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# Numerical simulations for the determination of chloride diffusivity in reinforced concrete under tensile load

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**Abstract.** In service conditions, reinforced concrete structures are multi-cracked due to the loads they are submitted to. It enables aggressive agents, such as chlorides, to penetrate the concrete cover and could initiate steel rebar corrosion leading to more structural damage. Some experimental programs focusing on chloride penetration were conducted on plain or cracked concrete, but mainly unloaded and unreinforced concrete specimens were used for the measurement. These tests highlight the linear dependence of chloride diffusivity to crack opening. However, they do not take into account the presence of rebar, and cracks are partially or totally closed up during the test, which is different from service conditions. This research project aims to understand the influence of micro- and macro-cracks on chloride diffusivity in conditions close to the service ones. To achieve this objective, three steady-state accelerated migration tests under electrical field are to be carried out on a same reinforced concrete specimen kept under a tensile load representative of a structural one. This non-standard chloride penetration test requires the adaptation of the experimental protocol. This paper presents preliminary adaptation work using numerical simulations developed with Comsol Multiphysics®. The impact of testing configuration and parameters, as well as cracking was investigated. Comparison of simulations and preliminary experimental results are also given.

**Keywords:** Simulations, Chloride migration, reinforced concrete, tensile load, cracking.

## 1 Introduction

Reinforced concrete structures are often multi-cracked because they are submitted to mechanical and environmental loads during their service life. These cracks are a preferential path for aggressive agents carried by water, such as chlorides, to enter the

concrete cover. When chlorides reach steel rebars in sufficient quantity, they initiate rebar corrosion, which progressively damages the structure. Chloride diffusivity measurements allow to quantify the chloride penetration capability and give an indicator of concrete durability. However, chloride diffusivity measurements are often conducted on plain concrete without reinforcement [1] and, in some cases, on cracked concrete without reinforcement. In the latter case, specimens are damaged with a splitting test and then unloaded before the diffusivity measure [2-4]. Through these studies, it has been shown that chloride diffusivity linearly increases with the crack opening until it reaches the chloride diffusivity value in water when the crack opening is over about 80  $\mu\text{m}$  [5]. Nevertheless, these studies do not reflect the reality of the concrete structures in service conditions, which are reinforced, cracked and loaded continuously.

This research project aims to understand the impact of the micro- and macro-cracks found in service conditions in reinforced concrete structures on chloride diffusivity. Accelerated migration tests are simultaneously conducted on three different parts of a reinforced concrete tie specimen, which is kept under a service-conditions tension load. The chloride diffusivity measurements are performed under an electrical field in steady-state conditions. Because the thickness of the tie-specimen, representative of concrete cover in real structures, is larger than specimens used in standard migration tests, and also due to the presence of three migration cells on the tie-specimen, the standard migration test had to be adapted for this project.

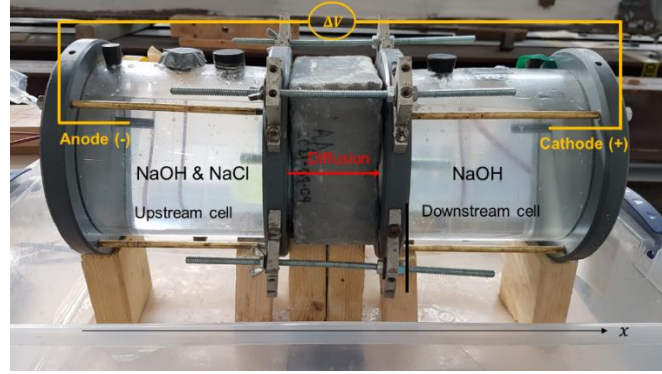
This paper presents preliminary numerical works conducted to evaluate the required adaptations to the NT Build 335 procedure [6]. It investigates variations in the electrical field and the upstream chloride concentration with Comsol Multiphysics® simulations. The effect of proximity between migration cells and the impact of a straight crack is also analysed. Comparisons of simulations and preliminary experimental results are given.

