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Development of a FE² Multiscale Model of Chloride Ions Transport in Recycled Aggregates Concrete

Arthur Fanara Fanara[1], Luc Courard Courard[1], Frédéric Collin Collin[1]

1 University of Liège

Abstract

Decreasing CO2 emissions and preserving natural resources are necessary to the well-being of our civilisations. In the construction industry, recycling old concrete members could be part of the solution to reach theses objectives. Recycled Concrete Aggregates (RCA), obtained by crushing of demolished concrete structures, can substitute the Natural Aggregates (NA) inside the so-called Recycled Aggregates Concrete (RAC). The durability of RAC is not guaranteed in the current state of research. RCA are indeed composed of natural aggregates partially embedded in an adherent mortar paste, increasing the porosity and water absorption of RAC.
This research aims to better predict the influence of RCA on chloride ions ingress inside concrete. It started with an experimental phase where multiple experiments have been performed to determine the transfer properties and the chloride ions diffusion coefficients of a mortar paste and concretes made from NA or 100% RCA. In this context, the microstructure of the RCA influences deeply the permeability, water content distribution and chloride ingress. Therefore, these properties must be included into a numerical model that integrates the microstructural information in a proper way. A numerical homogenization technique, based on the Finite Element square (FE2) method [5, 13], is implemented into a coupled multiscale model of water flows and advection/diffusion of chlorides in saturated concrete, in order to model the complex flow behaviour encountered.

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Summary

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Full Paper

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DEVELOPMENT OF A FE^2 MULTISCALE MODEL OF CHLORIDE IONS TRANSPORT IN RECYCLED AGGREGATES CONCRETE

Arthur FANARA*[1], Luc COURARD[2] and Frédéric COLLIN[3]

[1] Faculty of Applied Sciences, University of Liège, Belgium, arthur.fanara@uliege.be
[2] Faculty of Applied Sciences, University of Liège, Belgium, luc.courard@uliege.be
[3] Faculty of Applied Sciences, University of Liège, Belgium, f.collin@uliege.be

Key words: Multiscale Modeling, Concrete Structures, Recycled Aggregates, Waste Management, Durability, Chloride Attacks, Experimental Validation

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Once the numerical model has been developed and validated with an analytical solution, it is compared to experimental results and a sensitivity analysis of the RVE is performed.

1 INTRODUCTION

Chloride attacks are a major cause of degradation in the vicinity of roads (where de-icing salts are used in winter) and coastal areas [14, 15]. Chloride ions penetrate the concrete's porous system and concentrate near the steel rebars. This process creates pitting and loss of section of the reinforcements, thus decreasing their mechanical properties and possibly leading to a structural failure [2].
Recycled Concrete Aggregates (RCA) are produced from the recycling process of Construction and Demolition Waste (C&DW) as a mean to decrease the amount of waste landfilled and

provide a sustainable source of aggregates. Those RCA are coarse aggregates containing both Natural Aggregates (NA) and residual adherent mortar, the latter impairing their properties [12, 4]. RCA have an increased porosity and water absorption compared to NA, which favours the penetration of water and chloride ions, increasing its diffusivity inside Recycled Aggregates Concrete (RAC) [17, 1, 11, 19].

The microstructure of concrete, whether it is made of NA or RCA, is composed of a wide range of components: from nanometre-sized pores to centimetre-sized aggregates [9]. Concrete is therefore qualified as a highly heterogeneous material, and the modelling of its entire microstructure would be computationally impossible. This is why the concrete properties are often homogenized over the entire microstructure.
Multiscale modelling and computational homogenization techniques have been developed to allow homogenizing the concrete's microstructure over a smaller scale, and then up-scale it while keeping the computational cost acceptable [16, 5]. The differences between the computation at a macroscale and a microscale are the following:

1. Macroscale: the concrete is treated as a homogeneous medium, and the constitutive laws are supposed to represent the whole behaviour of the material. The mixture theory allows to account for multiple phases (e.g. liquid water and water vapour) percolating inside the porous system of the material studied [3]. This method is easy to implement and allows the use of general properties of concrete, determined experimentally for example. Unfortunately, it means that each modification of the microstructure requires a new experimental campaign to obtain the homogenized properties of the material.

