The Key Role of Surface Concentration in the Modelling of Chloride Penetration into Concrete

C. Andrade[1], M. Castellote[1], F. Tavares[1], I. Petre-Lazars[2], M.A. Climent[3]
[1]*Institute of Construction Science "Eduardo Torroja" (CSIC), Madrid, Spain;*
[2]*EDF-Marseille, France;* [1]*University of Alicante- Alicante, Spain*

ABSTRACT

Modelling of chloride penetration into concrete has been developed extensively during the last few years due to the need to predict evolution of existing structures and try to design more resistant elements. These models are based in assuming diffusion as the main mass transport mechanism, but they differ in the input and assumed parameters. As no calibration at long term has been possible yet, the suitability of the different models cannot be verified. A manner to overcome long term uncertainty is to compare the different models available in order to gain understanding, with the comparison of their predictions. In present paper comparison among different available models is presented based in the comparison of the scatter of a profile predicted from another one at an earlier age. The results indicate that it is not the D value applied which makes the differences between the models, but the value of the Surface Concentration, C_s, assumed at the second age. The risk of failure in the prediction is higher as higher is the difference between real and predicted C_s. A proposal is made to use the factor ($C_s \cdot D$) as the controlling parameter of the process.

Keywords: chloride, models, comparison, diffusivity by chloride concentration.

1. INTRODUCTION

Modelling of the service life of concrete structures is becoming one of the objectives with higher interest due to the economical consequences of premature repairs (1). In particular reinforcement corrosion is the most deleterious process regarding concrete durability and in consequence, is the deterioration mechanism more modelled.

The types of models available in the literature, although not very numerous, differ mainly: a) in the boundary or initial conditions (2), b) in considering more than one penetration mechanism (3-9) or c) in the "age factor" taken for the evolution of the variables (10). Thus, starting by the fundaments of more simple to more complex, there are models based in (11-15) empirical "data fitting" , other models use the quadratic relation between the penetration of the aggressive front and the time (square root law), other models use the classical solution of Fick's Second law having the "error function" in the resulting expression while other prefer numerical methods to compute the non steady diffusion and finally there are "multiescale" models considering the progression from the mixing of concrete raw materials, the development of the microstructure to end with the corrosion of the reinforcement. In summary, the offer of models is very diverse which can result in confusion of the user, in particular due to the lack of verification of the predictions by these models in real structures or the calibration of them with the behaviour in real conditions.

In spite of this lack of proper validation application of the models by design engineers is increasing and therefore it is urgent to look for some kind of cross checking of their ability to model the chloride penetration in order to give some guidance on the expected deviations from reality.

Present paper presents a kind of calibration of models on chloride penetration. The method selected has been to use two chloride profiles measured at two different ages in the same structure or specimen. The second profile has to be predicted from the first one. Deviations from the real profile are used to assess the reliability of the methods. Although the second profile is relatively closed to the first one, the exercise has enabled to find, in author's opinion, interesting conclusions for the sake of the modelling of service life.

2. EXPERIMENTAL CONDITIONS

For the sake of present paper 3 chloride profiles and 8 models have been selected. The chloride **profiles** at two ages are presented in figure 1. The first, figure 1a (series 1-case 1), corresponds to a real structure located in a beach suffering the tides and seasonal variations of temperature. This profile has a maximum in the concentration beyond the concrete surface. The second, 1b (series 1-case 3), is taken from the same structure but in another concrete type and environmental conditions: it does not present a maximum. The third (series 2-case 1) corresponds to a laboratory specimen submitted to controlled conditions of temperature and humidity. The exercise consists in predicting the profile at the second age using the Diffusion coefficient obtained from the profile at the first age.

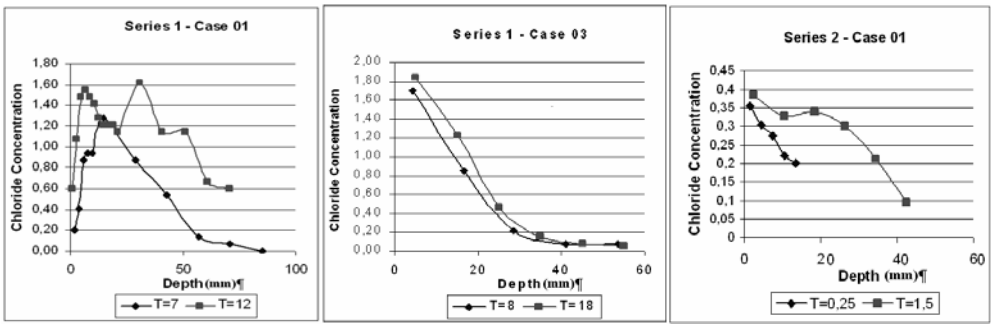


Figure 1. Profiles used in the exercise: The diamonds show the chloride profile at the earlier age and the squares show the one at later ages being T= age in years