## **2 Methodology**

### **2.1 Accelerated migration test**

Accelerated migration tests are generally carried out on cylindrical specimens with a thickness of 0.5 to 5 cm [1-7]. In this project, they are conducted on tie-specimens with thickness of 9 cm, offering a classical cover thickness (40 mm around a rebar of 10 mm in diameter). Migration test implies two cells attached to two opposite sides of the specimen. The first cell (upstream) contains a chloride solution, whereas the other one (downstream) contains a solution without chlorides. A constant electrical potential is then applied between these cells to accelerate the migration of chlorides from the upstream to the downstream cells through the concrete. The electrical potential is applied via an electrode placed in each cell: it is called anode in upstream cell and

cathode in downstream cell. Fig. 1 illustrates the set-up for a preliminary test carried out on a small 9 cm thick concrete prism.



**Fig. 1.** Accelerated chloride migration test device.

At the beginning of a migration test, downstream chloride concentration remains null until chlorides have begun to pass through concrete. Then concentration increases in a non-linear way during the non-steady state. Finally, downstream concentration in chlorides  $c_{down}$  [mmol/L] linearly increases with time  $t$  [s] at the steady state, during which the slope of the chloride concentration evolution is proportional to diffusivity  $D_e$  [m<sup>2</sup>/s] according to Eq. (1).

$$c_{down} = \frac{c_{up} \times \Delta V \times S \times F}{R \times T \times V \times e} D_e t \quad (1)$$

Where  $c_{up}$  [mmol/L] is the upstream concentration,  $\Delta V$  [V] is the potential difference,  $S$  [m<sup>2</sup>] is the surface of the specimen exposed to the diffusion tests,  $F$  [C/mol] is the Faraday constant,  $R$  [J/mol/K] is the molar gas constant,  $T$  [K] is the temperature,  $V$  [m<sup>3</sup>] is the downstream cell volume and  $e$  [m] is the thickness of the specimen.

Eq. (1) is derived from the Nernst-Planck equation and is applicable under the following assumptions:

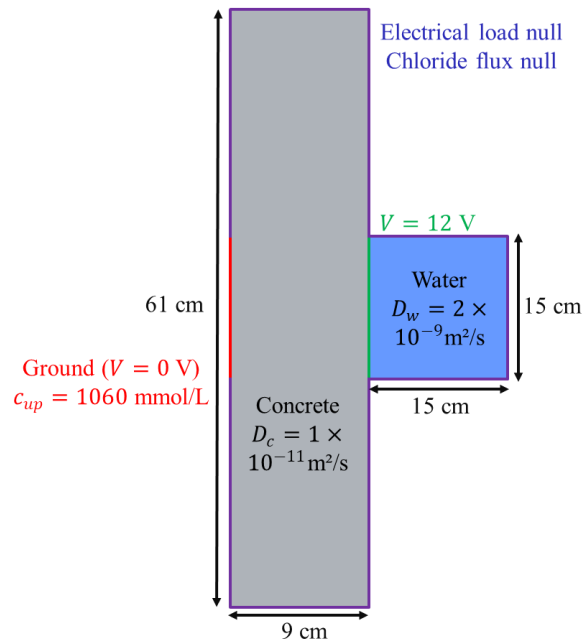
- Diffusion and electrical fields are both assumed to be unidirectional;
- The concrete is saturated, which means convection is negligible and is not considered in the modelling;
- Interactions between chlorides and cementitious matrix are neglected;
- Migration of the chlorides under the electrical field is predominant compared to natural diffusion;
- The upstream chloride concentration is considered constant.

In view of the numerous parameters involved in Eq. (1) and the various assumptions made, several numerical simulations were carried out to study the impact of electrical field and upstream concentration variations. The minimal distance between migration cells and the effect of a crack were also investigated.

