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2 - D MODEL FOR CARBONATION AND MOISTURE/HEAT FLOW IN POROUS MATERIALS

Anna V. Saetta[1], Bernhard A. Schrefler [2] and Renato V. Vitaliani [2]

(1) Dipartimento di Costruzione dell'Architettura
Istituto Universitario di Architettura - Tolentini 191 - 30135 - Venezia - Italy

(2) Istituto di Scienza e Tecnica delle Costruzioni
Università di Padova - Via Marzolo 9 - 35131 - Padova - Italy

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ABSTRACT

The previously-published one-dimensional finite element model for the analysis of the carbonation mechanism is extended to two-dimensional problems. The governing equations for the propagation of aggressive agents through concrete are rewritten for two-dimensional domains. A comparison is made with the one-dimensional model and some examples are developed to test the method. Finally, the study of a reinforcing bar placed at the corner of a concrete structure is presented in detail to show that the proposed numerical model is able to demonstrate the effects of the multidimensional moisture, heat and carbon dioxide transport through concrete.

Introduction

The analysis of deterioration mechanisms in concrete structures is of great concern in many fields of civil engineering. At present, predicting the durability of concrete in expensive structures such as waste containment plants is an important and hotly-debated issue.

Concrete deterioration generally stems from more than one cause, and it is usually very difficult to identify the initial reason why the concrete has no longer able to resist external or internal attack. However, published literature (e.g., [1] to [7]), shows that the most important cause of deterioration is corrosion of the reinforcing steel, followed by the effect of frost in cold climates, and the physical-chemical effects of external as well as internal phenomena on the hydrated cement paste. Damage to concrete structures due to corrosion of the reinforcing steel is generally apparent from the loss of concrete cover and from the loss of the bond between the concrete and steel. Such problems arise because the quality of the materials used and construction methods have not improved over time, whereas the environment has become more aggressive. Obviously, a marked corrosion does not develop unless the concrete is permeable from the beginning or becomes permeable in service, due to microcraking consequent to environmental effects. In fact, if the concrete quality and cover thickness are adequate, the three basic conditions for corrosion, i.e., iron available in the metallic state for the anode process, oxygen and moisture available for the cathode process and a low electrical resistivity for the electron flow, do not occur during service life. With regard to the anode process, the alkalinity of the cement paste near the steel must be reduced and the protective film of iron oxides or hydroxide must be destroyed before metallic iron becomes available (first condition). In saturated conditions with moisture available, the coefficient of oxygen diffusion is very low and oxygen is not readily available for corrosion; on the other hand, in dry conditions, when gas diffusion is facilitated, moisture is not available for the cathode process; moreover, dry conditions are inappropriate for a reduction in electrical resistivity.

Much research has been devoted to the identification of the influence of various factors (e.g., cement type and content, water/cement ratio, depth of cover, crack widths, environmental conditions) on corrosion phenomena, e.g., [1] to [3]. One of the most practical models to study and predict the corrosion process splits the duration phenomenon into two different periods: the corrosion initiation and propagation periods [4], which are influenced by different parameters. The corrosion initiation period depends essentially on the rate of diffusion of CO_2 (the carbonation process) and chlorides (responsible for depassivation of the steel), while the corrosion propagation period depends on the rate of diffusion of oxygen and water. By assuming this schematization of the corrosion process, the durability of a concrete structure is preserved, without needing intervention or maintenance, providing the time it takes to reach the start of the corrosion propagation period is close to the service life time of the structure.

The term "carbonation" of concrete means the chemical reaction between carbon dioxide in the air and hydration products of the cement. The main consequence of carbonation is the drop in the pH of the pore solution in the concrete from the standard values between 12.5 and 13.5, to a value below 9 in the fully carbonated zones, so that the passive layer that usually covers and protects the reinforcing steel from corrosion becomes unstable (first condition for corrosion). The most dangerous range of relative humidity for carbonation is 40% to 80%, since the carbonation reaction calls for the presence of water, while under higher atmospheric humidity the diffusion of carbon dioxide will be inhibited by the water that has filled the pores (second and third conditions for corrosion).