2. Microscale: the whole structure, including the heterogeneities (aggregates, porosity, ...) is directly represented in the model. Each microscopic constituent has its own constitutive equations. Although this increases the precision of the model, its computation cost is too high to be used on metre-sized structures.

Multiscale modelling therefore combines the best of both approaches. In this study, the chloride ingress inside RAC being highly dependent on the microstructure of concrete, a multiscale model is used. However, the microscale explained above will be replaced by a mesoscale according to the size of the constituents we model.

2 METHODOLOGY

2.1 RVE Generation

To each integration point of the discretized homogenized macrostructure is assigned a RVE, and finite element computations are performed separately for each RVE. The macroscopic pressure gradients and mean pressure are transformed into boundary conditions applied to the corresponding RVE, and the macroscopic fluxes are computed by averaging the results obtained for each RVE over their respective volume [18, 13].

The scales used in this work are:

- Macroscale: metre-sized reinforced concrete structures with single phase averaged effective properties;
- Mesoscale (RVE): centimetre-sized laboratory samples with properties relative to each specific phase. It is composed of homogenized porous mortar matrix (with homogenized properties as it is a composite material [20]) as well as impervious aggregates and adherent residual mortar (for the RCA). The ITZ between the different phases could be accounted for through interface elements, but their influence would be difficult to quantify experimentally.

The RVE must be representative of the microstructure of the material studied. It is therefore necessary to use, for its generation, properties related to the concrete studied. Those are the surface fraction, the aspect ratio and the particle size distribution of the aggregates. Each aggregate has a random size, position and orientation following the properties given above.
Using an algorithm similar to the one of Nilenius [16], a 2D RVE is generated and meshed by the software GMSH [10], according to the Frontal-Delaunay algorithm for quads, with a simple recombination algorithm applied to all surfaces, ensuring that all elements are quads.
The size of the RVE is dictated by the maximum aggregate diameter, so as to keep a size of at least 3 times that diameter. An example of a RVE with RCA of 8mm of maximum diameter is represented in the Figure 1.

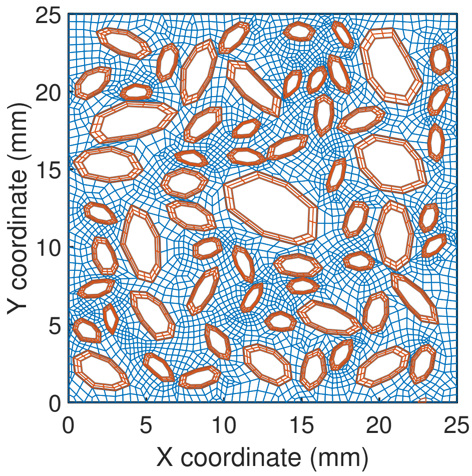

Figure 1: Example of an RVE generated for RAC.

Due to the octagonal form of the aggregates, that requires many points and elements, the mesh is more refined the closer to an aggregate we are. Even though the sample is small, its complexity is therefore resulting in a high number of nodes and elements, which is not ideal for the multiscale modelling, but required for precision purposes.

Concrete is a highly heterogeneous material, its 3D porous structure creating preferential paths along all directions. Therefore, a 3D model should be used when dealing with concrete. However, it would require a greater computational power and complicate the meshing procedure.

On the other hand, using a 2D model requires many hypothesis, such as the equality between a volume fraction and a surface fraction of aggregates, which is inaccurate due to the random geometry of aggregates. Moreover, other authors, such as [16], have done the comparison between 2D and 3D, yielding diffusivity coefficients up to 40% higher in 3D than in 2D. This is easily explained by the restriction created in 2D where the flow is required to by-pass the aggregates in the plane, while in 3D, an out-of-plane solution is possible.
Those hypotheses could be corrected by direct modelling methods and inverse modelling: the modelling of the experiments done will allow to verify that the sample is correct and if not, a penalisation will be applied to correct it.

