Field Validation of a Computer-based Prediction for Concrete Service Life

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INTRODUCTION

In spite of significant advances made in concrete technology in recent years, the problems of unsatisfactory durability of structures are still among the serious issues concerning the international community of engineers today. Deterioration of concrete structures in service may be the result of a variety of mechanical, physical, chemical or biological processes [1-5]. Corrosion of steel reinforcement is the most serious durability problem of reinforced concrete structures. It impairs not only the appearance of the structure, but also its strength and safety, due to the reduction in the cross-sectional area of the reinforcement, the deterioration of bond with the surrounding concrete, and the significant reduction of the steel ductility properties [5-7].

Over the past decades, an enormous amount of energy has been expended in laboratory and field studies on concrete durability. The results of this research are still either scattered widely in the journal literature or mentioned briefly in popular textbooks; having although partially included in the relevant industry consensus documents as well as in the relevant codes for construction. Moreover, the theoretical approaches of deterioration mechanisms with a predictive character are limited to some complicated mathematical models not widely applicable in practice. A significant step forward could be the development of appropriate software for computer estimation, including reliable mathematical models and strengthened by adequate supporting experimental data. Durability design should get as much attention as structural design since it has to quantify the anticipated functional lifespan. There is opportunity for both simulation computer-aided modelling as well as full-scale engineering corroboration both in the laboratory and in the field.

In the present work, the basis for the development of a computer estimation of the concrete service life is presented. After the definition of concrete mix design and structure characteristics, as well as the consideration regarding the environmental conditions where the structure will be found, the concrete service life can be reliably predicted using fundamental mathematical models that simulate the deterioration mechanisms. The prediction is focused on the basic deterioration phenomena of reinforced concrete, such as carbonation and chloride penetration. Basic principles of chemical and material engineering are applied to simulate the physicochemical processes, yielding simple and accurate mathematical models for design and prediction. Aspects on concrete strength and the production cost are also considered. Field observations and data collection from existing structures are compared with predictions of service life using the above model. A first attempt to develop a database of service lives of different types of reinforced concrete structure exposed to varying environments is finally included. In general, this work is aimed at construction engineers and building material manufacturers to enhance fundamental comprehension of materials behaviour. The work approach presented herein is in full compliance with the new European Standards, for cement: EN 197, and concrete: EN 206 [8, 9]; however, after a short modification it can be applied to any other standard.

Keywords: concrete, durability, estimation, modelling, service life, software, validation

CONCRETE DURABILITY AND THE EUROPEAN STANDARD EN 206 APPROACH

The type and rate of degradation processes of concrete and reinforcement determine the strength and the rigidity of the elements that compose the structure. These affect the safety, the serviceability, and the appearance of a structure, i.e., determine the performance of the structure. Concrete service life (or working life) is the period of time during which the performance of the concrete structure will be kept at a level
compatible with the fulfilment of the performance requirements of the structure, provided it is properly maintained. The ability of a structure to resist environmental attacks, without its performance dropping below a minimum acceptable limit, is called durability. The following three main factors affect the durability of concrete: the initial mixture proportions, the design, construction and maintenance of the structure, and the specific environmental conditions. Deterioration of concrete in service is every loss of performance, and it may be the result of a variety of mechanical, physical, chemical or biological processes [1-5].

The European Standard EN 206 [8] specifies requirements for the constituent materials of concrete, the properties of fresh and hardened concrete and their verification, the limitations for concrete composition, the specification of concrete, the delivery of fresh concrete, the production control procedure, the conformity criteria, and evaluation of conformity. It defines tasks for the specifier, producer, and user. During its development, consideration was given to detailing a performance-related approach to the specification of durability, but it was concluded that test methods to specify durability are not yet sufficiently developed to include them in the standard. However, this standard permits the continuation and development of performance-related methods for assessing durability, as does the present paper.

