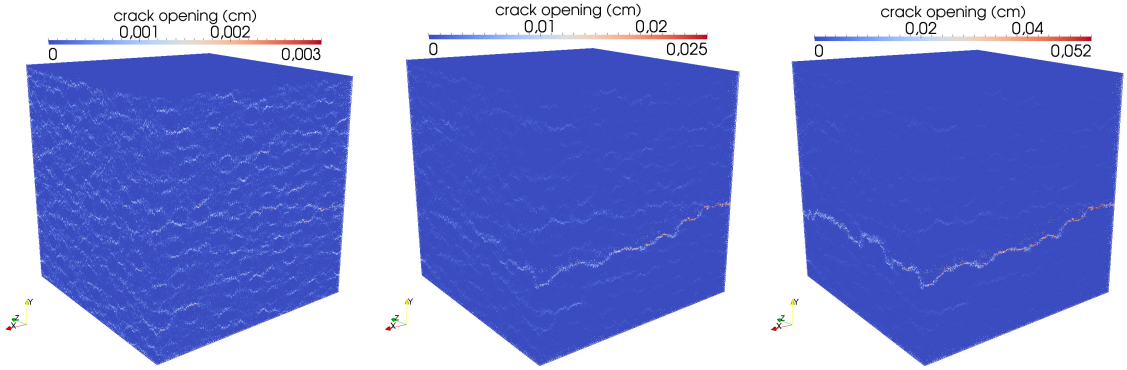
$$T_{cr} = T_\circ + T_{corr}$$

The principle interest of this section is to investigate the liaison between crack opening and the chloride-induced corrosion initiation time. The mean diffusivity tensor which resulted from the last section provide a good entrance to relate the service life end point to crack-induced diffusivity and crack width values using the aforementioned physical model, equation (14,15).

6. Numerical example

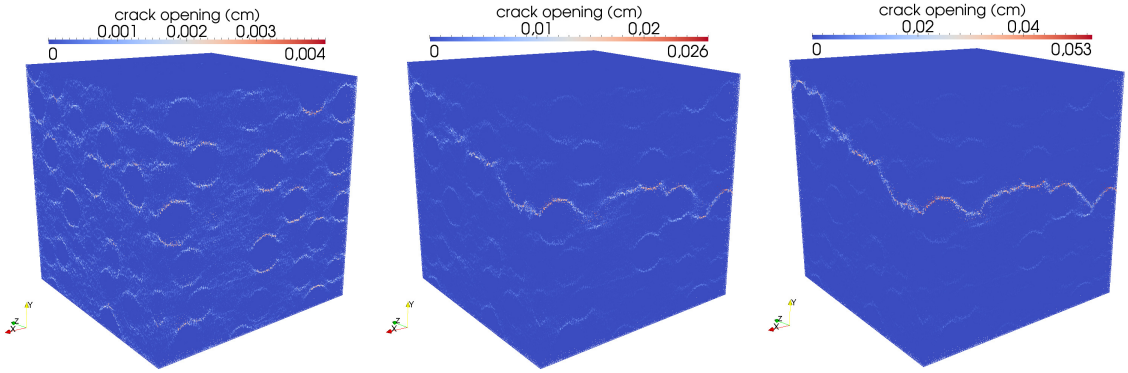
In this Section, the mechanical results and the upscaling method presented in section 4 is illustrated by means of numerical example. We consider a $100\times100\times100$ mm cubic domain of concrete-like materials with two types of heterogeneities (cracks and/or aggregates). This cube is composed of a mortar matrix with 35 $\%$ of spherical aggregates. Two aggregate diameters Φ are considered : 4 and 16 mm. Cracking is mechanically-induced by a tensile test. Once again, the numerical model presented in Section 2 is used for the simulation of the mechanical problem. The crack evolution for the cubic domain is shown in Figures 2 and 3 for Φ equals to 4 and 16 mm, respectively. It corresponds to the micro-cracked bar elements for which the strong discontinuity has been activated.

For each value of the crack width, the method presented above is applied ; the nine components of the macroscopic diffusivity tensor are computed. The numerical results are illustrated in Figures 4. They show diagonal components of the macroscopic diffusivity tensor $\underline{\underline{\boldsymbol{D}}}$ as a function of the crack width $[|u|]$ and the aggregate size for the $100\times100\times100$ mm cubic domain. We can observe from Figure ·4 that the macro-crack, which resulted from the evolution and coalescence of micro-cracks, gives an increase in the values of the diagonal components of mean diffusivity tensor.



(a) Micro-crack initiation around the aggregates (b) Micro-crack coalescence process (c) Macro-crack formation

Figure 2 – Crack pattern evolution and crack width values for the tensile test with Φ equals to 4 mm



(a) Micro-crack initiation around the aggregates (b) Micro-crack coalescence process (c) Macro-crack formation

Figure 3 – Crack pattern evolution and crack width values for the tensile test with Φ equals to 16 mm

The variation of the predicted service life (initiation and propagation phases) associated with the values of crack width for the same numerical example is investigated knowing that the following parameters is considered : concrete cover (d_c) 40(mm) and ($\frac{C_{th}}{C_s}$) 0.32, $j_r = 1.5 \times 10^{-15}(g/m^2.s)$, the corrosion product density $\rho_{cor} = 3600(kg/m^3) = 3.6(g/cm^3)$, the space of the steel bar , $s = 10(cm)$, as used by [LIA 09]. The results are illustrated in Figure (5 and 6). It is shown that the growing of crack width affects the critical time required to onset the corrosion-induced cracks largely after the value of $80\mu m$ for the diagonal diffusivity in the parallel direction with the crack principal plans (xx and zz).