2.2 Multiscale Ingress Modelling under Saturated Conditions

The first development of the models are performed under saturated conditions. The boundary conditions, i.e. water pressure and pollutant concentration variations, are applied on the macroscale. Gradients are then computed for each Gauss point and transmitted to the mesoscale, as well as the average pressure/concentration at that point. At the mesoscale, each integration point has an assigned value for the water pressure and pollutant concentration, based on the average pressure/concentration and their respective gradients localized from the macroscale. Once those conditions are applied, the resolution can start.

The model developed is described in details in Fanara et al. (2022) as well as the general FE^2 formulation [8].

3 DISCUSSION

3.1 Analytical Validation of the Model

The diffusion and advection of pollutants inside a saturated porous system has been largely studied in the literature, with analytical solutions easily available. One of those analytical solutions is the one used by Biver (1993) for a one-dimensional semi-infinite medium [6][7]:

$$C(x,t) = \frac{C_0}{2}\, \exp\left(\frac{ux}{2D}\right)\left[\exp\left(-x\frac{u}{2D}\right)\operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}} - \sqrt{\frac{u^2 t}{4D}}\right) + \exp\left(x\frac{u}{2D}\right)\operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}} + \sqrt{\frac{u^2 t}{4D}}\right)\right] \quad (1)$$

where C_0 is the limit state condition, u is the fluid flow, D is the diffusion coefficient and x and t are respectively the position and the time. Of course, if $u = 0$, then one recognises the Fick's second law solution. The value of the several parameters can be found in the Table 1.

Case	C_0 [mg/ml]	D [cm^2/s]	u [cm/s]
$u \neq 0$	100	1E-8	4E-11

Table 1: Values of the parameters used for the analytical validation of the model.

The results are displayed at the Figure 2, where the value of the water flows u has been obtained as follows:

$$u = \frac{k_{int}}{\mu_w}\frac{\partial P_w}{\partial x} = \frac{10^{-19}}{10^{-3}}\frac{105325 - 101325}{1} = 4 * 10^{-11} \text{ cm/s} \quad (2)$$

One can see that the multiscale model represents accurately the analytical solution. The model is therefore validated for pollutant diffusion and advection under saturated conditions.

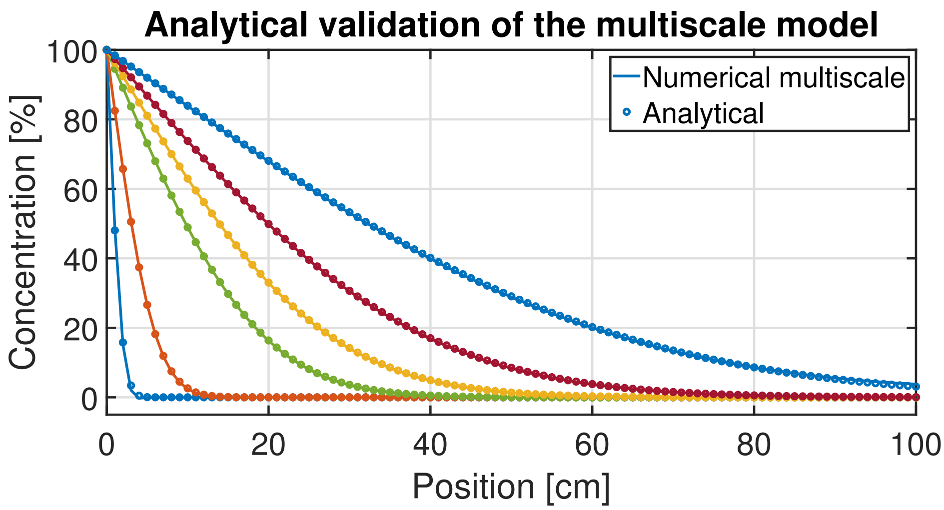

Figure 2: Results of the comparison between the multiscale model, the macroscale model and an analytical solution for the diffusion and convection of chloride ions.

3.2 Influence of RVE Size

While working with Representative Volume Elements, it is important to characterize their effects on the results, namely the size of the RVE. Indeed, a smaller RVE will result in less aggregates placed, and therefore a higher diffusive surface. This is expressed by the Figure 3, where one can see the Particle Size Distribution (PSD) of several RVEs, both from NAC and RAC. It is clear that the bigger the RVE, and the closer the PSD obtained is to the one given in input and representative of a real concrete.