## 2.2 Numerical simulation

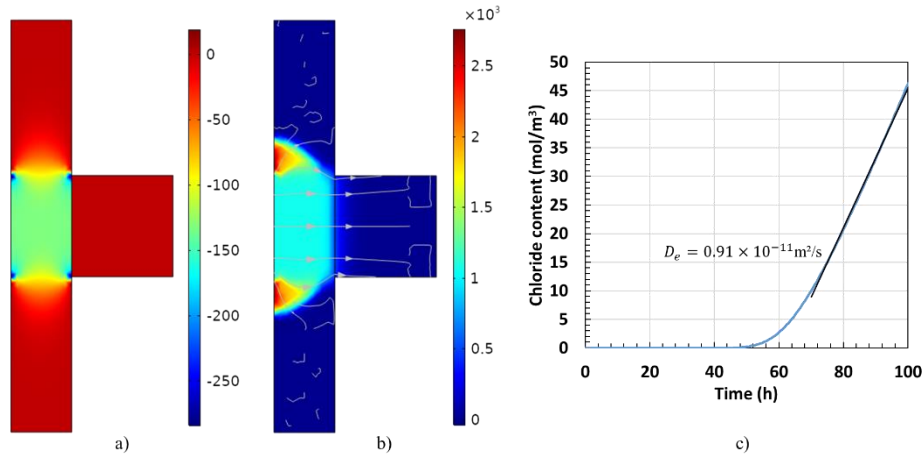
The following numerical simulations have been carried out using modules “Transport of Diluted Species in Porous Media” and “Electrostatic” in Comsol Multiphysics®.

The aim of this project is to make simultaneous migration tests on three different parts of a tie-specimen with a 9 cm x 9 cm cross-section and 61 cm length. Dimensions were chosen according to a previous project concerning water permeability measures [8]. A 2D reference simulation has thus been conducted with a concrete specimen with these dimensions (Fig. 2). This reference simulation considers only one migration test carried out at mid-height of the specimen (Fig. 2). The upstream concentration  $c_{up}$  (1060 mmol/L) and the electrical ground are imposed on a height of 15 cm corresponding to the diameter of the upstream cell (Fig. 1). It is generally recommended to impose an electrical potential difference of 12 V for 5 cm thick concrete specimens to keep natural diffusion negligible compared to migration transport [5-6]. That is why the electrical potential, imposed facing on the opposite side, has been chosen equal to 12 V. At the same location, the downstream cell, with dimensions of 15 cm by 15 cm, is modelled and filled with water, of which diffusivity is equal to  $D_w = 2 \times 10^{-9} \text{ m}^2/\text{s}$ . The surface average of chloride concentration is evaluated in the latter cell to determine diffusivity. Finally, the chloride flux and the electrical load are set to null on the rest of the specimen boundary. Concrete porosity is not physically considered in the modelling, it is included numerically by setting the chloride diffusivity  $D_c = 1 \times 10^{-11} \text{ m}^2/\text{s}$  to the concrete specimen.



**Fig. 2.** Geometry and parameters of the reference simulation.

Fig. 3 gives a 2D representation of the electrical field, and concentration 100h after the beginning of the simulation. Time-evolution of the chloride concentration in the downstream cell is also given.



**Fig. 3.** Result of a simulation, a) electrical field (V/m), b) chloride concentration ( $\text{mol/m}^3$ ) and flow lines for the reference test at  $t=100\text{h}$  and, c) chloride concentration evolution in the downstream cell.

The electrical field is constant between both cells, except on the borders where irregularities can be observed (Fig. 3a). This is linked to the end of the electrode and is expected also present in the experimental test. Indeed, field lines are parallel and regularly distributed in the middle of electrodes. But, on the electrodes rim, field lines are incurved and join the electrodes at the same place, leading to field lines concentration and a higher value of the electrical field. The same phenomenon can be observed with the chloride concentration: a higher value is noticeable close to the electrode ends (Fig. 3b). These perturbations at the extremities lead to a slight decrease in diffusivity. Thus, by evaluating the diffusivity from the evolution of the chloride concentration in the downstream cell, a value of  $D_e$  equal to  $0.91 \times 10^{-11} \text{m}^2/\text{s}$  is determined (Fig. 3c), which is 9% less than the one imposed for the concrete specimen in the simulation ( $D_c$  in Fig. 2).

### 3 Results of the sensitivity studies

This section aims to evaluate the impact of some testing parameters by modifying the reference simulation. Each different value of parameters (one point on following figures) corresponds to one simulation.