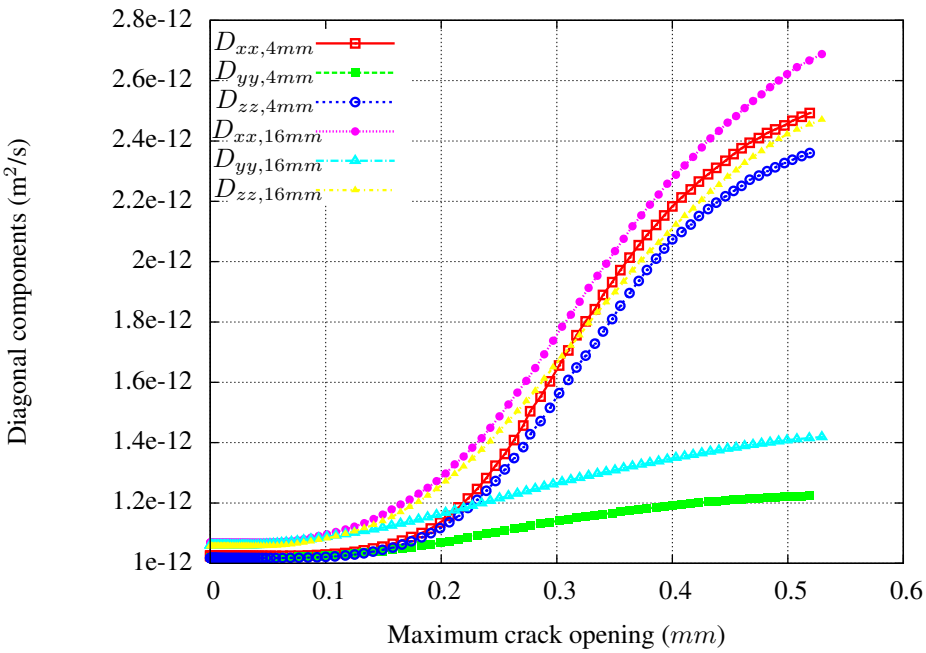


Figure 4 – Diagonal components in relation with the maximum crack width and the aggregates size

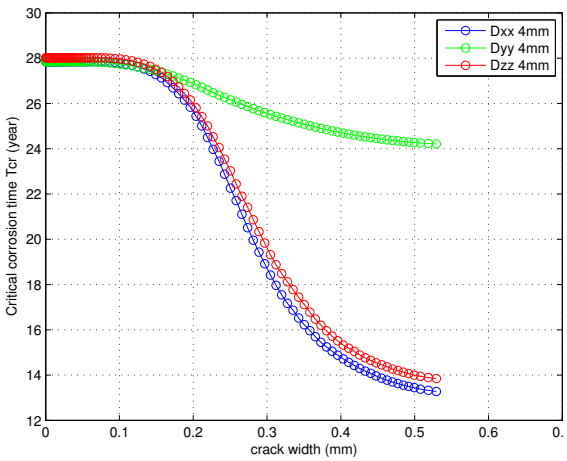


Figure 5 – Service life predicted related to crack width variation for 4mm aggr. size

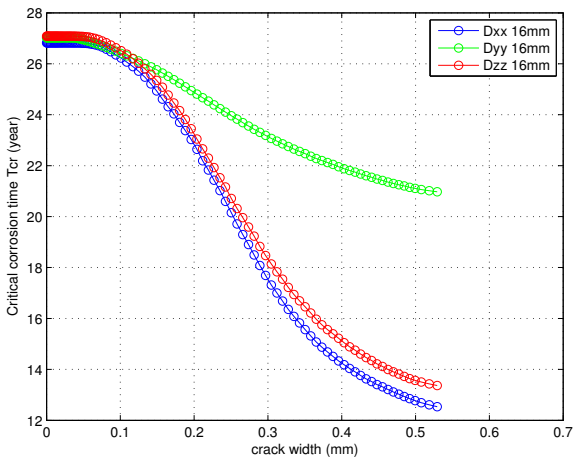


Figure 6 – Service life predicted related to crack width variation for 16mm aggr. size

7. Conclusion and perspective

We have presented in this paper a meso-macro numerical approach accounting for crack-induced diffusivity in heterogeneous quasi-brittle materials such as concrete. This numerical approach relied firstly on the strong discon-

tinuity approach for modelling the evolution of the micro-cracks pertaining to the meso-scale coupling according to work of Benkemoun et al. [BEN 10], and secondly, on an upscaling method developed by Pouya et al. [POU 02] for calculating macroscopic information as a mean diffusivity tensor. The results obtained in a two-phase mechanically induced crack domain (stiff aggregates embedded into a mortar matrix). We have presented several numerical examples showing the ability of the numerical upscaling process to model anisotropic macroscopic diffusivity tensor for realistic cracks. Concerning the chloride ions transport model, only diffusion mechanism is taken into account in this work, so it remains to realize other numerical simulations on specimens considering the integration of transport model by migration and the effect of chloride binding.
Finally, and concerning the service life prediction, a Bazant's classical formulas were used to investigate the corrosion initiation and propagation period as a function of crack-induced diffusivity to examine the effect of crack width on service life of RC structures.

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