COMPUTER MODELLING OF CONCRETE SERVICE LIFE

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ABSTRACT: In all concrete constructions besides the common strength problems, in presence or not of seismic activity, serious problems from environmental attack may be presented which significantly decrease their durability and service lifetime. In the literature, there is a vast number of papers dealing with degradation mechanisms, attempting either to study them experimentally or to simulate them using fundamental or empirical models. The lots of experimental results and the complicated mathematical models on the other hand, make difficult their wide use from the concrete engineers, who want to predict the concrete service life. It is time all this information to be included in a software package, where the user, by giving the minimum required data, to receive the concrete mix design reliably, ensuring the specified strength level and service lifetime, at the minimum cost. General guidance on the use of alternative performance-related design methods with respect to durability is already given in the European Standard EN 206 and it could be evolved in further generation standards. In this paper, such a first approach is presented, i.e., a computer software package for reliable concrete design achieving a specified concrete strength, service life and production cost.

Keywords: Computer, Concrete, Design, Durability, Modelling, Service Life.

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INTRODUCTION

Over the past 50 years, an enormous amount of effort has been expended in laboratory and field studies on concrete durability [1-5]. The results of this research are still either widely scattered in the journal literature or mentioned briefly in the standard textbooks. 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 an appropriate software for computer-based estimation, including reliable mathematical models and adequate experimental data.

In the present work, the basis for the development of a computer model for the estimation of 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 and rate. The prediction is focused on the basic deterioration phenomena of reinforced concrete, such as carbonation and chloride penetration, and on various chemical attacks. Aspects on concrete strength and the production cost are also considered. This approach enables mixture proportions to be accurately specified and concrete performance reliably predicted. Basic principles of Chemical and Material Engineering are applied to simulate deterioration processes, yielding mathematical models for design and prediction, and furthermore the software for estimation of the concrete service life. Finally, results from computer runs regarding the recommendations of the European Standard EN 206 [6] for various compositional and environmental parameters are presented.

CONCRETE DURABILITY AND THE EUROPEAN STANDARD EN 206 APPROACH

The type and rate of degradation processes of concrete and reinforcement determine the resistance and the rigidity of these materials, the sections and the elements that compose the structure. This reflects in the safety, the serviceability and the appearance of a structure, i.e., determines 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 to drop below a minimum acceptable limit, is called durability. The following three main factors define the durability of concrete: the initial mix design, 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], see Fig. 1.

The European Standard EN 206 [6], specifies requirements for the constituents 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 work.