According to EN 206, environmental actions are those chemical and physical actions to which the concrete is exposed and that result in effects on the concrete or reinforcement or embedded metal that are not considered as loads in structural design. The main deterioration actions considered are corrosion of reinforcement induced either by carbonation or chlorides, cyclic freezing and thawing, and chemical attack. The environmental actions are classified in exposure classes [8]; their selection depends on the provisions valid where concrete will be used. Durability is then specified either through the traditional practice of limiting values of concrete composition (more widely used) or by performance-related methods. The requirements shall take into account the intended service life of the concrete structure.

Limiting Values for Concrete Composition

In the absence of European standards for absolute performance testing of concrete, requirements for the method of specification to resist environmental actions are given in EN 206 in terms of established concrete properties and limiting values for concrete composition. The requirements for each exposure class shall be specified in terms of permitted types and classes of constituent materials, maximum water-cement ratio, minimum cement content, minimum concrete compressive strength class (optional), and, if relevant, minimum air-content of the concrete.

Due to lack of experience on how the classification of the environmental actions on concrete reflect local differences in the same nominal exposure class, the specific values of these requirements for the applicable exposure classes are given in the provisions valid in the place of use. A recommendation for the choice of limiting values for concrete composition and properties is given in Annex F (informative) of EN 206. These values are based on the assumption of an intended service life of the structure of 50 years, and refer to the use of cement type CEM I conforming to EN 197 [9].

Performance-related Design Methods

The requirements related to exposure classes may be established by using performance-related methods for durability and may be specified in terms of performance-related parameters, e.g., scaling of concrete in a freeze/thaw test. Guidance on the use of an alternative performance-related design method with respect to durability is given in Annex J (informative) of EN 206 [8]. The application of an alternative method depends on the provisions valid in the place of use of the concrete.

The performance-related method considers each relevant deterioration mechanism, the service life of the element or structure, and the criteria which define the end of this service life, in a quantitative way. Such a method may be based on satisfactory experience with local practices in local environments, on data from an established performance test method for the relevant mechanism, or on the use of proven predictive models.

A general guidance and some applications are given:

- Some aggressive actions are best dealt with a prescriptive approach, e.g., alkali-silica reaction, sulphate attack, or abrasion.
- Performance-related design methods are more relevant to corrosion resistance and possibly, freeze-thaw resistance of concrete. This approach may be appropriate where:
  - a service life significantly differing from 50 years is required;
  - the structure is "special" requiring a lower probability failure;
  - the environmental actions are particularly aggressive, or are well defined;
- standards of workmanship are expected to be high;
- a management and maintenance strategy is to be introduced, perhaps with planned upgrading;
- significant populations or similar structures, or elements, are to be built;
- new or different constituent materials are to be used;
- method based on limiting values for concrete composition has been used in design, but there has been a failure to conform.

In practice, the level of durability achieved depends on a combination of design, materials, and execution.

The sensitivity of the design concept, the structural system, the shape of members and structural/architectural detailing are all significant design parameters for all methods of durability design.

Compatibility of materials, the construction method, the quality of workmanship, levels of control and quality assurance are significant parameters for all methods of durability design.

The required durability performance depends on the required service life, on the possible future use of the structure, on the particular protective measures, on the planned maintenance in service, and on the consequences of failure, in the particular local environment.

For any required level of performance, it is possible to derive alternative equivalent solutions from different combinations of design, material and construction factors.

The level of knowledge of the ambient and local micro-climate is important in establishing the reliability of performance-related design methods.

The performance-related methods that may be used include:

- The refinement of the method of limiting values for concrete composition, based on long-term experience of local materials and practices, and on detailed knowledge of the local environment.
- Methods based on approved and proven tests that are representative of actual conditions and have approved performance criteria.
- Methods based on analytical models that have been calibrated against test data representative of actual conditions in practice.

The orientation of the present work is towards the development of performance-related methods based on predictive models that have been calibrated against test data representative of actual conditions in practice.