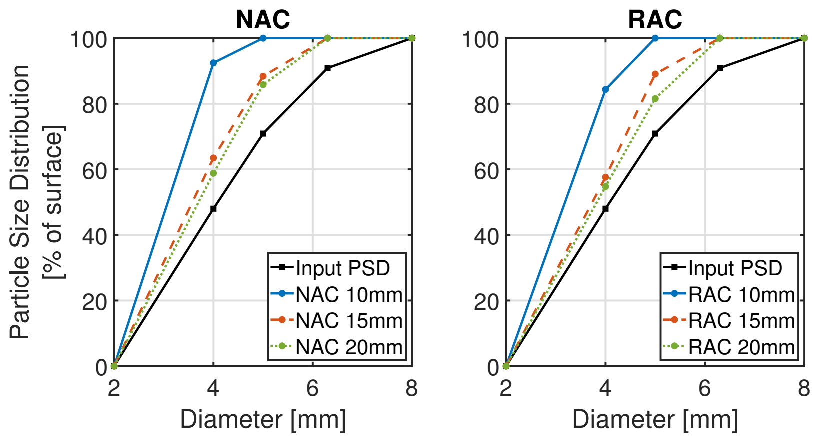

Figure 3: Influence of the RVE Size on a diffusion simulation on RAC RVE.

A simple diffusion simulation was performed on three RVEs representing NAC and RAC, the size ranging from 10mm to 20mm by a 5mm increment. The results are visible in the Figure 4, where the y-axis is the mean value of the concentration on the whole macroscopic sample.
One can see that for the RVE representing RAC, the results do not vary excessively when the size varies. However, for the NAC, there is a huge difference between a 20mm and a 10mm RVE. In that case, more simulations must be done to obtain the RVE size at which the results converge, but the numerical cost is quite high. There is indeed a compromise to be made between the accuracy of the results and the cost of the computation, as shown in the Figure 5.

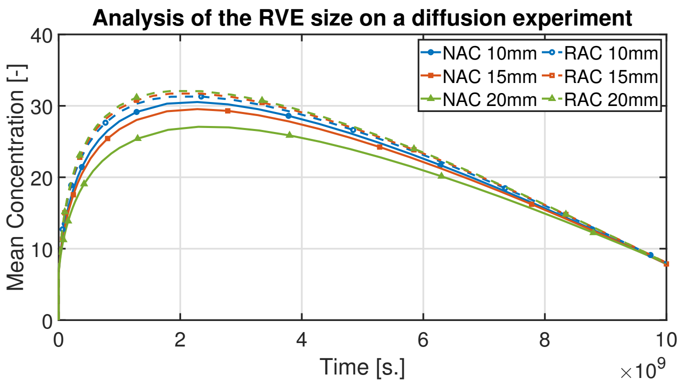

Figure 4: Influence of the RVE Size on a diffusion simulation on NAC RVE.

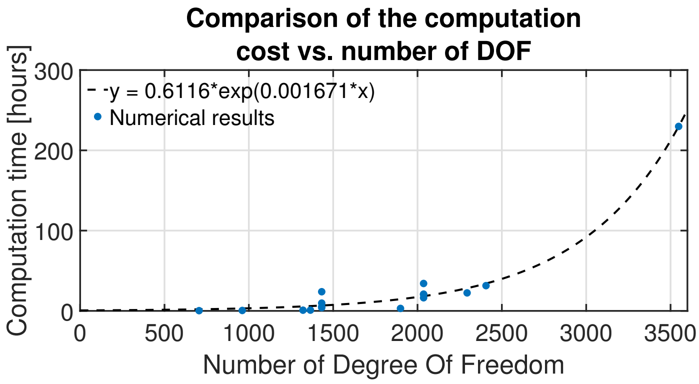

Figure 5: Influence of the number of DOF in the RVE on the computation time.