#### 3.1 Electrical field

In this section, the voltage was changed while keeping the same configuration as the reference simulation to study the impact of the potential difference on the diffusivity.

Fig. 4 illustrates the modification of the diffusivity when increasing the potential difference.

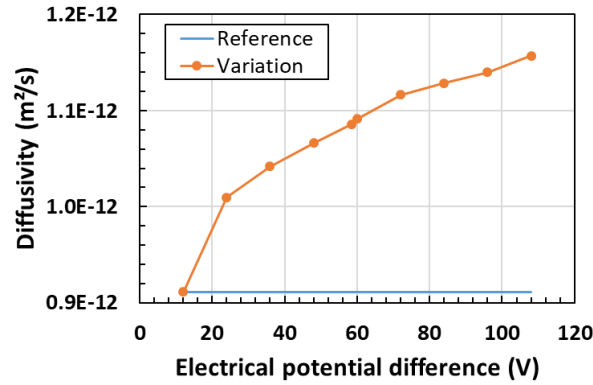


Fig. 4. Evolution of diffusivity according to the electrical potential difference.

The diffusivity value increases with the potential difference to reach a 27% higher value than the reference when increasing the electrical potential difference to 110V. It means that the results obtained during migration tests are very sensitive to voltage variations and can be overestimated for high potential differences. Therefore, even if a high potential is a way to achieve test results more quickly, it will be essential to use reasonable value as well as same potential difference to compare results in experimental tests.

Considering the previous conclusions as well as the risk of formation of undetectable chlorinated compounds such as dichlore or hypochlorite when the voltage is too high, a potential difference of 58.5V was chosen for all the experimental tests [9]. This electrical potential value was numerically tested with Comsol Multiphysics® and involved a diffusivity equal to  $1.09 \times 10^{-11} \text{m}^2/\text{s}$  and a difference of 19% with the reference value, as shown in Fig. 4.

### 3.2 Chloride upstream concentration

The influence of upstream chloride concentration has been studied and shown in Fig. 5. The upstream cell chloride concentration does not influence chloride diffusivity in the concrete. However, it is assumed that upstream concentration is constant during the simulation, which is not the case experimentally when the upstream solution is not regularly renewed.

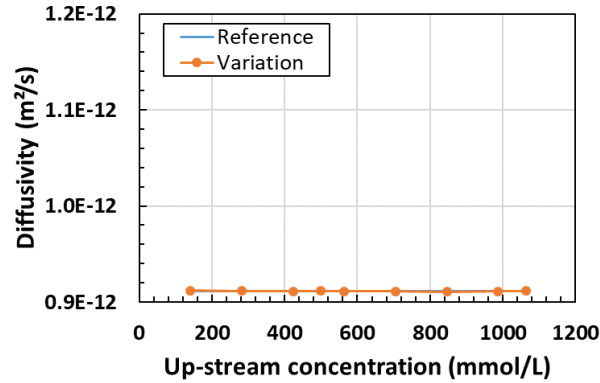


Fig. 5. Evolution of diffusivity according to upstream concentration.

Another simulation with an upstream cell filled initially with a chloride solution and free to equilibrate with the system has shown a decrease in concentration with time, as shown in Fig. 6. This decrease reaches 9% of the initial upstream chloride content after 100h of migration test. Afterwards, this linear decrease was set as a chloride content boundary evolution instead of a constant one. The diffusivity obtained was  $0.88 \times 10^{-11} \text{m}^2/\text{s}$ , which is only 3% lower than the reference value. This observation means that variation of chloride concentration in the upstream cell should have a negligible effect in experiments.

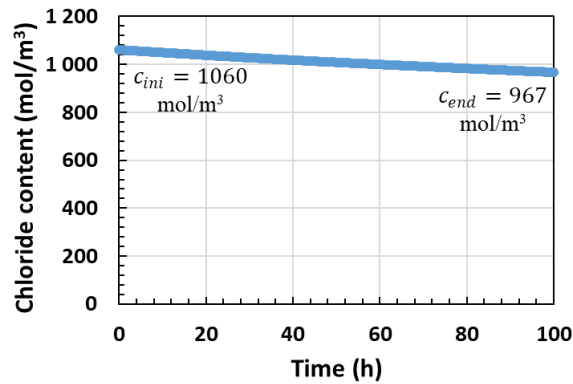


Fig. 6. Decrease of the chloride concentration in the upstream cell.