MODELLING OF DETERIORATION RATE AND COMPUTER DESIGN

All physical and mechanical mechanisms for concrete deterioration, except direct loading and imposed deformations, may exhibit their effect on concrete performance during the first year of the service life [1-5]. Chemical and biological mechanisms actually start from the beginning; however, their detrimental results are observed typically long after the first year. In reinforced concrete, the most serious deterioration mechanisms are those leading to corrosion of the reinforcement, which occurs after depassivation due to carbon dioxide or chloride ion penetration. It is therefore necessary, if a long service life is required, that the modelling attempts to address corrosion initiation mechanisms and chemical/biological attack processes.

Fig. 1 shows the logic diagram followed in the software program development (EUCON, [10]) for the estimation of concrete service life. First, the essential parameters that characterize a concrete composition (mixture proportions) are selected, and this is the main source on which all other concrete characteristics depend. Thereafter, the main chemical and volumetric characteristics of concrete are calculated (chemical composition of hydrated cementitious materials, porosity and related characteristics) and this is also another source to receive more information. Based on the selected mixture proportions (cement type and strength class, cement content, water-cement ratio, air content, aggregate type, type and activity of additions, etc.), the compressive strength class of concrete is estimated [11].

For each significant deterioration mechanism, according to the specific environment where the structure would be found, an appropriate proven predictive model is used [11-15]. Concrete carbonation and chloride penetration are the most common causes for reinforcement corrosion onset, and for further concrete deterioration. The service life of the structure found in these environments, which cause either carbonation or chloride penetration, is calculated. The degree of deterioration from a possible chemical attack is also estimated, either as a reduction in the effective concrete section (in the case of acid or biological attack) or as a reduction in strength of the affected concrete (in the case of sulphate or alkali attack). Finally, cost and environmental aspects regarding concrete composition are analysed. Now, for the initially selected concrete composition, the most essential properties have been predicted, such as strength, service life and cost. The designer can then modify the concrete composition accordingly to improve further every required property.
Mix Design and Basic Calculations

Concrete is the material formed by mixing cement, aggregates and water, with or without the incorporation of admixtures and additions, which develops its properties by hydration of the cement. For the present application, a concrete volume is assumed that contains certain amounts of cement, additions (optional), aggregates, water, and admixtures (optional) only, see Fig. 2. To the above materials entrained or entrapped air should be added. All these materials have to comply with the corresponding standards for the constituent materials. In Fig. 2, the part (tab) of the logic flowchart for the concrete mix design is presented and it contains:

- a field that the user introduces the input data for cement, additions, admixtures, water, aggregates, etc.
- a calculation button, and
- a field of the output results including the aggregate content in order to achieve the mass balance requirements (the composition of 1 m³ of fresh concrete).

Fig. 1. Logic diagram for computer-based estimation of concrete service life.
In “Physicochemical Characteristics” part (tab) of the software, the chemical and volumetric composition of concrete is estimated. The tab contains:

- A field that the user introduces the input data for cement composition and oxide analysis, and additions activity and oxide analysis.
- A calculation button, and
- A field of the output results including the reaction degree of supplementary cementing materials and the various additions (either in cement or concrete), the calcium hydroxide and calcium-silicate-hydrate content, the chemically-bound water content and the concrete porosity.

Despite the fact the main aim of the present calculation concerns service life, a strength approach is also welcome, as some lower limitations in strength have been put in many standards, including EN 206, in order to attain a minimum of service life. A reliable prediction of concrete strength based on contribution of each individual compound of hydrated cement is very difficult, because this contribution is not simply additive and has been found to depend on age and the curing conditions [3, 16]. Moreover, a generally applicable strength prediction equation is not possible due to interaction between the various compounds, including additions and cement’s SCM, the influence of alkalis and gypsum, the influence of the particle size of cement and the influence of particle size and shape of aggregates, etc. Many attempts have been made to generate strength prediction of cement paste, mortar and concrete, but without a generally accepted validity. On the other hand, many empirical expressions have been proposed for strength prediction, presenting the most crucial dependences of strength from concrete compositional parameters and calculating the adjustable parameters from experiments [3, 16]. In all empirical expressions the water/cement (W/C) ratio turns out to
be the most important parameter. Probably the first formulation of the relation of strength, \( f_c \) (mean compressive strength, MPa) and the concrete constituents was made by Feret \([4, 17]\):