3.3 Comparison of NAC and RAC under Saturated Conditions

An other important parametric study of the RVE is based on the type of concrete represented. Indeed, at equivalent properties, the representation of one type of concrete or another may change the results. An example of an RVE made from NA (respectively RCA or RCA with 20% more adherent mortar than the other) is shown in the Figure 6 (resp. Figure 7 or Figure 8). On the Figures respective to the RAC, one can see the adherent mortar around the aggregates in orange.

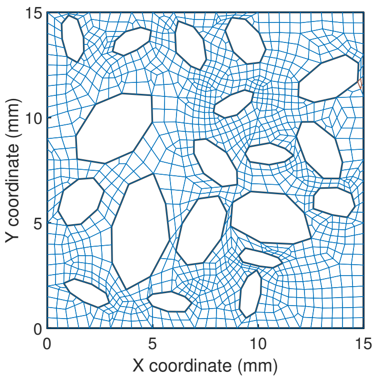

Figure 6: RVE - NAC.

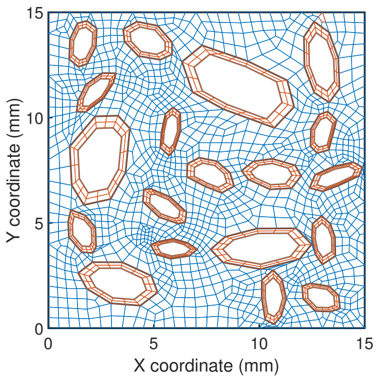

Figure 7: RVE - RAC.

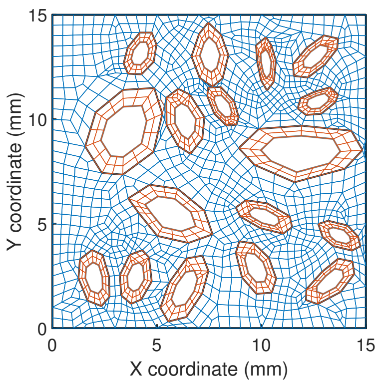

Figure 8: RVE - RAC+20%.

Those RVEs are then used inside a macroscale mesh to perform a 1D diffusion and convection of chloride ions. Initially, the water pressure is equal to the atmospheric pressure and there is no chloride ions inside the sample. The applied conditions, on the left border, are:

- From 0s. to 50s.: linear increase of the chloride content from 0 [-] to 100 [-];
- From 50s. to 1E+5s.: linear increase of the water pressure from 101325 Pa to 202650 Pa;
- From 1E+5s. to 1E+10s.: the water pressure and chloride content are kept constant.

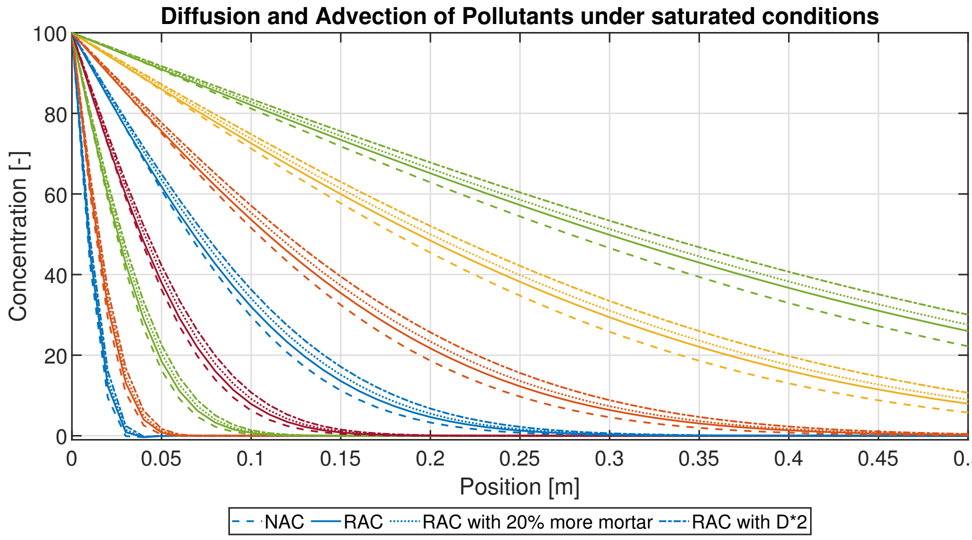

Figure 9: Results of the diffusion of chloride ions inside two different RVE (NAC and RAC) under increasing water pressure and chloride content at the left border.