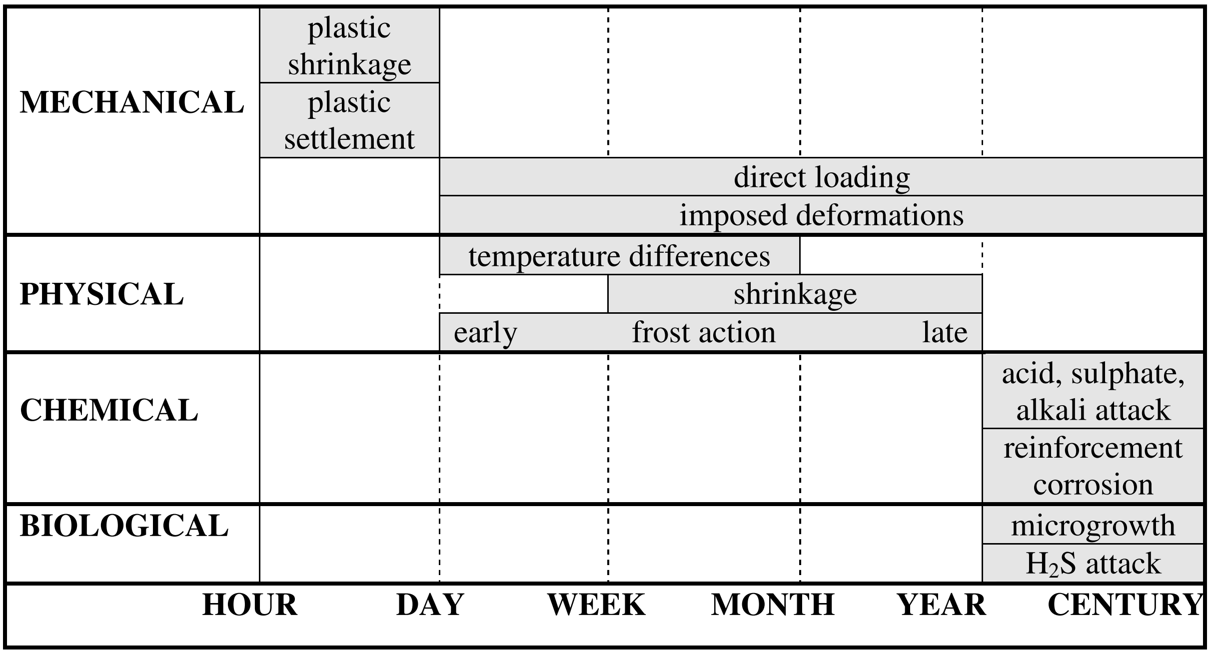


Figure 1 Deterioration mechanisms and possible time of appearance of cracking or damage.

According to EN 206, environmental actions are those chemical and physical actions to which the concrete is exposed and which 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, freeze/thaw and chemical attack. The environmental actions are classified in exposure classes [6]; their selection depends on the provisions valid in the place of use of the concrete. 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 the 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 [7].

Performance-related Design Methods

Guidance on the use of an alternative performance-related design method with respect to durability is given in Annex J (informative) of EN 206. The application of an alternative method depends on the provisions valid in the place of use of the concrete. The performance-related method should consider 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.

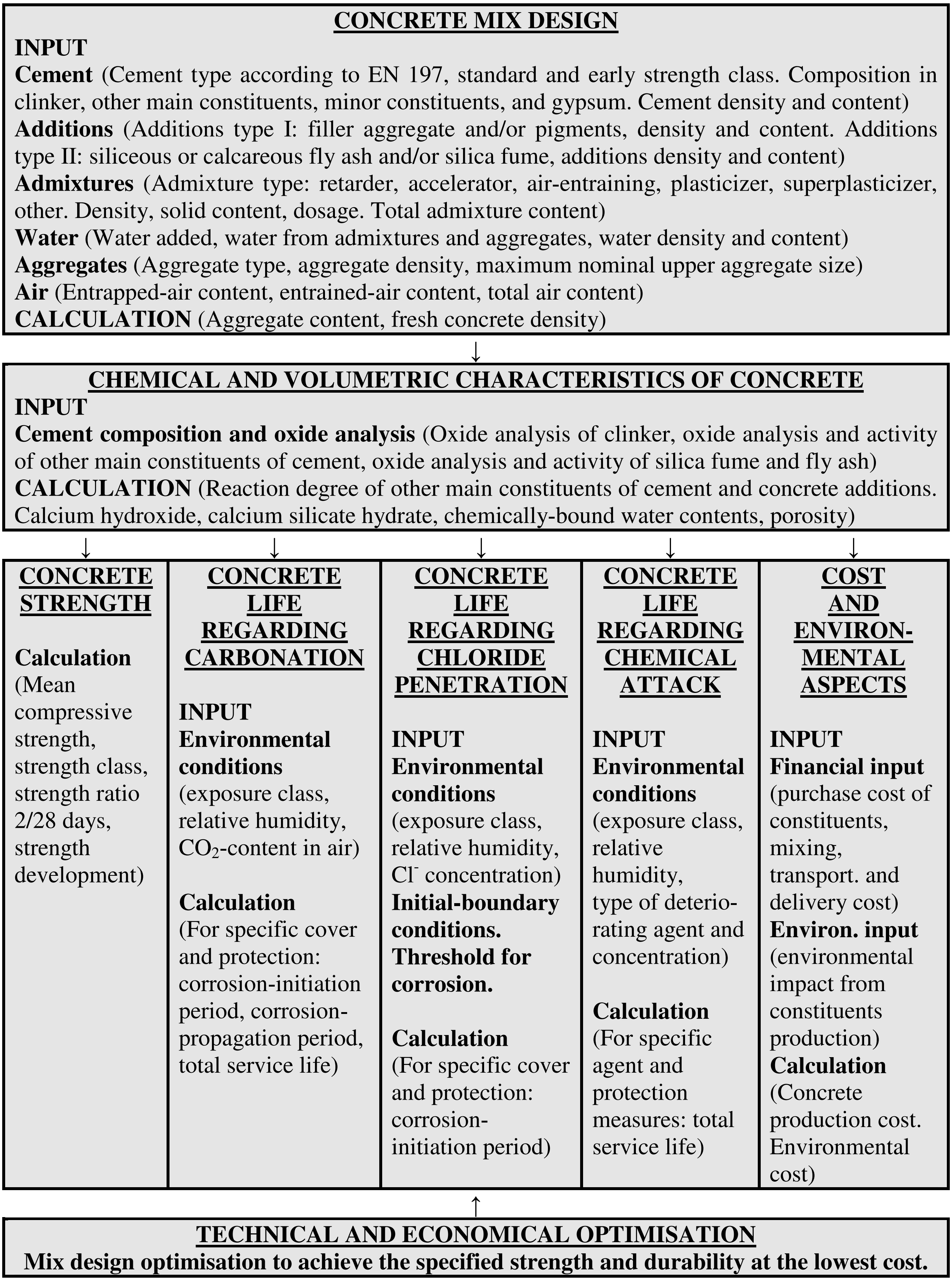
The orientation of the present work is towards the development of performance-related methods based on predictive models that have been calibrated against test data representative of actual conditions in practice.

