Proc. of the Intl. Conf. on Advances In Civil and Structural Engineering - CSE 2014.

ISBN: 978-1-63248-006-4 doi: 10.15224/ 978-1-63248-006-4-63

Modeling and simulation of chloride diffusion in concrete with recycled aggregates.

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***Abstract*— The concrete along with steel, are the responsibility structural material required to respond to mechanical stresses; specifically, the tensile stresses are borne by the steel, and it is this material that involvement of durability can lose their resilience. Corrosion of steel is one of the main causes of this affectation in the steel, and this is caused by the entry of chloride ions in the called phenomenon diffusion.**

This phenomenon is governed by the diffusion equations of the Fick's first and second law [1]; for these, there are several models that describe the behavior of chloride diffusion in conventional concrete, but nevertheless, not in the recycled concrete.

In this paper, are used as basis, the models of Janzhuang Xiao et al. [2] and Long-Yuang Li et al. [3] to model and simulate the phenomenon of chloride diffusion in concrete with recycled aggregates; for which it has been used a five-phase model for the aggregate: old and new Interfacial Transition Zones (ITZ), new and old mortar, and original aggregate. Furthermore, in this model were considered as variables the Thickness of the Interfacial Transition Zone (T_{ITZ}), the rate of old mortar adhered, the volume fraction of the aggregates and the continuity of the ITZ. The model considered, was composed by a "slice" square 10x10 mm with a unit thickness, and in it, was assessed the effect of each of the study variables separately with respect to the chloride diffusion of this recycled concrete.

Keywords—Chloride diffusion, recycled concrete, Interfacial Transition Zone.

I. Introduction

Concrete is a composite material resulting from the mixture of one or more binders (usually cement) with stone aggregates (gravel, gravel and sand), water and, optionally, additives and additions [4]. Of this, about three quarters of the volume is occupied by aggregates, which are natural material stone selected subject to processes such as disintegration, screening, crushing and washing [5].

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Moreover, at present and environmental requirements, several studies indicate than is favorable the use of recycled aggregates from demolition for use as road base, as fill material in a new Recycled Aggregate Concrete (RAC); in the latter case, new applications are being found [6].

The concrete is combined with steel to support efforts to stress, but this can cause corrosion problems in the system, one of the causes of this corrosion is due to chloride diffusion [7]. This chloride diffusion is described by Fick's second law, and is expressed in Equation (1) in its one-dimensional form:

$$\frac{\partial C_x}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C_x}{\partial x} \right) \qquad (1)$$

Where C_x is the concentration in the X position of a species and D is the diffusion coefficient.

The Determine the kinetics of chloride diffusion allows set up the onset of corrosion of steel in reinforced concrete, to thereby estimate her durability of the structure. The fact establish a model describing the phenomenon of diffusion of chlorides in the RAC, based on previously reported diffusivity values, this could help reduce time and costs in sustainable construction.

Modelling is defined as the process of producing a prototype which is a representation of the construction and operation of a system of interest. Furthermore, the simulation of a system is the operation of the system model itself. The contribution of these processes is that the model can be reconfigured and experienced; while in general would be impossible, too expensive or impractical to reconfigure and experience in a real system [8].

A technique for the simulation is the Finite Element Method (FEM), which is based on the decomposition of the domain into a finite number of subdomains (elements) for which the systematic approximate solution is constructed by applying the residual variational methods or weighted to [9].

The mechanism of diffusion of chloride in RAC is more complex than that of with Natural Aggregates Concrete (NAC). In general terms, comparing a NAC with RAC, the latter is more porous (caused by old cement paste adhering to the surface of the aggregates), therefore, the microstructure of the area of interfacial transition (ITZ) in RAC will be different from the CAN [10].

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In previous researches [2], have proposed models of a RAC, which defines it as composite material of five phases by treating old and new ITZs as interfaces, new mortar, old mortar attached and original aggregate as continuous phase , as shown in Figure 1

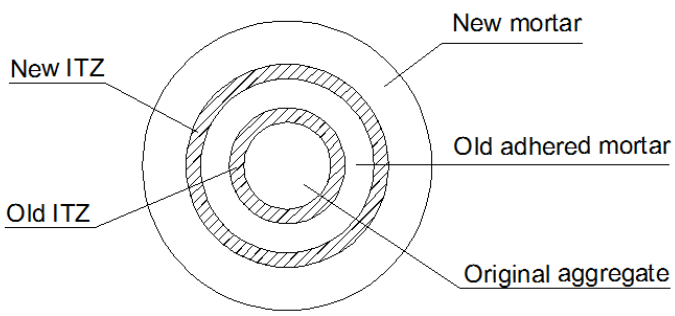

Figure 1 Five-phase composite sphere model, own elaboration from [2].