\[
f_c = \frac{b}{[1 + (W/C)(d_C/d_W) + \varepsilon_{air}(d_C/C)]^2}
\]

where \( C \) and \( W \) are the cement and water contents in concrete (kg/m\(^3\) concrete), \( d_C \) and \( d_W \) the densities of cement and water respectively (kg/m\(^3\)), \( \varepsilon_{air} \) the air content in concrete, and \( b \) is a parameter adjustable from experimental results. In the lack of experimental results the information from the cement strength class may be used to estimate a safe lower limit for concrete strength and thus to approach the corresponding value of compressive strength class. European Standard EN 196-1 prescribes a compressive strength test for cement on mortar specimens of fixed composition. The specimens are tested as 40 mm equivalent cubes, and are made with a “CEN standard sand”, natural, siliceous, and rounded. The W/C ratio is 0.5 and the sand/cement ratio is 3. The specimens are cured in water at 20 °C until testing on 2 or 7, and 28 days. Through this approach the cement strength class is defined \([9]\). However, when strength results from mortars are compared with ones from concretes made each with the same W/C ratio, a significant difference is observed. The concrete strength is higher than the mortar strength, mostly due to greater amount of entrapped air in mortar \([3]\). Using for example all the above information to the Feret’s formula, a lower value for parameter \( b \) can be estimated.

\[
f_c = \frac{b}{[1 + (W/C)(d_C/d_W) + \varepsilon_{air}(d_C/C)]^2} \geq SS
\]

\[\text{i.e., } \quad b \geq 7.84 \text{ SS} \] (2a)

\[b \geq 7.84 \text{ SS} \] (2b)

where SS is the standard strength class (at 28 days) of cement (MPa). Using Eq. (2), the minimum compressive strength class of concrete (at 28 days) can be estimated at another values of W/C, C or \( \varepsilon_{air} \) from the following equation:

\[
f_c \geq 7.84 \text{ SS} / [1 + (W/C)(d_C/d_W) + \varepsilon_{air}(d_C/C)]^2
\]

(3)

If rounded aggregates are used for concrete the above estimation has to decrease by a factor of 13% \([4]\). On the other hand, if a strength result from the above mortar specimens is known at another age (2, 7, or 90 days), this could be used in Eq. (3), as SS, in order to estimate the compressive strength at the same age and for other W/C values. In this way, the strength development can be predicted.

Several other empirical expressions may be used as above, i.e., Abrams’, or Bolomey’s, etc. \([3, 4, 16, 17]\). However, Feret’s formula, as it contains only one adjustable parameter, permits a rather safer approximation from the other models with more than one adjustable parameters. On the other hand, it contains the effect of air content (\( \varepsilon_{air} \)) predicting that 1% variation in air content results in a variation of about 4.5% of the compressive strength as many experimental results have shown \([3, 17]\). In any case, this approach is just a first rough approximation, valuable for the initial test proportioning, and a detailed experimental verification is required. It has also to be emphasized that the above approach can be applied for any cement type, but it refers only to concrete without any active additions such as fly ash or silica fume.

When in a concrete, made with CEM I type of cement, a Type II addition is used (silica fume and/or fly ash), the Eq. (3) is not valid anymore, in this form. The pozzolanic action of addition shall be taken in consideration as it gives strength components. In the previous tab, a simplified scheme describing the activity of supplementary cementing materials (SCM) in terms of chemical reactions was proposed, yielding quantitative expressions for the estimation of the final chemical and volumetric composition of such SCM-concretes. However, a practical approach to the effect of SCM on the strength of portland cement systems and on their resistance against carbonation and chloride penetration can be achieved, using the concept of the SCM efficiency factor. The efficiency factor (or k-value) is defined as the part of the SCM that can be considered as equivalent to portland cement (CEM I), providing the same concrete properties (obviously k=1 for portland cement). The quantity of the SCM in the concrete mixture can be multiplied by the k-value to estimate the equivalent cement content, which can be added to the cement content for the determination of the water-to-cement ratio, minimum required cement content, etc. In the case of SCM-concrete, the following expression for compressive strength can be used which involves the concept of k-value:

\[
f_c \geq 7.84 \text{ SS} / [1 + (W/(C+k_F ACT+k_S ACT))][d_C/(d_W)] + \varepsilon_{air}[d_C/(C+k_F ACT+k_S ACT)]]^2
\]