MODELLING OF DETERIORATION RATE AND COMPUTER DESIGN

As observed in Fig. 1, 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. The chemical and biological mechanisms actually start from the beginning; however, their detrimental results are observed 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 prediction is required, the modelling attempts to turn towards the corrosion initiation mechanisms and the chemical/biological attack processes.

In Fig. 2, the logical diagram followed in the software program development [8] for the estimation of concrete service life is presented. First, the essential parameters that characterize a concrete composition (mix design) 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 mix design (cement type and strength class, cement content, water/cement ratio, air content, aggregates type, type and activity of additions, etc.), a first approximation of the compressive strength class of concrete is estimated [9].

For each significant deterioration mechanism, according to the specific environment where the structure would be found, an appropriate proven predictive model is used [9-13]. Concrete carbonation and chloride penetration are the most common causes for reinforcement corrosion and further concrete deterioration. The service life of the structure found in these environments, which cause either carbonation or chloride attack, is calculated. The degree of deterioration from a possible chemical attack is also estimated. Finally, cost and environmental aspects regarding concrete composition are fully 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. In the following, typical results are presented concerning various exposure classes and compositional parameters.



CONCRETE MIX DESIGN

INPUT

Cement (Cement type according to EN 197, standard and early strength class. Composition in clinker, other main constituents, minor constituents, and gypsum. Cement density and content)

Additions (Additions type I: filler aggregate and/or pigments, density and content. Additions type II: siliceous or calcareous fly ash and/or silica fume, additions density and content)

Admixtures (Admixture type: retarder, accelerator, air-entraining, plasticizer, superplasticizer, other. Density, solid content, dosage. Total admixture content)

Water (Water added, water from admixtures and aggregates, water density and content)

Aggregates (Aggregate type, aggregate density, maximum nominal upper aggregate size)

Air (Entrapped-air content, entrained-air content, total air content)

CALCULATION (Aggregate content, fresh concrete density)

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CHEMICAL AND VOLUMETRIC CHARACTERISTICS OF CONCRETE

INPUT

Cement composition and oxide analysis (Oxide analysis of clinker, oxide analysis and activity of other main constituents of cement, oxide analysis and activity of silica fume and fly ash)