Extensive work has been done in recent years on the theoretical and experimental analysis of carbonation in relation to durability, but most of the papers dealing with the numerical simulation of deterioration phenomena, like most of the existing service life models, only consider the effect of one variable at a time, making it difficult to take into account any effects of temperature and humidity, which can often be significant.

In this context, previous works by the present authors [8 to 10] dealt with defining a numerical model to predict the initiation of corrosion due to the carbonation process. Such a model, based on the works of Houst and Wittmann [11, 12] and of Bažant et al. [13] and Bažant [14], considered the interaction between many processes, namely CO_2 diffusion, moisture and heat transfer, the mechanism of $CaCO_3$ formation and the availability of $Ca(OH)_2$ in the pore solution due to its transport by water movement. It was restricted to the one-dimensional case, but can also be successfully applied to investigate the deterioration of many concrete structures. However, for particular situations, such as the case of a steel bar placed in the corner of a building, the one-dimensional model underestimates the actual depth of carbonation.

The purpose of the present paper is to extend the theory presented in [8] to two-dimensional problems in order to gather the effects of multidimensional attack on the corner reinforcing bars of concrete structures and to simulate all the phenomena involving the multidimensional transport of moisture, heat and carbon dioxide through concrete.

The difficulties frequently encountered in the numerical simulation of deterioration phenomena, i.e., in dealing with the non-linearity and the coupling of the differential transport equations, are solved by means of a finite-element procedure which proves very reliable and effective. The two-dimensional study of the corner of a typical concrete structure is performed and compared with the one-dimensional analysis. Some numerical tests in different environmental conditions are also presented.

A complete service-life model might also incorporate the synergetic effects of two or more simultaneous corrosive elements (e.g., chloride attack and carbonation), and this will be the subject of a later work.

Field equations

Assuming the existence of carbonation reactions, the governing differential equation of moisture, heat and carbon dioxide flow in a two-dimensional porous material can be written in the same form as in Ref. [8]:

$$\frac{\partial h}{\partial t} = \operatorname{div}(C \operatorname{grad} h) + \frac{\partial h_s}{\partial t} + K\frac{\partial T}{\partial t} + \frac{\partial h_c}{\partial t} \tag{1}$$

$$\rho C_q \frac{\partial T}{\partial t} = \operatorname{div}(b \operatorname{grad} T) + \frac{\partial Q_h}{\partial t} + \frac{\partial Q_c}{\partial t} \tag{2}$$

$$\frac{\partial g}{\partial t} = \operatorname{div}\left[D_g \operatorname{grad}(g)\right] - \frac{\partial g_c}{\partial t} \tag{3}$$

but here the relative humidity h, the temperature T and the carbon dioxide concentration g are all functions of x, y and t. The diffusivities of the relative humidity C and carbon dioxide (CO_2) D_g are assumed to be strongly dependent not only on pore humidity, but also on temperature, on the degree of cement hydration (i.e., on the equivalent curing time), and on the relative calcium carbonate content c to take into account the reduction of the porosity due to carbonation. These latter two factors produce a slowing of the carbonation phenomenon for long-term results. The equations for the diffusivities are:

$$\begin{aligned} C(h,T,t_e,c) &= C_{28} \cdot F_1(h) \cdot F_2(T) \cdot F_3(t_e) \cdot F_4(c) \\ D_g(h,T,t_e,c) &= D_{g28} \cdot F_1^*(h) \cdot F_2(T) \cdot F_3(t_e) \cdot F_4(c) \end{aligned} \tag{4}$$

where C_{28} and D_{g28} are the diffusivities in standard conditions, after 28 days. The functions:

$$F_1(h) = \alpha_0 + \frac{1-\alpha_0}{1+\left[(1-h)/(1-h_c)\right]^n} \qquad F_2(T) = \exp\left(\frac{Q}{RT_0} - \frac{Q}{RT}\right) \tag{5a}$$

are semi-empirical expressions, proposed by Bažant [13, 14]. The other functions have been obtained on the basis of the available references on the carbonation phenomenon [1, 11, 12] and the results of experimental tests:

$$F_1^*(h) = (1-h)^{2.5} \qquad F_3(t_e) = \chi + (1-\chi)\sqrt{\frac{28}{t_e}} \qquad F_4(c) = 1 - \zeta \times c \tag{5b}$$

In particular $F_1^*(h)$ takes into account the decrease in CO_2 diffusivity as the relative humidity increases, $F_3(t_e)$ the slowing of the diffusion as the degree of hydration of the cement proceeds and $F_4(c)$ the decrease in CO_2 diffusivity due to the reduction in the porosity caused by the carbonation. The graphic representation of these functions is given in figure 1.

The evaluation of the free parameters in Eqs. (4) to (6) is based on the results of experimental tests carried out on different specimens, using both available data and data provided by ad hoc laboratory tests. It is worth noting that such parameters depend on the features of the concrete (i.e., mix design), not on exposure conditions, so the model allows for the analysis of different types of external condition for the same concrete, i.e., by using the same parameters.

Moreover, [8], the last terms in eq.(1), (2) and (3) have the following meaning:

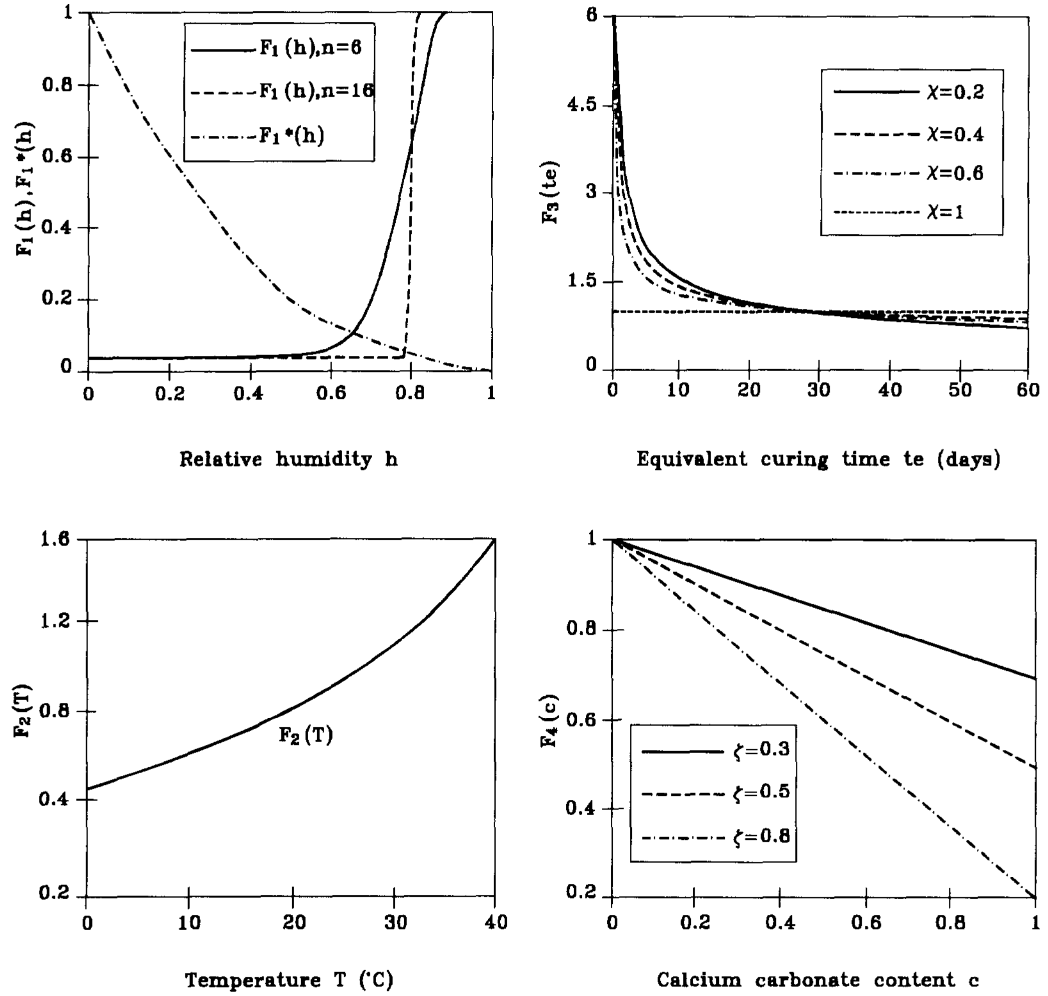

FIG. 1

Basic tendencies given by equations (5a) and (5b) in terms of the variables h, T, t_e and c

- $\partial h_c/\partial t = \alpha_2 \partial c/\partial t$, $\partial Q_c/\partial t = \alpha_3 \partial c/\partial t$, $\partial g_c/\partial t = \alpha_4 \partial c/\partial t$ are respectively the changes in relative humidity, temperature and CO_2 concentration due to carbonation per unit of time;
- α_2, α_3, α_4 are non-dimensional parameters that vary between 0 and 1, according to the features of the concrete, like the parameters introduced by Wittmann, [11]; these parameters are calibrated by means of experimental results [8, 9, 11, 12];
- $\partial c / \partial t$ is the rate of carbonation given by:

$$\frac{\partial c}{\partial t} = v = \alpha_1 \times f_1(h) \times f_2(g) \times f_3(c) \times f_4(T) \tag{6}$$

In this equation α_1 is a non-dimensional parameter that depends on the influence of the features of the concrete on the rate of reaction, and the functions $f_1(h)$, $f_2(g)$, $f_3(c)$ describe the influence of water, carbon dioxide, degree of carbonation c and temperature on the process of calcium carbonate formation. These functions are defined in more detail in [8].

The model

In this study, the standard finite element method was applied both in time and in two-dimensional space. The system of coupled ordinary differential equations in time that governs the phenomena is as follows [8]:

$$\begin{aligned}
&\mathbf{Q}\mathbf{h}+\mathbf{I}\frac{d\mathbf{h}}{dt}-\mathbf{TH}\frac{d\boldsymbol{\mathcal{T}}}{dt}-\mathbf{CH}\frac{d\mathbf{c}}{dt}-\frac{\partial\mathbf{HG}}{\partial t}=0\\
&\mathbf{L}\mathbf{g}+\mathbf{I}\frac{d\mathbf{g}}{dt}+\mathbf{CG}\frac{d\mathbf{c}}{dt}=0\\
&\mathbf{I}\frac{d\mathbf{c}}{dt}+\mathbf{S}\mathbf{c}-\mathbf{CJ}=0\\
&\mathbf{TR}\boldsymbol{\mathcal{T}}+\mathbf{TS}\frac{d\boldsymbol{\mathcal{T}}}{dt}-\mathbf{CT}\frac{d\mathbf{c}}{dt}-\frac{\partial\mathbf{TG}}{\partial t}=0
\end{aligned} \tag{7}$$

where **h**, **c**, **g** and $\boldsymbol{\mathcal{T}}$ are respectively the discrete relative humidity, carbonate concentration, relative carbon dioxide concentration and temperature nodal vectors; the matrices of diffusivity for relative humidity, carbon dioxide and heat flow are defined as:

$$\mathbf{Q}=\int_{(V)}(\nabla\mathbf{N})^T\mathbf{C}(\nabla\mathbf{N})\,dV \qquad \mathbf{L}=\int_{(V)}(\nabla\mathbf{N})^T\mathbf{D}_g(\nabla\mathbf{N})\,dV \qquad \mathbf{TR}=\int_{(V)}(\nabla\mathbf{N})^T\boldsymbol{\Lambda}(\nabla\mathbf{N})\,dV \tag{8}$$

and the matrices of coupling between the rate of carbonation and the humidity diffusion phenomenon, the carbon dioxide diffusion phenomenon and the heat transfer are respectively:

$$\mathbf{CH}=\int_{(V)}\mathbf{N}^T\alpha_1\mathbf{N}\,dV \qquad \mathbf{CG}=\int_{(V)}\mathbf{N}^T\alpha_2\mathbf{N}\,dV \qquad \mathbf{CT}=\int_{(V)}\mathbf{N}^T\alpha_4\mathbf{N}\,dV \tag{9}$$

S and **CJ** are the matrices representing the influence of relative humidity and temperature at the previous time-step on the carbonation process. For the detailed expression of the other matrices **I**, **TH**, **HG**, **TS**, **TG**, which are the usual matrices of the discretized mass and heat transfer equations, see References 9, 14 to 16.

Numerical examples

Validation tests

Two finite element meshes are used to simulate a one-dimensional diffusion process, with the two-dimensional model, in order to validate the extension of the one-dimensional procedure by reproducing the experimental tests reported in [16]. Eight-noded isoparametric elements are used for both the meshes: the first mesh, 50 mm x 5 mm is made with elements very stretched in one direction; the second, 50 mm x 50 mm, is made with quadratic elements.

The samples of concrete made with Ordinary Portland Cement (OPC) and with a water - cement (w/c) ratio of 0.5, are subjected to three one-dimensional exposure conditions (see [16] for detailed information about the exposure characteristics). Both the two-dimensional finite element meshes are only subjected to flux boundary conditions along the right side and the numerical results obtained with the two meshes are very similar. Comparison with the experimental tests provides excellent results, as shown in table 1, where the experimental and numerical findings, in terms of carbonation depth after two years, are very similar.

Only four of the curing conditions studied in [16] are reported here: A0: curing in air for 28 days; A3: 3 days in a mould and then curing in air for 25 days; W0: 5 days in water and 23 days of curing in air; W3: 3 days in a mould and then 5 days in water and 20 days of curing in air.

TABLE I

Carbonation depth (mm) after 2 years of exposure

	Exposure Conditions					
	External sheltered from rain		*External exposed to rain*		*Internal, controlled-climate*	
Curing	experim.	numerical	experim.	numerical	experim.	numerical
A0	7.5	8.0	2.5	2.6	12.0	12.1
W0	3.0	3.2	1.5	1.5	5.0	5.0
A3	3.5	3.5	1.0	1.3	6.0	5.9
W3	2.5	2.6	1.0	1.0	3.5	3.5

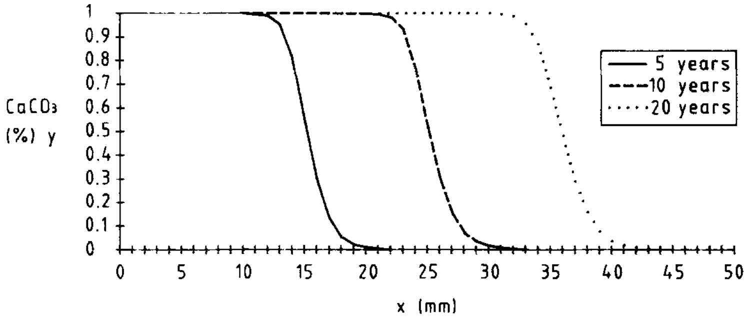

FIG. 2

Carbonation depth reached after 5, 10 and 20 years of exposition

It is worth noting that carbonation is much faster if the structures are sheltered from the rain than if they are exposed to rain. This is because the water in the pores slows down the penetration of carbon dioxide in the concrete, allowing the cement hydration to proceed. It is also apparent that the most dangerous situation is exposure under controlled-climate conditions, see results shown in figure 3 in terms of carbonation depth reached after 5, 10 and 20 years of exposure.