(4)

where \( F_{ACT} \) and \( S_{ACT} \) are the active contents of concrete additions fly ash and silica fume (kg/m\(^3\)), having an efficiency factor \( k_F \) and \( k_S \) respectively. These active contents are calculated in the previous tab “Physicochemical Characteristics”. Using this equation, and plenty of experimental results, the k-values for
various SCM can be estimated [18, 19]. For siliceous fly ashes, a k-value of 0.5 was calculated for 28 days' strength. However, as time proceeds, higher k-values are calculated for these fly ashes approaching those of high-calcium fly ashes (0.7 for 91 days and 1.1 for 1 year). For calccareous fly ashes, the k-values are around unity (1) at early ages and they exceed it as time proceeds. This means that up to a certain level, these specific pulverized fly ashes can substitute, equivalently, for portland cement. In the case of silica fume very high k-values were calculated (3 at 28 days).

As shown in Fig. 3 an excellent agreement is observed between strength measurements and predictions of the computer program that based on the above Eq. (4), for two cement types. In the second case of CEM II/32.5, the software predictions constitute a safe lower bound, actually because the real cement strength is higher than the nominal cement strength class.

![Graph showing comparison between predictions and measurements](image)

**Fig. 3.** Comparison between predictions of the compressive strength using Eq. (4) and experimental measurements.

**Reinforcement Corrosion Induced by Carbonation**

Reinforcing bars in concrete are protected from corrosion by a thin oxide layer that forms on their surface due to the high alkalinity, i.e., the high pH-value, of the surrounding concrete. Corrosion may start when this protective layer is destroyed:

- either by chloride penetration (and the chloride content exceeds a critical value), or
- due to a reduction in the pH value of concrete to values below 9. Such a reduction in alkalinity is the result of carbonation of the Ca(OH)$_2$ in the concrete mass, i.e., of its reaction with the atmospheric CO$_2$ that diffuses through the concrete pores.

Papadakis et al. [12, 13] were the first to develop a reaction engineering model of the processes leading to concrete carbonation. These processes include the diffusion of CO$_2$ in the gas-phase of pores, its dissolution in the aqueous film of these pores, the dissolution of solid Ca(OH)$_2$ in pore water, its ultimate reaction with the dissolved CO$_2$, and the reaction of CO$_2$ with CSH. The mathematical model yields a nonlinear system of differential equations in space and time and must be solved numerically for the unknown concentrations of the materials involved. For the usual range of parameters (especially, for ambient relative humidity RH≥55%), certain simplifying assumptions can be made, which lead to the formation of a carbonation front, separating completely carbonated regions from the ones in which carbonation has not yet started. For one-dimensional geometry, the evolution of the carbonation depth, $x_c$ (m), with time, $t$ (s), is given by the following analytical expression, proven widely by many laboratory and field measurements [12, 13]:

$$x_c = \frac{2D_{c,\text{CO}_2} (\text{CO}_2 / 100) t}{0.33CH + 0.214CSH}$$

(5)
where, CO₂: the CO₂-content in the ambient air at the concrete surface (%), Dₑ,CO₂: the effective diffusivity of CO₂ in carbonated concrete (m²/s), CH and CSH: the content of calcium hydroxide and calcium-silicate-hydrate, respectively, in concrete volume (kg/m³). CO₂-content varies between 0.03%-0.15% (mean value for urban areas: 0.08%, whereas in countryside: 0.035%). In an ambient relative humidity, RH (%), the diffusivity is given by the empirical equation:

\[ D_{e,CO_2} = 6.1 \times 10^{-6} \left( \frac{\varepsilon_c - \varepsilon_{air}}{1 - \frac{A}{d_A} - \varepsilon_{air}} \right)^3 (1 - RH/100)^{2.2} \]  