CALCULATION (Reaction degree of other main constituents of cement and concrete additions. Calcium hydroxide, calcium silicate hydrate, chemically-bound water contents, porosity)

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CONCRETE STRENGTH	**CONCRETE LIFE REGARDING CARBONATION**	**CONCRETE LIFE REGARDING CHLORIDE PENETRATION**	**CONCRETE LIFE REGARDING CHEMICAL ATTACK**	**COST AND ENVIRONMENTAL ASPECTS**
Calculation (Mean compressive strength, strength class, strength ratio 2/28 days, strength development)	**INPUT** **Environmental conditions** (exposure class, relative humidity, CO_2-content in air) **Calculation** (For specific cover and protection: corrosion-initiation period, corrosion-propagation period, total service life)	**INPUT** **Environmental conditions** (exposure class, relative humidity, Cl^- concentration) **Initial-boundary conditions. Threshold for corrosion.** **Calculation** (For specific cover and protection: corrosion-initiation period)	**INPUT** **Environmental conditions** (exposure class, relative humidity, type of deteriorating agent and concentration) **Calculation** (For specific agent and protection measures: total service life)	**INPUT** **Financial input** (purchase cost of constituents, mixing, transport. and delivery cost) **Environ. input** (environmental impact from constituents production) **Calculation** (Concrete production cost. Environmental cost)

↑

TECHNICAL AND ECONOMICAL OPTIMISATION

Mix design optimisation to achieve the specified strength and durability at the lowest cost.

Figure 2 Logical diagram for computer design of concrete mix for specified strength class, service life and cost.

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 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. [10, 11] were the first to develop a reaction engineering model of the processes leading to concrete carbonation, yielding a nonlinear system of differential equations in space and time that must be solved numerically. For the usual range of parameters, certain simplifying assumptions can be made, which lead to the formation of a carbonation front; the evolution of this is given by a simple analytical expression [10, 11]. This approach is the basis in the software [8] for estimation of the corrosion-initiation period.

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 period of time required to crack the concrete cover is equal to the period required for the carbonation front to reach the bar (period to initiation of corrosion, $t_{cr,carb}$) plus the period of time necessary for the layer of rust to build up around the bar until to split the cover (corrosion propagation period, $t_{pr,carb}$). According to various researchers [14, 15], 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 shortly followed 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 narrow lower bound (minimum) to the service life of reinforced concrete.

Corrosion is much faster than carbonation at higher water contents of concrete pores, and consequently at higher relative humidity (RH) of the ambient air. This was taken into account in the definition of the exposure classes in EN 206. We propose to use a measurable characteristic of the environment regarding its humidity state, i.e., the mean RH, in order to convert the somehow indefinite exposure classes of EN 206. In order to investigate if the EN 206 recommendations for limiting composition values would ensure a service life of 50 years, the above software [8] was used, and the results are presented in Table 1. Two common cement types are examined, CEM I 42.5N and CEM II/B-M 32.5N, for concrete production, using common crushed aggregates of maximum nominal upper size of 31.5 mm. We suppose a non-protected concrete surface, exposed to urban environment (CO_2-content: 0.08%).

For the exposure class XC1 and dry environment (we propose: $45\% \leq RH < 65\%$, mean value: 55%), carbonation is more rapid, however, in this region the corrosion rate is slight due to insufficient moisture. According to Parrot [14], the critical corrosion depth of the reinforcing bar that causes visible deterioration is 100 μm, and as the corrosion rate is about 0.3 μm/y in this RH region, the propagation period is $t_{pr,carb} > 100$ years. Typical example of this case is the concrete inside buildings or structures where RH remains low during the whole working life. For the same exposure class, XC1, but for permanently wet environment (we propose: $RH \geq 98\%$, value for computations: 98%), carbonation is almost fully inhibited due to water-filled pores which decrease significantly the CO_2 diffusion, and the corrosion process is also very slow for the same reason, as regards O_2 diffusion. Typical examples of this case are concrete members that will be submerged at all times during the working life.