Two-dimensional test

The use of a two-dimensional analysis enables the effect of local shape on the advancing of the carbonation front to be studied. Such an aspect of carbonation should be taken into account in preliminary studies on the durability of certain concrete structures, since a decrease in the time it takes for the carbonation front to reach the reinforcing bars could be significant, and the estimated service life of the structures could drop to an unacceptable level.

Moreover, the possibility of discretizing two-dimensional domains enables the simulation of a surface layer with different characteristics, e.g., an impermeable surface coating, and the analysis of its influence on the progress of carbonation, especially if such a coating is not evenly spread over the concrete surface. The presence of different boundary conditions along the sides of the structures considered can also be easily reproduced with two-dimensional analysis.

The difference between the effects of a one- and a two-dimensional carbonation process can be emphasised by studying the L-shaped mesh of figure 3 (made with OPC, w/c = 0.5, cured in air for 28 days), subjected along two sides to the controlled-climate conditions described in the

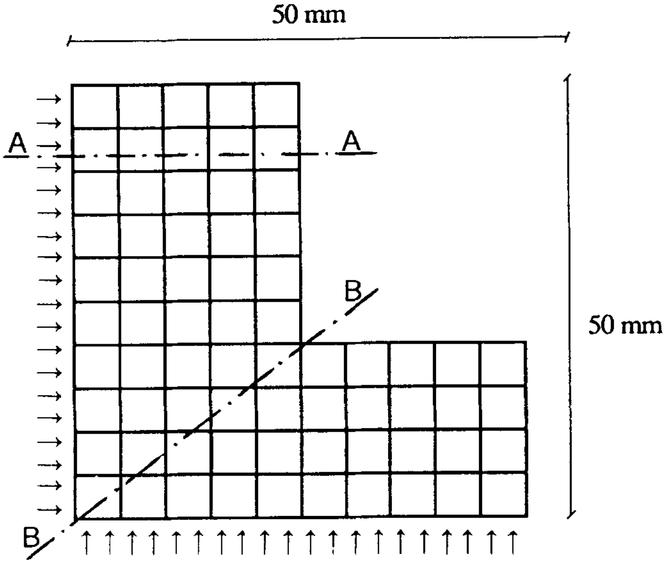

FIG. 3

Finite element mesh for the two-dimensional diffusion process

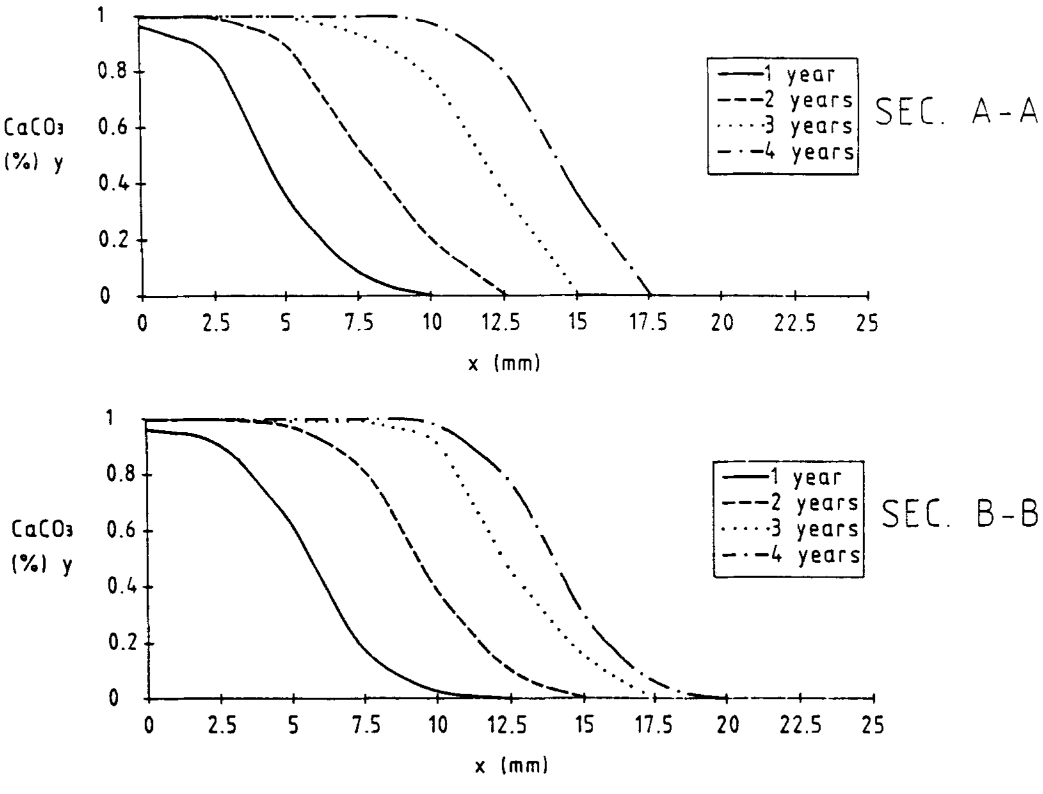

FIG. 4

Carbonation depth along the line of the horizontal section A-A and the diagonal section B-B previous example, and by comparing the carbonation depth along the line of the horizontal cover section A-A, which is almost in a one-dimensional situation, and along the line of the diagonal cover section B-B.

As shown in figure 4, the carbonation front is more advanced in section B-B, because of the effect of two-dimensional flow. The increase in penetration from the one-dimensional to the two-dimensional diffusion process can be estimated to be approximately 40%.

Corner analysis

The finite element mesh of the corner of a concrete structure is shown in figure 5.

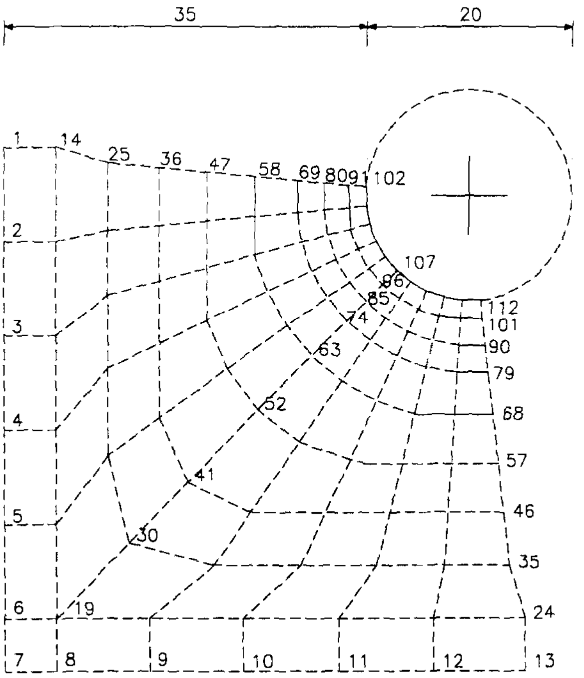

FIG. 5
Finite element mesh for the corner reinforcing steel example

The cover of the reinforcing bar is about 35 mm. The concrete is assumed as being made with OPC, with two different water-cement ratios, w/c = 0.4 and 0.5, and cured 3 days in a mould and then in air for 25 days.