(6)

where, \( \varepsilon_c \): the porosity of the carbonated concrete, \( \varepsilon_{air} \): the content of concrete in entrapped or entrained air, \( A \): the aggregate content in concrete volume (kg/m³), and \( d_A \): the aggregate density (kg/m³). The above equations are valid for both portland and blended (with supplementary cementing materials - SCM) cements, as well when additions of SCM are used separately in concrete. The critical time, \( t_{cr,carb} \) (s), required for the carbonation front to reach the reinforcement located at a distance \( c \) (concrete cover to reinforcement, m), can be estimated by (RH ≥ 55%):

\[ t_{cr,carb} = \frac{(0.33CH + 0.214CSH)c^2}{2D_{e,CO_2}(CO_2/100)} \]  

(7)

It is concluded:

- The service life of a concrete structure, regarding corrosion of reinforcement induced by carbonation, is at least \( t_{cr,carb} \).
- As far as the steel bars have been depassivated, the corrosion progress depends on the relative availability of both water and oxygen.

In reinforced concrete structures, it can be reasonably assumed that major repair will be necessary once corrosion of the reinforcement causes generalized cracking of the concrete cover, signalling the end of the service life of the structure. The time required to crack the concrete cover is equal to the time required for the carbonation front to reach the bar (period to initiation of corrosion, \( t_{cr,carb} \)) plus the time necessary for the layer of rust to build up around the bar and split the cover (corrosion propagation period, \( t_{pr,carb} \)). According to various researchers [20, 21], the corrosion rate in carbonated concrete at high relative humidity values is so high that the arrival of the carbonation front at the bar is followed shortly by splitting of the concrete cover. Therefore, the time \( t_{cr,carb} \) required for the carbonation front to penetrate the concrete cover, \( c \), can be considered with good approximation as a lower bound (minimum) to the service life of reinforced concrete. This approach is the basis in the software [10] for estimation of the corrosion-initiation period. In Fig. 4, the part (tab) of the logical flowchart of the program is presented for the calculation of the concrete carbonation depth and the estimation of the service life as regards corrosion induced by the carbonation-initiation mechanism. The tab contains:

- a field that the user introduces the input data as regards the environmental conditions where the concrete structure is exposed.
- a field that the user is informed on the main concrete characteristics and CO₂ diffusivity that influence concrete carbonation.
- a calculation button, for estimation of concrete service life for a given cover to reinforcement.
- a calculation button, for estimation of carbonation depth at a given concrete age.
- There is also the possibility to estimate the above results in the case of use of a protection measure, such as waterproof sealants or cement – lime mortar coatings.

As shown in Table 1, an excellent agreement is observed between the carbonation depth predictions using the above software and the field measurements in real concrete structures of various ages up to 70 years old. The initial concrete composition parameters (mostly C and W/C) were approached indirectly, by measuring strength and porosity and running the software for various parameter values until satisfactory agreement. This table presents also the results of a first attempt to develop a database of service lives of different types of reinforced concrete structure exposed to varying environments.
Fig. 4. General view of the tab “CONCRETE CARBONATION” of the EUCON program.

Tab. 1. Comparison between predictions of the carbonation depth using Eq. (5) and real measurements.