Table 1 Estimated minimum of concrete service life for various cement types and exposure classes, in the case of carbonation-induced corrosion of reinforcement [8].

MIX AND DESIGN CHARACTERISTICS	XC1 (dry)	XC1 (p. wet)	XC2	XC3		XC4
Cement type CEM I 42.5N						
Maximum ratio W/C	0.65	0.65	0.60	0.55	*0.50*	0.50
Minimum content C (kg/m^3)	260	260	280	280	*300*	300
Minimum strength class	C20/25	C20/25	C25/30	C30/37	*C30/37*	C30/37
$t_{cr,carb}$ (years) for c = 15 mm	5	>100	>100	22	*34*	84
$t_{cr,carb}$ (years) for c = 20 mm	8	>100	>100	38	*61*	>100
$t_{cr,carb}$ (years) for c = 25 mm	12	>100	>100	60	*95*	>100
Cement type CEM II/B-M(W-P-LL) 32.5N						
Maximum ratio W/C	0.65	0.65	0.60	0.55	*0.50*	0.50
Minimum content C (kg/m^3)	260	260	280	280	*300*	300
Minimum strength class	C20/25	C20/25	C20/25	C25/30	*C25/30*	C25/30
$t_{cr,carb}$ (years) for c = 15 mm	2	>100	77	9	*13*	32
$t_{cr,carb}$ (years) for c = 20 mm	4	>100	>100	16	*23*	57
$t_{cr,carb}$ (years) for c = 25 mm	6	>100	>100	25	*36*	89

W/C: water to cement ratio by weight, C: cement content in concrete, c: concrete cover to reinforcement, $t_{cr,carb}$: initiation period for carbonation-induced corrosion of reinforcement.

For the exposure class XC2 (wet, rarely dry, we propose: 90%≤RH<98%, value for computations: 90%), both the carbonation and corrosion rates are greater than in the XC1 environment (permanently wet), however for the compositional parameters of Table 1, the $t_{cr,carb}$ is almost >100 years. Typical examples of this case include concrete reservoirs and water towers that will be full most of the time, and foundation members below ground level.

For the exposure class XC3 (moderate humidity, we propose: 65%≤RH<85%, value for computations: 70%) carbonation is faster than XC2, and lower than XC1 (dry environment). For c=25 mm and the EN 206 recommendations, $t_{cr,carb}$=60 years for CEM I and much lower, $t_{cr,carb}$=25 years, for CEM II/B-M (for CEM II/A-M, $t_{cr,carb}$=40 years and for CEM IV/B, $t_{cr,carb}$=15 years [8]). The corrosion rate is also at its high level due to presence of both oxygen and water. It is worth to note that in such an environment of high humidity, the corrosion rate is rather fast, almost 5-20 μm/y [4,1 4], that gives propagation periods of the order of 5-20 years (as 100 μm is the critical corrosion depth). Morinaga [15], estimates even shorter periods of 2 years! Typical examples of this case are external concrete surfaces sheltered from rain and internal concrete with higher than normal relative humidity. As these exposure conditions are rather common, and the corrosion rate is high enough, more onerous limiting values for concrete composition have to be applied (see proposal in Table 1, *italics*), than those recommended by EN 206, as also proposed in British Standard BS 8500 [4, 16].

For the last exposure class XC4 (cyclic wet and dry, we propose: 75%≤RH<90%, mean value: 80%) carbonation is still medium due to dry periods. The corrosion rate is at its maximum level due to the presence of both oxygen and adequate water. It has also to be emphasized that concrete takes water from the environment more rapidly than it loses it and thus the internal humidity could be higher than the average ambient humidity. This higher internal moisture speeds up the corrosion rate. Typical examples of this case are external concrete surfaces exposed to rain and many other, mostly industrial, applications.

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 [3, 5, 9]. 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.