The results are displayed in the Figure 9. First of all, if we compare a RVE representing NAC and one representing RAC, we can see that at equal properties (even for the mortar of the recycled aggregates), the increased diffusive surface of the RAC increases the diffusivity of the concrete, which was to be expected. We can then play with the RCA themselves: we first increase the adherent mortar content by 20%. The diffusivity therefore increases by 17.6% in average. We can also, on the other hand, use the same adherent mortar content but with a diffusivity two times bigger than the one of plain mortar. In that case, the diffusivity of the concrete is increased by 23% in average.

3.4 Modelling of Experimental Results

The final results to be presented are the modelling of some experimental results obtained. Three compositions were tested under an unsteady-state chloride diffusion experiment: an equivalent mortar (E-M), a concrete made from NA (NAC) and one from RCA (RAC).

The results are displayed in the Figures 10 and 11 for the NAC and RAC respectively. The black data points are the experimental results obtained after 15, 29 and 91 days. Then, the Fick analysis is represented in plain line. It represents a multiscale simulation with an homogeneous microstructure, and whose properties are directly the homogenized properties resulting from the experiments for the NAC and RAC respectively. It is therefore the closest we could get to the experimental points using our model.

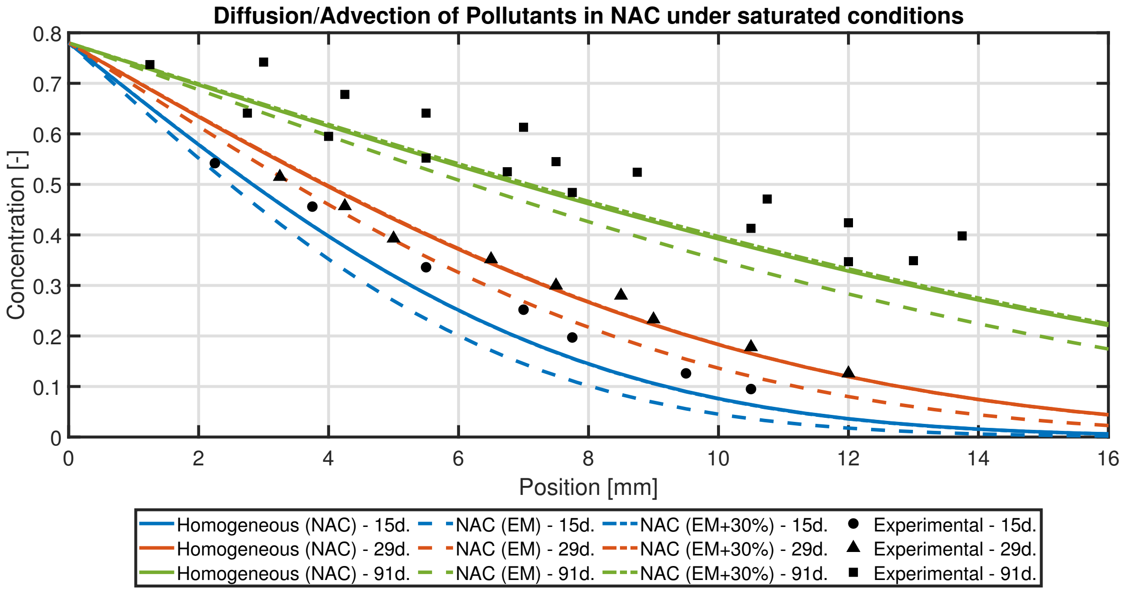

Figure 10: Comparison between experimental results on a NAC and numerical results with an RVE representing that NAC.

Then, we used microstructures related to the concrete studied, and therefore the properties used were the one of the equivalent mortar as only our mortar is meshed in the RVEs. For the NAC (Figure 10), one can see that the results in dash lines are not as accurately representing the experimental results as it should. It is because of the 2D model, in comparison to the experiments being 3D. Therefore, according to some studies, the diffusion coefficient used were increased by 30% to account for out-of-plane diffusion paths [16]. This gave results accurately representing the experiments, in dash-dot lines.