<table>
<thead>
<tr>
<th>Building/Construction</th>
<th>Age (years)</th>
<th>Carbonation depth Prediction (mm)</th>
<th>Carbonation depth Measurement (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooling tower of Public Electricity Enterprise in Megalopolis, Greece inside tower</td>
<td>25 (1995)</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Outside tower</td>
<td></td>
<td>16.9</td>
<td>18</td>
</tr>
<tr>
<td>Technical School, Nafpaktos, Greece</td>
<td>30 (1995)</td>
<td>16.9</td>
<td>18</td>
</tr>
<tr>
<td>Palamaiki School, Messolonghi, Greece</td>
<td>66 (1998)</td>
<td>50.5</td>
<td>52</td>
</tr>
<tr>
<td>General Hospital, Lixouri, Greece</td>
<td>51 (2004)</td>
<td>43.1</td>
<td>45</td>
</tr>
<tr>
<td>Ladopoulos papermill, Patras, Greece non-protected, uncoated with cement-lime mortar coating</td>
<td>70 (2005)</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>City Hall, Neapolis Vion, Greece</td>
<td>38 (2005)</td>
<td>32</td>
<td>35</td>
</tr>
<tr>
<td>Stela Maris Hotel, Galatas, Greece</td>
<td>37 (2005)</td>
<td>32</td>
<td>30</td>
</tr>
<tr>
<td>City Hall, Sami, Greece</td>
<td>40 (2005)</td>
<td>50</td>
<td>55</td>
</tr>
</tbody>
</table>
Reinforcement Corrosion Induced by Chlorides

Numerous surveys have indicated that chloride ions (Cl\(^{-}\)), originating from de-icing salts or seawater, are the primary cause of reinforcing steel corrosion in highways and marine or coastal structures [1-5, 11]. Chlorides, transported through the concrete pore network and microcracks, depassivate the oxide film covering the reinforcing steel and accelerate the reaction of corrosion and concrete deterioration. Chloride penetration is a process which takes place in totally or partly water-filled pores. This is the main reason that as a process is much slower than carbonation, where CO\(_2\) molecule may penetrate faster via air-filled pores.

In many studies, chloride transport in concrete is modeled using Fick’s second law of diffusion, neglecting the chloride interaction with the solid phase. However, the latter process is very important including binding of chlorides by cement hydration products, ionic interaction, lagging motion of cations and formation of an electrical double layer on the solid surface, etc. Pereira and Hegedus [22] modelled chloride diffusion and reaction in fully saturated concrete as a Langmuirian equilibrium process coupled with Fickian diffusion. Papadakis et al. [14, 15] extended this approach to more general conditions, offering a simpler solution, proven experimentally. The physicochemical processes of diffusion of Cl\(^{-}\) in the aqueous phase, their adsorption and binding in the solid phase of concrete, and their desorption therefrom are described by a nonlinear partial differential equation for the concentration of Cl\(^{-}\) in the aqueous phase \([\text{Cl}^-\text{(aq)}]\) (in kg/m\(^3\) pore solution), from which that of Cl\(^{-}\) bound in the solid phase \([\text{Cl}^-\text{(s)}]\) (kg/m\(^3\) concrete) can be computed algebraically:

\[
\frac{\partial}{\partial t} \left[ \frac{\text{Cl}^-\text{(aq)}}{\text{Cl}^-\text{(s)}} \right] = \frac{D_{e,\text{Cl}^-} (1 + K_{eq} \left[ \text{Cl}^-\text{(aq)} \right])^2}{K_{eq} \left[ \text{Cl}^-\text{(s)} \right]_{sat} + \varepsilon (1 + K_{eq} \left[ \text{Cl}^-\text{(aq)} \right])^2} \frac{\partial^2 \left[ \text{Cl}^-\text{(aq)} \right]}{\partial x^2}
\]

where:

\[
\left[ \text{Cl}^-\text{(s)} \right] = \frac{K_{eq} \left[ \text{Cl}^-\text{(aq)} \right]}{1 + K_{eq} \left[ \text{Cl}^-\text{(aq)} \right]} \left[ \text{Cl}^-\text{(s)} \right]_{sat}
\]

*initial condition:* \([\text{Cl}^-\text{(aq)}] = [\text{Cl}^-\text{(aq)}]_{in} \) at \(t = 0\) (initial concentration)

*boundary conditions:* \([\text{Cl}^-\text{(aq)}] = [\text{Cl}^-\text{(aq)}]_{0} \) at \(x = 0\) (concrete surface)

\(\frac{\partial [\text{Cl}^-\text{(aq)}]}{\partial x} \) at \(x = M\) (axis of symmetry)