The **models** selected were five numerical and three analytical, including the standard “error function” (model 2). In the figures the line noted as “Model 0” is the real profile at the second age, that is, the reference. The models selected are briefly described in Table 1.

Model characteristic	*Basis of the Model*	*Time dependence of D or equivalent*	*Time dependence of C_s*	*Chloride binding*
Model 1	Square root, does not need a Diffusion coeff.	Yes	Yes	Yes
Model 2	Classical error function	Yes	Yes	Apparent D
Model 3	Fick’second Law, theoretical	No	No	Apparent D
Model 4	Fick’second Law, empirical	Yes	Yes	No
Model 5	Fick’second Law, numerical	Yes	Yes	Yes
Model 6	Fick’second Law, numerical	No	Yes	Yes
Model 7	Fick’second Law, numerical	Yes	Yes	No
Model 8	Fick’second Law, analytical	Yes	No	Yes

Table 1. – Some characteristics of the models used for the comparison.

They have been selected to represent a range of different assumptions. The models are fitted to the profile at the earlier age and the Diffusion coefficient values obtained are used for the prediction of the profile at the second age.

Criteria for the comparison

The method used for the comparison is based in the bias of the predicted profiles (areas encountered by the profiles) of each model with respect to the real one. This comparison of areas enables to quantify in some manner the deviation. Thus, each model can be compared with the measured profile by comparing the value of the Area between the model and the real profile at the second age in a certain range of depth (from X1 to X2 as showed in the figure 2). The values $S1 = |A1| + |A2|$ and $S2 = A1 + A2$ are used to compare the addition of the areas A1 and A2 in absolute value (S1) or being positive or negative with respect to the real profile (S2). Thus, S1 gives the information about how near the model is from the measured data and S2 gives the information about how higher or bellower the model is, compared with the measured data.

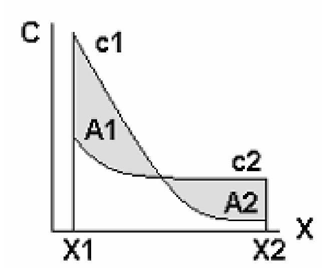


Figure 2 – Diagram of the example of comparison of areas between the real profile at the second age and the predicted profile by each model tested.

where :

c1 : measured curve (total chlorides)

c2 : model curve (total chlorides)

A1 : area between the measured curve and model curve which measure data is lower (negative sight)

A2 : area between the measured curve and model curve which measure data is higher (positive sight)

X1, X2 : validation range. The validation range adopted is:

- X1 = 10mm (this value was adopted to not take into account the skin effect)
- X2 = 50mm (except in the situation when the depth of the measure data is lower).

C, X : concentration and depth axis respectively.

The C1 and C2 profiles are fitted to the points in the profile using the cubic spline interpolation of measured C1 and model C2 data points.

3. RESULTS

Figure 3 depicts the comparison of the predicted profiles of all the models of the Series 1 case 1. The models 1 and 7 seem to be that picking best the real profile. The rest of the models obtain profiles too conservative (too low chloride concentration at a certain depth) with respect to the real profile. This information is better illustrated by figure 4 where the representation of the calculated S1 and S2 is given.

There are large differences in the prediction of each model tested. Roughly there are some that have correctly predicted the change in C_s and therefore they fit better in the Real Profile, while other, not having picked the new C_s, they predict very out of the real profile the deepest part of the profile.

For the Series 1 – Case 2 (figure 5) the best seems model 3 and after Model 7. In present case Model 1 deviates very much at a certain depth. All the rest have well predicted the value of Cs and then the prediction is reasonable good.