Moreover, it has also investigated the effect of moisture transport due to the concentration gradient, capillary suction and pressure gradient in the penetration of chlorides in concrete partially saturated [11], and the experimental results showed that the moisture transport has no effect on the penetration of chloride and chloride concentration gradient is the mechanism most dominant for the penetration of chloride into the concrete.

II. Methodology

Is modeled a RAC as a material composed of five phases (old and new ITZ, old and new mortar, and original aggregate). The diffusivity of the above components, will be collated and compared with the reported in previous studies [2, 3], in order to clarify and provide validation of this phenomenon of diffusion of chlorides in a RAC.

A. *Materials and equipment*

The basic elements necessary to carry out this investigation were the following specifications: computer with operative system windows 7 64-bit, 8 GB RAM, and Intel CORE i5-2450M CPU@2.50 GHz with software for modeling and simulation by the finite element method.

Access database and meta-search engines provided by the National Consortium of Scientific Information Resources and Technology (CONRICYT, for its acronym in Spanish) and access through the Autonomous University of Sinaloa.

B. *Modeling process*

A RAC is modeled with only one aggregate (see Figure 2) to evaluate the effects that cause the different variables studied separately with regard to the phenomenon of diffusion. The variables included in this research were: the position where is measured chloride concentration, the thickness of the old and new ITZ, the rate of adhesion of old mortar and the volume fraction of recycled aggregates. For this, it was used the diffusion equation of Fick's second law (Equation 1) and taking into account the perceptions and principles of related previous work [2].

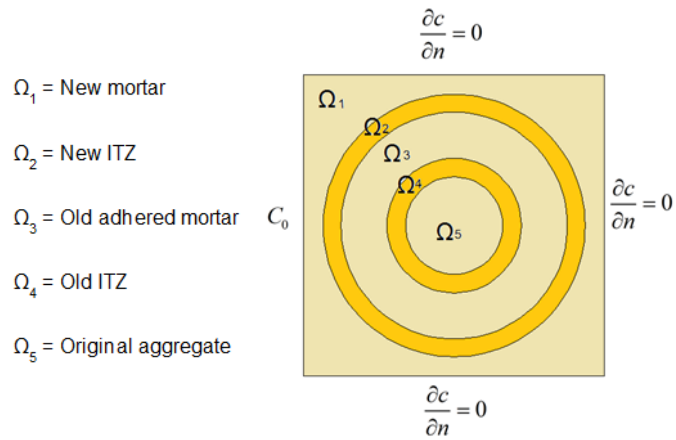

Figure 2 representative model of the problem, domains and boundary conditions.

In the above scheme is positioned in the center of the natural aggregate (Ω_5) surrounded by the old ITZ (Ω_4), immediately the old mortar attached (Ω_3), which in turn is covered by the new ITZ (Ω_2) and finally all covered by the new mortar (Ω_1). The assembly represents than in the left contour has an initial concentration (C_0), and finally the remaining contours are considered provided insulation ($\partial c/\partial n=0$).

Model parameters proposed in previous work are presented [2] in Table 1, which served as the initial basis for defining the general framework of the proposed model; these have the following meaning and implication in the simulation: initial concentration in the boundary of the problem under study; the range of old mortar adhesion is the portion of old mortar adhered around to the original aggregate ; ITZ is the area located between mortar and aggregate, and is usually considered a particular segment with weaker property, the average value of the thickness of this zone is 30 microns, however in this work is considered to 50 microns for computing facility, except for the case IV wherein the effect of the thickness of this area is evaluated.

Table I. Parameters used in modeling [2].

Case	Concentration ($x10^{-1}$ mg/mm^3)	Recycled aggregate shape	Adhesive rate of old adhered mortar (R_{rm})	Thickness of both new and old ITZ (microns)	Recycled aggregate volume fraction (F_{ra})
I	0.03	Round	0.68	50	0.4
II			0.12		0.3, 0.4, 0.5 0.6
III			0.04, 0.12, 0.2, 0.28, 0.36, 0.44, 0.52, 0.6, 0.68, 0.76, 0.84, 0.92		0.4
IV			0.68	20, 35, 65	

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Moreover, in addition to the above parameters that define the model, have also been used the following parameters that define the coefficients of diffusion of each phase of the model (see Table II).