In these equations, \(x\) is the distance from the concrete surface (m), \(t\) is the time (s), \(D_{e,\text{Cl}^-}\) denotes the intrinsic effective diffusivity of Cl\(^{-}\) in concrete (m\(^2\)/s), \(K_{eq}\) the equilibrium constant for Cl\(^{-}\) binding (m\(^3\) of pore volume/kg), \([\text{Cl}^-\text{(s)}]_{sat}\) the saturation concentration of Cl\(^{-}\) in the solid phase (kg/m\(^3\) concrete), and \(\varepsilon\) the concrete porosity (m\(^3\) pore volume/m\(^3\) concrete). In the case of “complete” hydration and Pozzolanic action, the above parameters can be calculated using the mathematical expressions given elsewhere [13-15].

Eq. (8) can be solved only numerically, e.g., using a finite difference method as does the aforementioned software [10]. Typical model results are presented in Fig. 5. The solution of the above system allows estimation of the time (critical time for chloride-induced corrosion, \(t_{cr,\text{chlor}}\)) required for the total chloride concentration surrounding the reinforcement (located at a distance \(c\) from surface) to increase over the threshold for depassivation. A way of threshold expression is by measurement of the total chloride ion content in concrete required for the onset of reinforcement corrosion, and a mean value of 0.4-1% by weight of binder is often adopted [5, 23]; although this subject is still an open issue [24]. We can state that the service lifetime of a structure, regarding chloride penetration, is at least \(t_{cr,\text{chlor}}\). Afterwards, the propagation of corrosion process takes place at a rate that depends strongly on the availability of both oxygen and water. The possible mechanism of chloride ion interaction with the reinforcement and passive layer has not been fully resolved [5]. Moreover, the estimation of the propagation period and the definition of the end of the service life due to chloride-induced corrosion contain a lot of uncertainties [1, 5, 24]. Therefore, as in the case of carbonation, the time \(t_{cr,\text{chlor}}\) required for Cl\(^{-}\) to exceed the critical value at the concrete cover, \(c\), can be considered in good approximation as a lower bound to the service life of reinforced concrete.

A comparison between experimental measurements and model predictions of chloride concentration in various concrete specimens is presented elsewhere [11, 14, 15], that proves the validity of the above approach. An ongoing research is also taking place in order to perform a more extended comparison with real structures as in the case of carbonation, see Table 1.
CONCLUSIONS

Computer software [10], based on proven predictive models, has been developed for estimation of concrete service life, strength and cost, and it may be included in performance-related methods of EN 206 for assessing durability. Its structure is in full compliance with the European Standards EN 197 for cement (applicable to all 27 types of cement) and EN 206 for concrete (including addition use, such as silica fume and fly ash, various admixtures use, etc.). The logic diagram, however, can be easily applied to any other national standard. The software offers the possibility of investigating the efficiency of various protection measures, such as waterproof sealants, cement-lime mortar coatings, inhibitors, etc. Comparing the software results with field measurements from various real structures, a satisfactory general agreement is observed.

The paper’s aim is not to put itself against the few (not many) other similar software packages [as for example DuCOM; 25, Life-365; 26] but to turn people in informatics applications on concrete design. The basic scope of this presentation is thus to pass a message to the relevant researchers to use computer-based estimations of concrete properties that, potentially, may include a vast quantity of information data (mathematical models and many experimental data). Using these software packages, including the present one, an optimum concrete design can be achieved by estimating reliably the concrete strength, durability and production cost.

It has also to be emphasized again that the introduction of performance-related design methods, such as proven predictive models in the form of user-friendly software, is absolutely necessary when [8]:

- a service life significantly differing from 50 years is required;
- the structure is “special” requiring a lower probability failure;
- the environmental actions are particularly aggressive, or are well defined;
- a particular management, maintenance or protection strategy is to be introduced;
- significant populations of structures or similar structures or elements are to be built;
- new or different constituent materials are to be used; and
- a method based on limiting values for concrete composition has been used in design, but there has been a failure to conform.

REFERENCES