The exposure conditions are assumed to be sinusoidally variable with time:

external temperature $Tx = Ty = 15° + 10° \sin(\pi t / 12)$

external relative humidity $Hx = Hy = 65\% + 25\% \sin(\pi t / 12)$

atmospheric carbon dioxide content $g_0 = 0.035\%$

The iso-carbonation lines, i.e., the lines with the same calcium carbonate content (variable from 0.1 to 1) are shown in figure 6, after fifteen years of simulation time, for the case of water-cement ratios of 0.4 and 0.5 respectively.

The carbonation front, defined as the distance between the iso-carbonation lines with a calcium carbonate content of 0.1 and 1 can be estimated as approximately 1 cm.

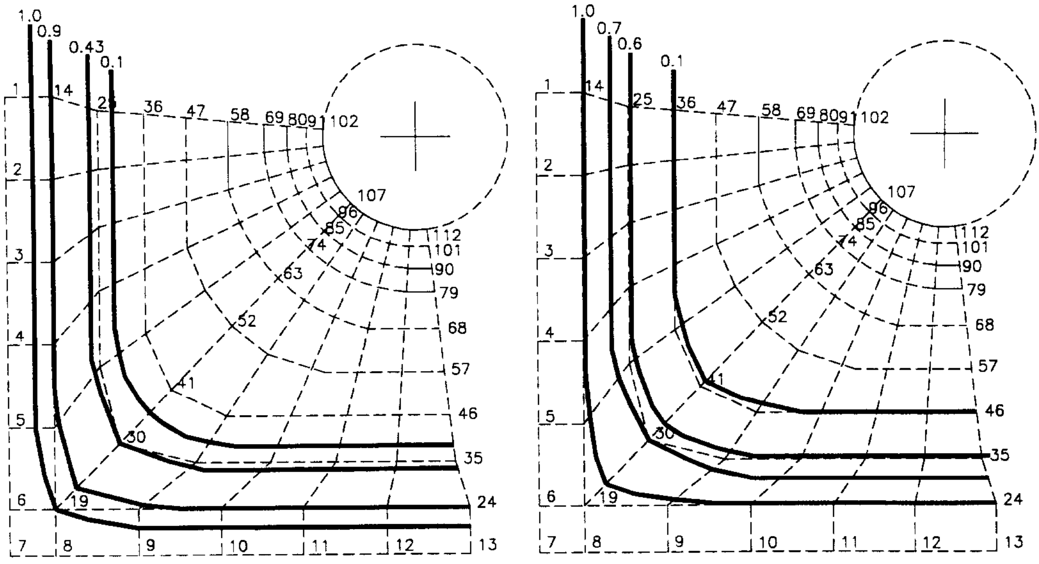

FIG. 6

Iso-carbonation lines after fifteen years for w/c ratios of 0.4 and 0.5

The corrosion initiation time, i.e., the time it takes for the carbonation front to reach the reinforcing bar, can be identified as being after forty years for the case of a water-cement ratio of 0.5 and after ninety years for the case of a water-cement ratio of 0.4.

These times can be defined as approximations of the service life of the two concrete structures made with OPC and a w/c ratio of 0.4 and 0.5 respectively, subjected to two-dimensional carbonation attack.

Conclusions and discussion

The technical service life of a structure with regard to corrosion of the reinforcement can be evaluated by means of a mathematical model, where the influencing factors are the thickness of the concrete cover, the quality of the and the environmental conditions. One of the central aims of structural durability studies now in progress is consequently the development of such mathematical models for the estimation of the service life of structures.

For existing structures in particular, the aim should be to study the current safety level, and to predict the evolution of deterioration phenomena in time in order to plan restoration work or program future inspections. For new constructions, on the other hand, the aim should be to design a concrete mix able to guarantee the required service life in the environment concerned and to simulate the evolution of deterioration phenomena in time.

The present work, in which the two-dimensional extension of the finite element model developed in [1] to simulate the diffusion of aggressive substances (i.e., carbon dioxide) in concrete, enables particular situations to be studied, such as corner reinforcing bars, for which the one-dimensional model overestimates the service life (i.e., it underestimates the actual depth of carbonation).

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