Table II. Parameters used in modeling [2].

Phase	Diffusivity ($x10^{-6}$ mm^2/s)
Original aggregate	0.2
Old ITZ	367.75
Old mortar	23
New ITZ	73.55
New mortar	5

To corroborate the effect of the position, the volume fraction of recycled aggregate (F_{ra}), the adhesive rate of old mortar (R_{rm}) and the T_{ITZ}, the cases I, II, III and IV of the Table I were used respectively, resulting in the model to be used and presented in Figure 3; in which it is noted that the origin is positioned in the center of the model, and the radii of each phase (R_1, R_2, R_3, R_4) is determined from this.

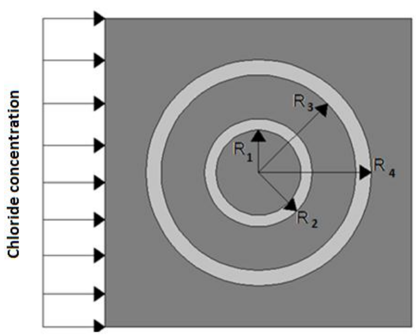

Figure 3 Model of RAC of five phases with their radios.

In addition of the previous model, was assessed the variation of the same through using another model of type cubic face-centered (see Figure 4) in order to evaluate the effect of continuity and discontinuity of the ITZ. This model is defined with the hypothesis that the ITZ can in a RAC, be or not be interconnected between them, and therefore closer to reality simulation of the behavior of these concrete.

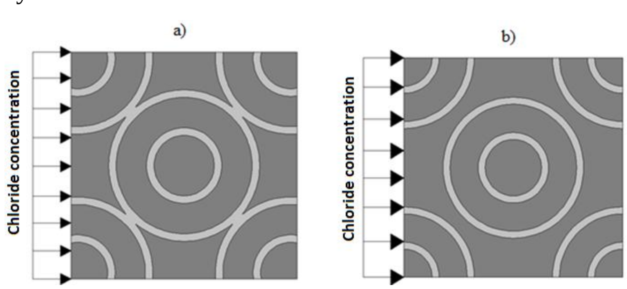

Figure 4 cubic face centered Model a) ZTI continuous b) discontinuous ZTI.

Finally, a more complex variant of the model is performed, which were disposed various aggregates together with order to close more the simulation study to reality. This model was disposed through theoretical circular aggregates with variation of the particle size distribution; the resulting model is representative of a square cross section of 15x15 cm (see Figure 5).

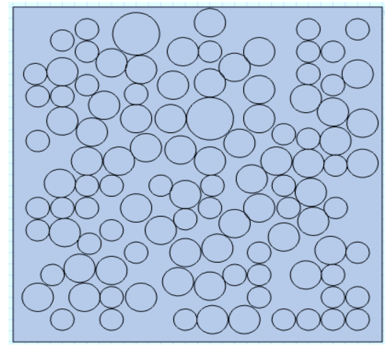

Figure 5 Geometry Model 15x15 cm.

III. Results and discussion

For the initial modeling of a single aggregate, in Figure 6A the distribution of concentration is observed. In Figure 6B a drop is observed in the concentration of the curve where Y = 0 and this is due to that the curve passes through the center of the original aggregate and this can be considered an element of less diffusion than the rest of the other phases . It is also noteworthy that despite the drop in concentration, variation when X = 5 mm is very similar in Y = 0, 2.5, and 5 mm.