### 3.3 Distance between 2 cells

In this section, two sets of chloride migration cells are considered in the simulations and the impact of the distance between cells is studied. Cells are located in such a way that geometry is symmetrical to the middle horizontal axis, which means migration phenomena are the same in both migration cells by symmetry. Results of diffusivity are given according to the distance between cells in Fig. 7.



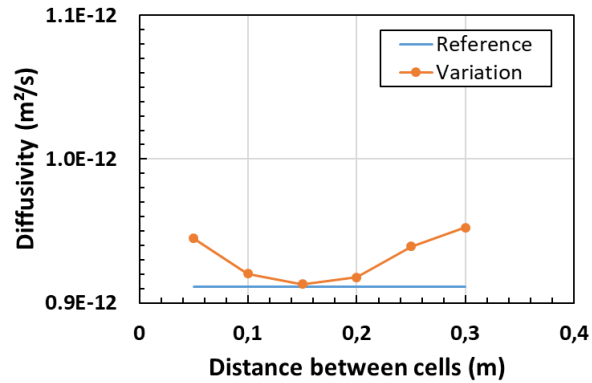


Fig. 7. Impact of the distance between 2 cells on the chloride diffusivity.

When cells are closer than 10 cm, diffusivity is higher than the reference simulation including only one set of migration cells. Indeed, electrical fields of both sets of cells are superposed and locally higher, which drives more easily chlorides and lead to an overestimation of diffusivity. For larger distance between the sets of cells, the diffusivity decreases until it reaches the reference value for a distance of 15 cm. Then, it starts to increase again when the sets of cells become close to the top and bottom specimen border. Indeed, a reflection against the top and bottom surfaces reduces the chloride transit time from the upstream to the downstream cells, artificially raising the diffusivity.

The same simulations were thus conducted on a 2m-long specimen to eliminate the specimen length effect (Fig. 8).

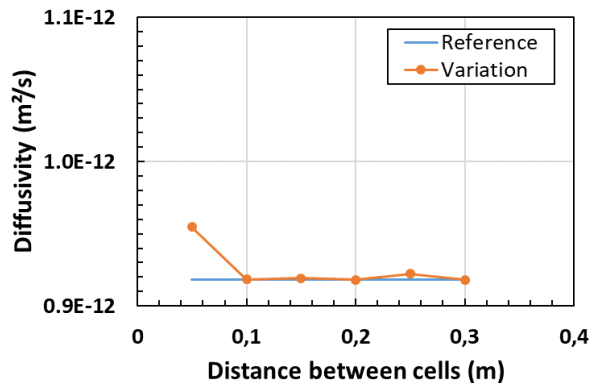
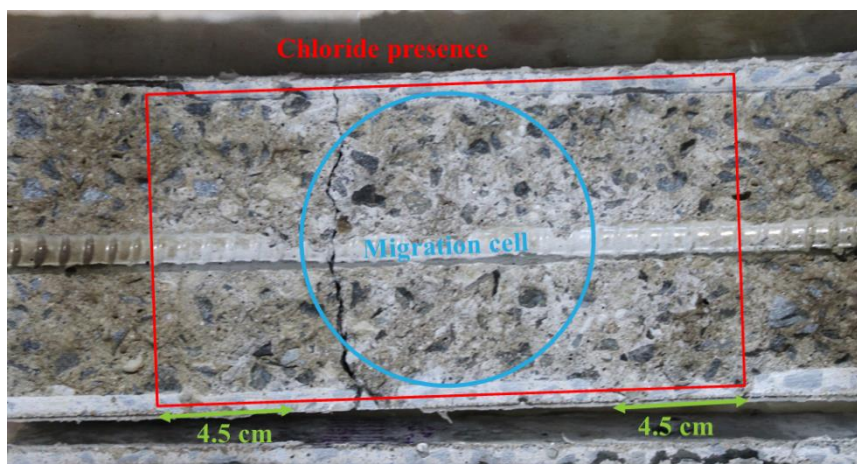


Fig. 8. Impact of the distance between 2 cells on the chloride diffusivity in a 2m-long specimen.