For the RAC, the same results are represented, and the properties of the adherent mortar from the RCA was taken equal to the one of the mortar matrix of the concrete. In that case, the results are, accordingly to the one of the NAC, not accurately representing the experiment. We then increased the diffusivity of both mortar phase by 30%, as for the NAC, and obtained similar results than for the natural concrete. Finally, we decided to increase the diffusivity of the adherent mortar paste from the aggregates by 50% instead of 30%, because the aggregates are often more porous and therefore diffusive that plain mortar. The results were not far from the one discussed before, and the influence of this increased diffusivity is to be tuned appropriately to obtain the best results.

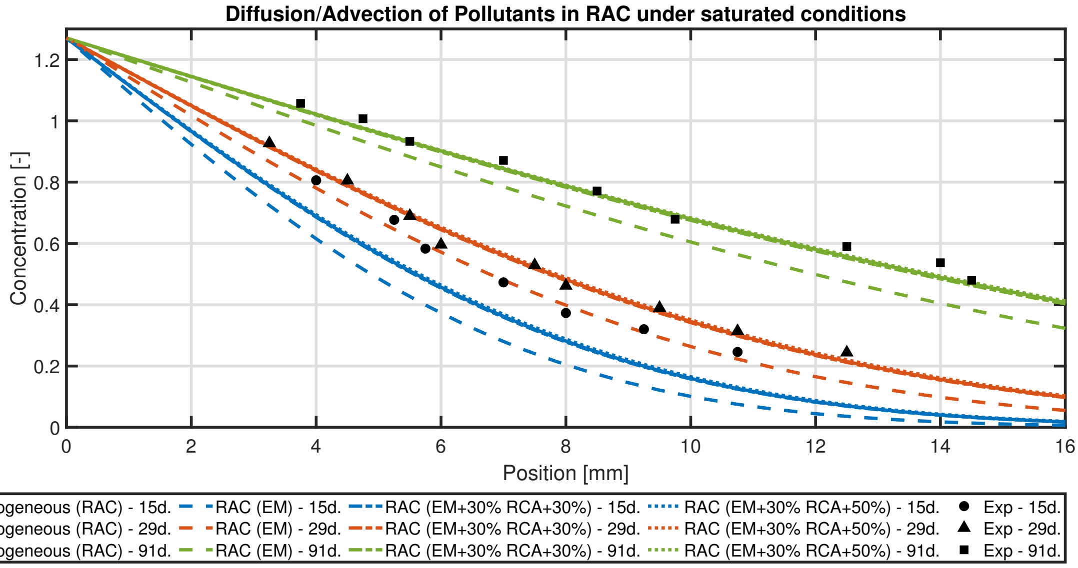

Figure 11: Comparison between experimental results on a RAC and numerical results with an RVE representing that RAC.

4 Conclusion

In this paper, the use of our numerical model (defined in [8]) was presented. It was validated for the diffusion and advection of chloride ions inside a saturated porous medium. Then, the influence of the RVE on the results was analysed, from a point of view of its size and its type (NAC or RAC). Finally, the model was used to replicate experimental results.

For the sensibility analysis of the RVE, it was found that the bigger it is, the more accurate it can represent the reality but the greater the computation time is. Therefore, a compromise is necessary until parallelisation of the code is performed. Furthermore, the influence of the RVE size on the results was found to be more pronounced for the NAC than for the RAC.
The analysis on the RVE type showed, on the other hand, that the added diffusive surface due to the RCA obviously increases the diffusivity of concrete. Furthermore, an increase adherent mortar content seemed to have an important role on the overall response.

Finally, it was found that the use of a RVE allows to replicate the behaviour of a concrete, using homogenized properties for the mortar paste only. The influence of a two dimensional model compared to a three dimensional one was also studied, and it was concluded that the diffusion properties should be increased by approximately 30% in order to replicate the experimentation accurately.

Therefore, one could conclude that the use of Recycled Concrete Aggregates inside concrete promotes the diffusion of chloride ions inside its porous system, notably because of the added diffusion volume/surface.

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