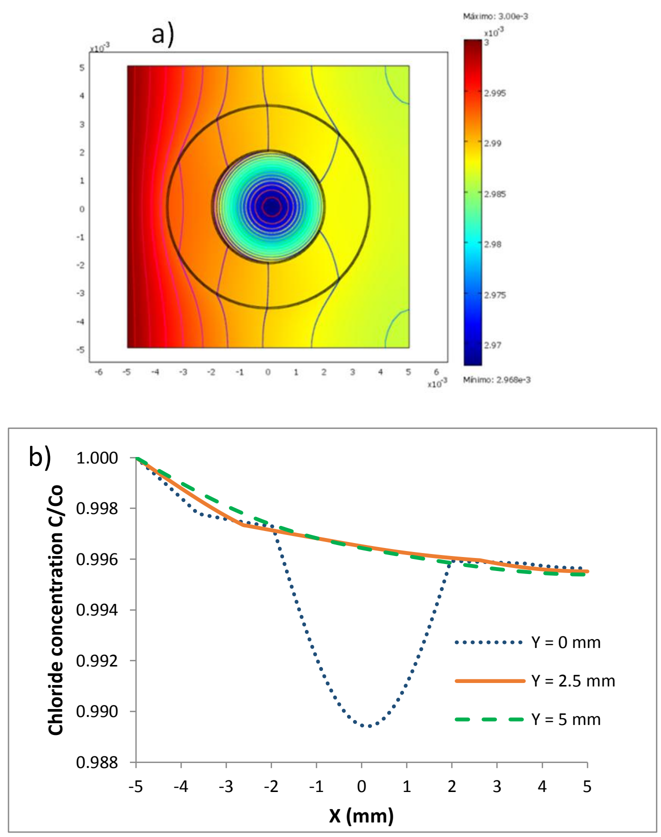

Figure 6 Position effect.

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With respect to the chloride concentration of studied model, Figure 7 shows the decrease of this with respect to increased F_{ra}. Interpreting than the valleys of the profiles is due to the original aggregate restricts diffusion of chloride ion, and these are directly correlated with increased Fra; with the pass of a Fra = 0.3 to 0.6 produces in the chloride diffusivity a considerable decrease

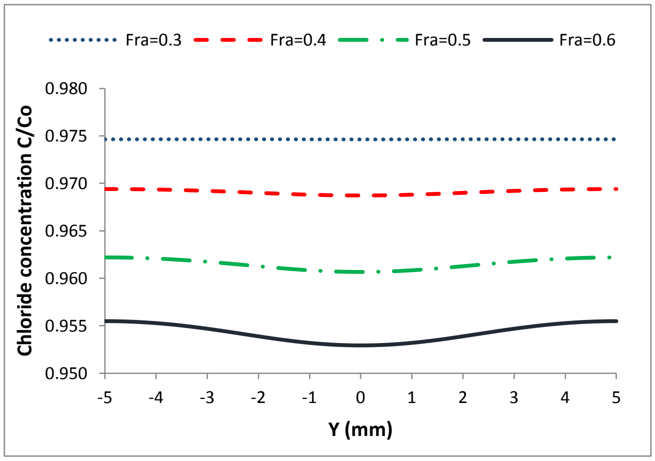

Figure 7 Effect of the volume fraction of the aggregates.

As shown in Figure 8, the distribution curve is concave downward when R_{rm} is less than 0.44 and is convex upward when R_{rm} is greater than 0.44, this behavior is due to that the R_{rm} is the smaller, the original aggregate is more large so that concentration decreases, which shows that the adhesive rate of the old mortar influences the behavior of the diffusion of chloride in a RAC, so that when R_{rm} value is larger, the chloride concentration is bigger.

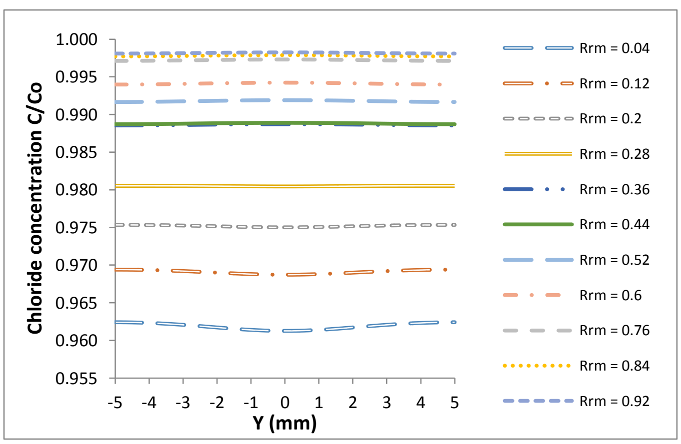

Figure 8 Effect of adhesive rate of old mortar.

Figure 9 shows that the distribution of the concentration of chloride is increased when the thickness of the ITZ is larger, so that the diffusivity is correlated with the increased thickness of the ITZ. This is consistent with the fact that this area is usually considered as more porous and mechanically weaker of a concrete.