Increasing the specimen length from 0.6 to 2 m brings a very little change in the value of  $D_e$  when in presence of one centred cell ( $0.92 \times 10^{-11} \text{m}^2/\text{s}$  in comparison to  $0.91 \times 10^{-11} \text{m}^2/\text{s}$  for the 0.61m-long specimen). The new value of  $0.92 \times 10^{-11} \text{m}^2/\text{s}$  was then used as the reference in Fig. 8 for proper comparison of the effect of two cells versus one cell on the 2m-long specimen. As observed in Fig. 7, diffusivity still decreases in

Fig. 8 when the distance between cells increases up to 10 cm. However, it then remains constant. This confirms that the increase of diffusivity observed in Fig. 7 when the sets of cells were moved away from each other (for distances superior to 15 cm) is related to the specimen length effect. Consequently, recommendation for the minimal distance between migration sets of cells is 10 cm to avoid spurious effects, whereas the minimal distance to specimen border is 5 cm.

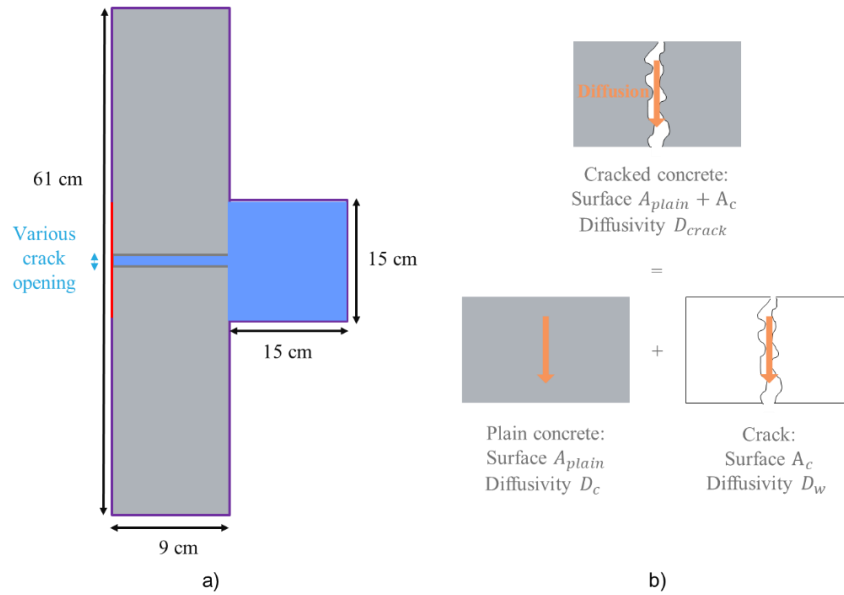
These values have been experimentally verified. A migration test has been carried out on ordinary concrete, reinforced with a 10M epoxy-coated steel rebar. The water/binder ratio was 0.60 and the cement was a standard North American GU type Portland cement. At the end of the test, the specimen was split. A solution of silver nitrate was then sprayed to determine which part of the concrete had been reached by chlorides. The surface of concrete contaminated with chlorides becomes white due to the formation of silver chloride, whereas it stays brown in the absence of chloride [10]. Fig. 9 shows that chloride diffused in concrete in a zone wide of 17 cm, corresponding to a distance of 4.5 cm outside the cell. Therefore, sets of cells must be spaced at least by more than 9 cm and located at more than 4.5 cm from the specimen top and bottom surfaces to avoid interferences. This is consistent with numerical results.



**Fig. 9.** Concrete contaminated with chloride (white surface) and without chlorides (brown) revealed by the addition of silver nitrate.