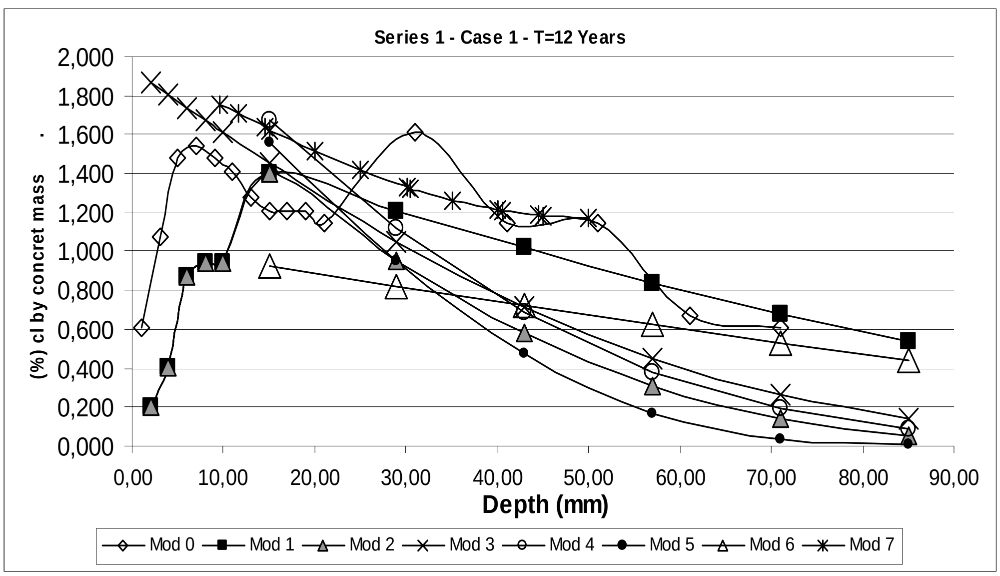
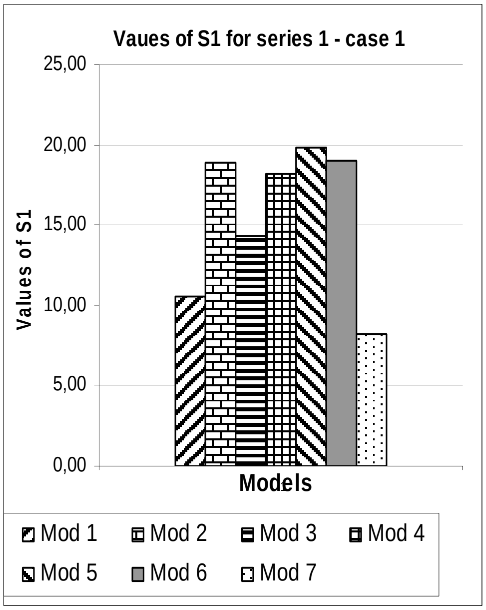


Figure 3. Series 1/Case 1: Comparison of the results of the prediction of the second profile from the values obtained by each model by fitting the profile at the earlier age.

For Series 1 – Case 3 (Figures 5 and 6) the most accurate model is Model 2. In particular Model 4 deviates very much from real C_s value although the prediction of the deepest part of the profile does not result too badly.



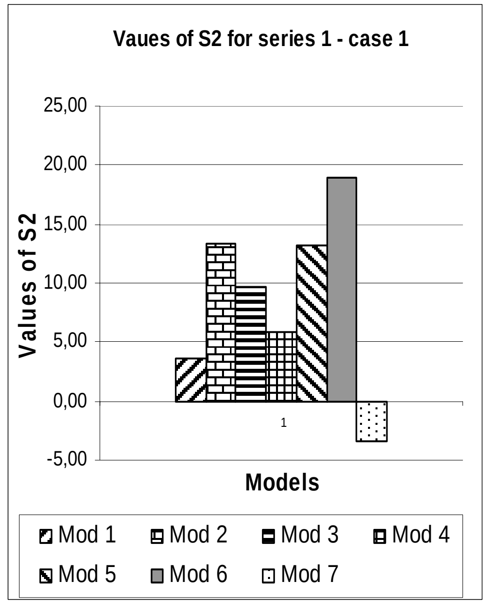


Figure 4. - Values of S1 and S2 which enable to deduce that the best fitting is made in present case by models 1 and 7.