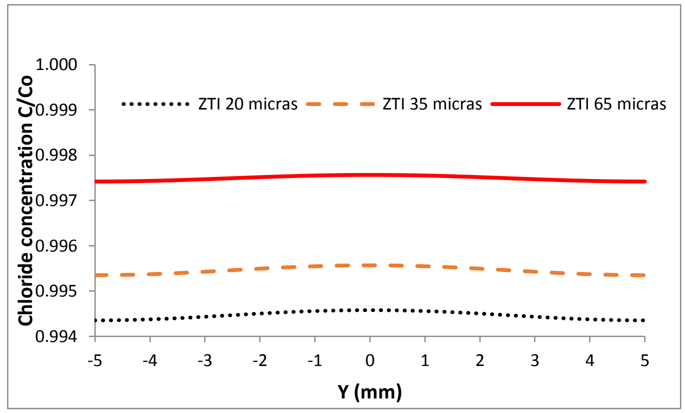

Figure 9 Chloride concentration profile as a function of thickness of the ITZ.

In the case of modeling with ITZ continuous or discontinuous, can be seen in Figure 10 that when the ITZ are continuous, chloride concentration is higher than when the ITZ are discontinuous; this allows to confirm that a concrete can be more durable if is reducing the ITZ continuous.

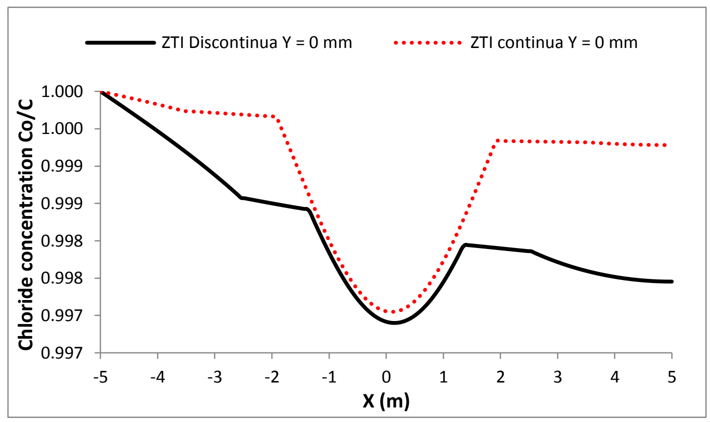

Figure 10 Comparison between model with ITZ continuous and ITZ discontinuous.

Model results of several aggregates are shown in Figure 11, comparing the concentration of chloride between a model with a normal size distribution of aggregates with one ½ "and ¾", in it is observed that the concentration between the models have a variation nonsignificant, to present a similar trend. This may mean that the effect of the aggregate's distribution is not significant in the diffusivity.

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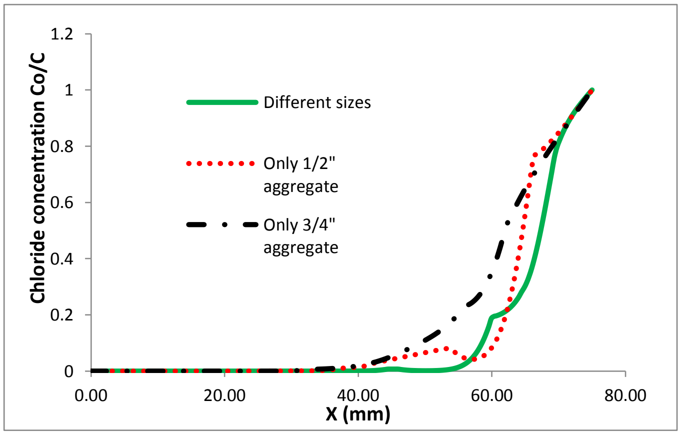

Figure 11 Comparison of various aggregates model with cross section of 15x15 cm.

IV. Conclusions

A recycled aggregate surrounded by mortar can be understood as composite material consisting of five phases.

Usually, the concrete is considered as a homogeneous medium of diffusion characterized by an apparent single value; however, in the model used for RAC can predict the propagation diffusion in the time of a more complex way and not homogeneous.

The diffusivity decreases with increasing of volume fraction of the aggregates, but it heightens with increased of adhesion range of old mortar and with the ITZ thickness; finally, it verifies that the chloride diffusion may become greater when the ITZ is interconnected or are continuous.

The distribution of aggregates does not has significant variation by showing a similar trend in the evaluated models.

Acknowledgment

The authors express thanks to: research project S-01117 from CTT-UPC, to FIM-UAS and to the scholarships program for Master Degree studies by CONACYT.

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