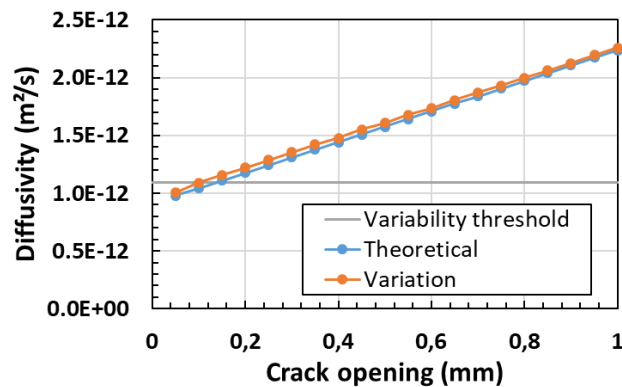
### 3.4 Influence of a straight crack

A straight and constant opening crack filled with water was added at mid-height of the specimen with a unique set of migration cells (Fig. 10a). Several numerical simulations were performed for crack openings ranging from 0.05 mm to 1 mm. A comparison of those simulations with the theory is made. For this, a parallel theoretical model is used: it considers two plain concrete surfaces surrounding a water surface corresponding to the crack. The diffusivity of the cracked concrete is then deduced from the diffusivities of the plain concrete and the water [5] (Fig. 10b).



**Fig. 10.** Impact of crack, a) cracked specimen simulated, b) decomposition of cracked concrete in plain concrete and crack.

Diffusivity can be obtained from the theoretical model and compared to simulations in Fig. 11. A good consistency between simulation and theoretical values of diffusivity as a function of crack opening in cracked concrete was obtained. This means that Comsol Multiphysics® simulations reproduce correctly the impact of perfect crack (straight crack with smooth surfaces with no chemical and physical interaction with water and chloride).



**Fig. 11.** Comparison between theoretical and simulated diffusivity values with a crack opening in the specimen. A variability threshold corresponding to 20% of the reference diffusivity has been added.

The variability in diffusivity appears to be between 12.4 and 19.5% [11]. To be sure to quantify the effect of a crack and not the variability, a variability threshold equal to 20% of the reference diffusivity value was considered (Fig. 11). It means the crack opening has to reach 0.1 mm to cause a significant diffusivity variation compared to inherent concrete variability. Experimental loading will be adapted to reach the crack opening.

## 4 Conclusion

This research project aims to understand the impact of micro- and macro-crack on chloride diffusion in reinforced concrete structures in service conditions. To this end, three simultaneous accelerated migration tests under an electrical field are carried out on the same reinforced concrete tie-specimen under tensile load. These non-standard migration tests have required some numerical work to establish the optimal testing configuration. Comsol Multiphysics® was used to model chloride migration in the concrete specimen in different conditions. A set of electrical and transport parameters were imposed to the specimen, whereas the evolution of downstream chloride concentration provides an estimation of chloride diffusivity based on the Nernst-Planck equation.

A reference simulation was used to evaluate the impact of the different sets of parameters. The electrical field map in the specimen allows reporting the boundary effect of electrodes with a field lines concentration, leading to a locally higher concentration. Diffusivity found in the simulation is slightly lower than the one imposed, but other diffusivity estimations will be compared to this reference value.

Several electrical potential differences in migration test, as well as upstream cell chloride concentrations, were tested. While upstream cell chloride concentration has no impact on the diffusivity, this latter increases with the potential difference. Therefore, keeping the same voltage during the experimental campaign will be mandatory to compare results with each other. The assumption of constant upstream concentration was also verified. Even if the chloride content has decreased by 9% 100h after the beginning of the accelerated migration test, diffusivity is almost not impacted. It means that the change of upstream cell solution is not necessary during the experimental test.

In the final experimental configuration, at least two sets of migration cells will be installed simultaneously on the same specimen. Therefore, the impact of one on the other was verified by simulations. Interferences between the cells are observed when they are separated by less than 10 cm. Furthermore, spurious effects are noticed when sets of cells are too close to specimen extremities. The addition of silver nitrate on a concrete specimen after a migration test showed chloride diffusion up to 4.5 cm around each cell. It corroborates the simulation results.

A concrete specimen with a straight crack was also simulated and compared to a theoretical model. Numerical and theoretical results are similar. The conclusion is that the crack opening must reach 0.1 mm to modify significantly the diffusivity in view of the variability of the diffusivity of plain concrete.

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