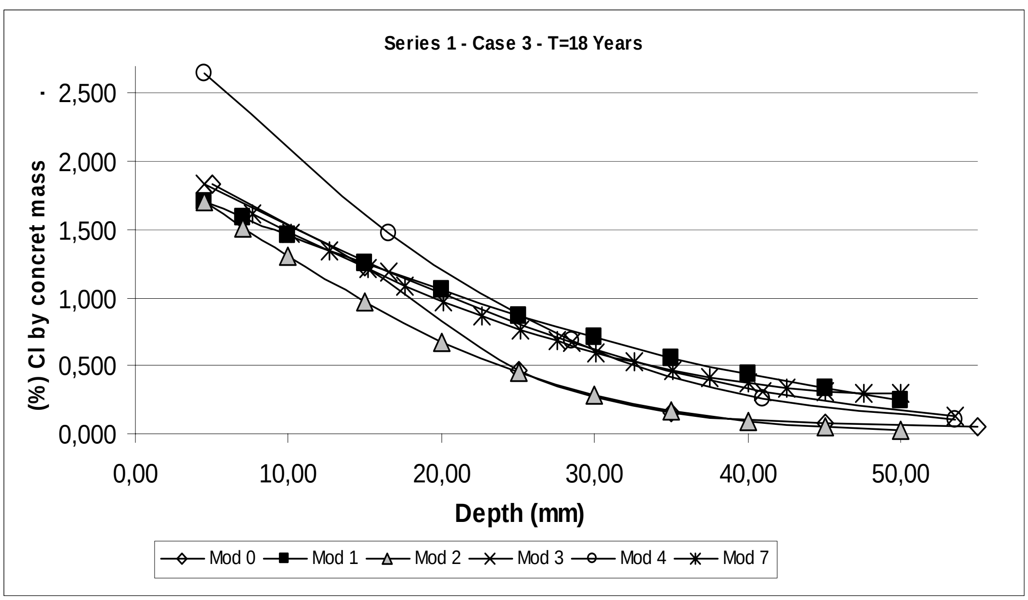
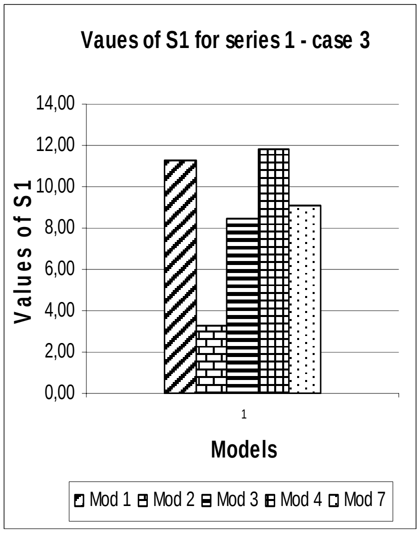


Figure 5 Series 1 - Case 3: Comparison of the results of the prediction of the second profile from the values obtained by each model by fitting the profile at the earlier age.



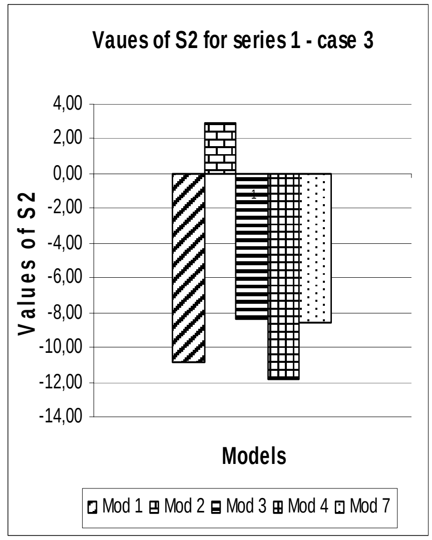


Figure 6 Values of S1 and S2 which enable to deduce that the best fitting is made in present case by model 2.

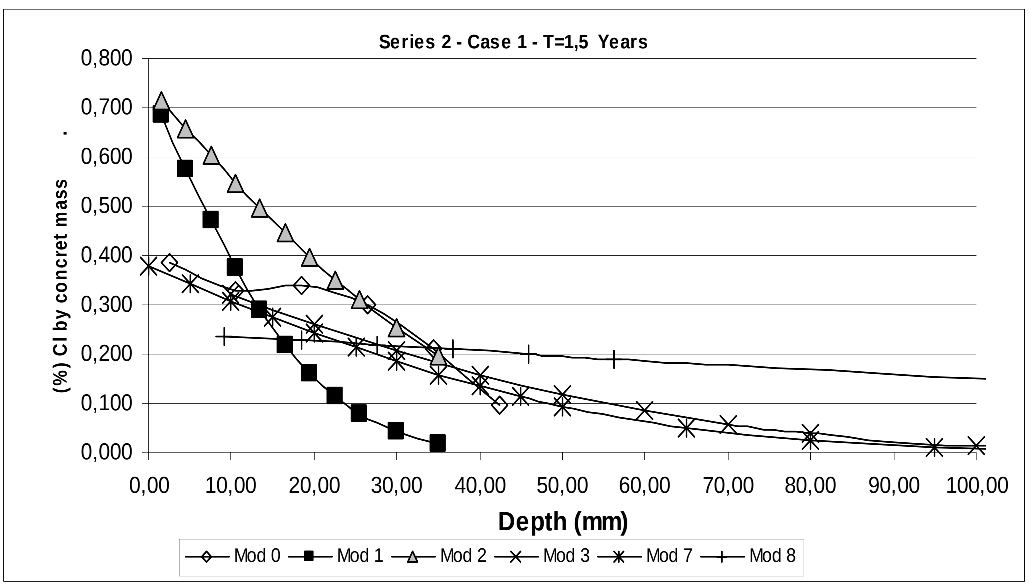


Figure 7 Series 2 - Case 1: Comparison of the results of the prediction of the second profile from the values obtained by each model by fitting the profile at the earlier age

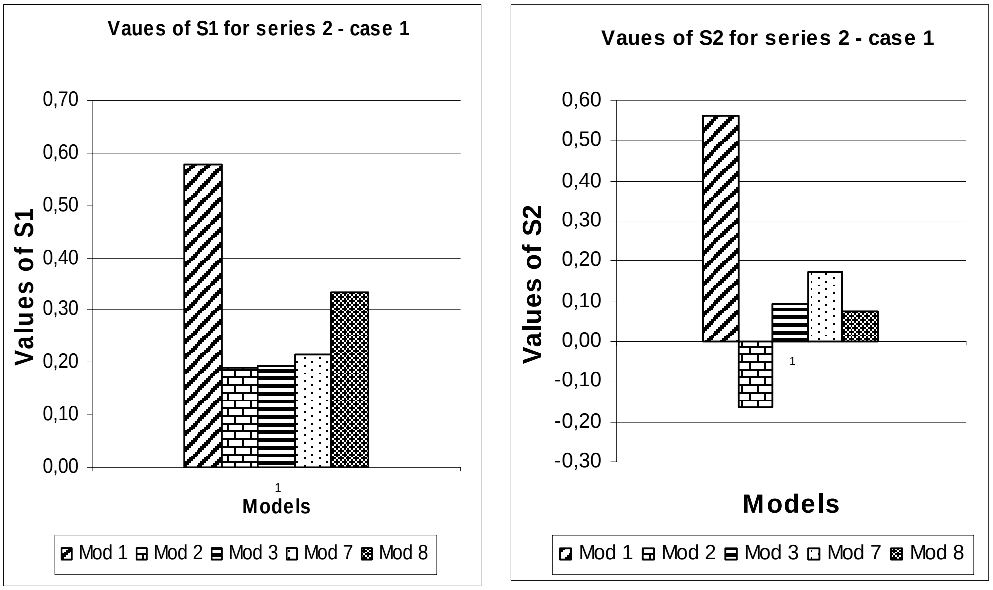


Figure 8 Values of S1 and S2 which enable to deduce that the best fitting is made in present case by models 2 and 3 being Model 1 very deviated.

For the <u>Series 2: - Case 1</u> the best models resulted Model 2 and Model 3 being Model 1 very deviated from reality, Looking at the results in a more integral manner it can be noticed that when the models pick correctly the value of the surface concentration C_s, the prediction has a high probability of being more correct than when the calculations of the models consider values of C_s very far from the reality.

4. DISCUSSION

In present exercise the most important result is that any of the models tested have shown to be consistently more accurate than the other. Some have been good at least in three occasions (Models 1 and 2). Other have been never good (Models 5 and 6) but those being able to predict well one case are not good in other occasions. This is interpreted to be due that the reality is very variable and that the process of chloride penetration is not purely diffusive, depending on many circumstances how the evolution is proceeding, even in laboratory conditions (Series 2-case 1).

Studying more in detail the different models used in the exercise, almost all of them are based in considering a quadratic relation between depth reached by a certain chloride concentration and the time passed. On the other hand, apart from the mathematical tool for making the calculations, the different models differ mainly in:

- The main parameter controlling the diffusivity (usually the Diffusion coefficient)
- The binding ability by cement phases
- The law introduced for accounting on the decrease of D with time
- The law of variation of C_s with time

In order to analyze the results it is necessary to consider the effect of the C_s and that of the decrease of the D value with time. As an example, and using the standard “error function solution”, regarding the effect of the surface concentration, in figure 9 a chart is given, in which, for different depths (three curves at x=2, 3 and 4 cm), pairs of values of D and C_s satisfy the condition of a determined concentration of chloride ions (theoretical chloride threshold value) at a specified time (50 years). This figure illustrates very well the crucial importance of the $C_{s,}$ because if the models do not pick it correctly, the deviations from the reality can be very high.

However, the evolution of C_s with time and type of environment has not attracted so many studies in the past. Perhaps this lack of models for C_s is due a certain lack of definition of what means this parameter and to the fact that the surface concentration is not always the maximum of the profile at the surface. In any case, it seems that in order to improve the prediction ability of chloride models in the future, more research has to be devoted to study the evolution of C_s as it is the most crucial parameter in the prediction.

Due the uncertainty on the C_s, it seems of interest to consider for concrete specification of diffusivity threshold values, a new parameter: the multiplication of $(D \cdot C_s) = \delta$ = diffusivity by chloride concentration. This parameter will enable to compare tests made in different conditions.

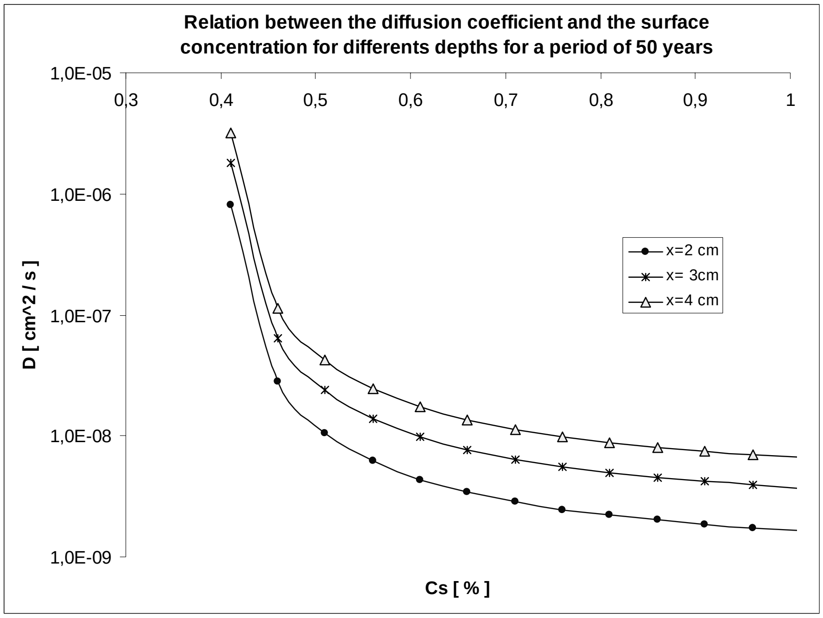


Figure 9.- Pairs of values of D and C_s that satisfy the condition of 0.4% Cl^- at 50 years for different depths.

CONCLUSIONS

In present paper an exercise to study the differences in the predictions made with different models is presented. It has comparative purposes in order to illustrate the reliability of the models. The predictions have been made at relative short term (not much difference between first and second profiles). The calibration at long term will be necessary. The most relevant conclusions deduced are:

1. The methodology used to make the benchmarking has resulted very helpful to compare the models. S1 is an indicator informing on the accuracy and S2 informs on how conservative the prediction is. Combination of both quantities serve to appraise how appropriate are the predictions.
2. The predictions from the models taken as examples differ considerably.
3. With respect to the sensitivity of the models to the variation of the constitutive parameters, it seems that the most influencing is the C_s value. On the ability of the models to predict, all of them, do or not, depending on the value of C_s calculated.
4. The values of D are much less influencing than the C_s values.
5. Finally, a new mode of approaching the prediction is made by proposing a parameter that encounters the whole phenomena by being the multiplication of ($D \cdot C_s$). This parameter has been named δ = diffusivity by chloride concentration.

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