Papadakis et al. [12, 13] presented a generalized model of chloride diffusion and reaction in saturated or non-saturated concrete. This model can be solved only numerically, e.g., using a finite difference or element method, as does the software [8]. The solution allows estimation of the time (critical time for chloride-induced corrosion, $t_{cr,chlor}$) 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 0.6% by weight of binder is adopted [9, 17].

Chloride penetration is a process which takes place in totally or partly water-filled pores. This is the main reason that the process is much slower than carbonation, where CO_2 molecule may penetrate faster via air-filled pores. The RH of the environment and the origin of Cl^- were taken into account in the definition of the exposure classes in EN 206. In order to investigate whether the EN 206 recommendations for limiting composition values would ensure a service life of 50 years, the above software [8] was used, and the results are presented in Table 2. The same cement types are examined, CEM I 42.5N and CEM II/B-M 32.5N, using common crushed aggregates of a maximum size of 31.5 mm.

In the case of concrete containing reinforcement and subjected to contact with chlorides from sea water, for all exposure classes: XS1: exposed to airborne salt but not in direct contact with sea water (structures near to or on the coast), XS2: permanently submerged (parts of marine structure), XS3: tidal, splash and spray zones (parts of marine structure), the recommendations of EN 206 ensure a service life greater than 50 years (even 100 years); for an adequate cover, see Table 2. We suppose a non-protected concrete surface, exposed to Atlantic Ocean environment (Cl^- concentration: 20 kg/m^3). It has to be emphasized that on the contrary to the carbonation results, cement types that contain supplementary cementing materials (SCM: silica fume, fly ash, etc.) exhibit significantly longer initiation period than pure Portland cement.

In the case of concrete with reinforcement and subjected to contact with water containing chlorides including de-icing salts, from sources other than from sea water, for all exposure classes: XD1: moderate humidity (concrete surfaces exposed to airborne chlorides), XD2: wet, rarely dry (swimming pools, concrete exposed to industrial waters containing chlorides), XD3: cyclic wet and dry (parts of bridges exposed to spray containing chlorides, pavements, car park slabs), the recommendations of EN 206 ensure a service life greater than 50 years (in some cases even 100 years); for an adequate cover, see Table 2. Especially for XD2, in spite of the low initiation period, the total life is much longer due to prolonged propagation period; however, a denser design may be required. We suppose a non-protected concrete surface, exposed to a Cl^- concentration of 100 kg/m^3, lasting for 1/5 of the year. In this case also blended cements with SCM, or when an SCM is added separately to the concrete mixture, the estimated initiation period is greater than in the case of pure Portland cement use.

Table 2 Estimated minimum of concrete service life for various cement types and exposure classes, in the case of chloride-induced corrosion of reinforcement [8].

MIX AND DESIGN CHARACTERISTICS	XS1	XS2	XS3	XD1	XD2	XD3
Cement type CEM I 42.5N						
Maximum ratio W/C	0.50	0.45	0.45	0.55	0.55	0.45
Minimum content C (kg/m^3)	300	320	340	300	300	320
Minimum strength class	C30/37	C35/45	C35/45	C30/37	C30/37	C35/45
$t_{cr,chlor}$ (years) for c = 30 mm	63	25	32	43	8	32
$t_{cr,chlor}$ (years) for c = 35 mm	80	35	46	57	12	43
$t_{cr,chlor}$ (years) for c = 40 mm	100	48	58	72	16	53
$t_{cr,chlor}$ (years) for c = 45 mm	>100	58	70	90	20	64
$t_{cr,chlor}$ (years) for c = 50 mm	>100	69	81	>100	24	77
Cement type CEM II/B-M(W-P-LL) 32.5N						
Maximum ratio W/C	0.50	0.45	0.45	0.55	0.55	0.45
Minimum content C (kg/m^3)	300	320	340	300	300	320
Minimum strength class	C25/30	C30/37	C30/37	C25/30	C25/30	C30/37
$t_{cr,chlor}$ (years) for c = 30 mm	70	38	35	54	15	46
$t_{cr,chlor}$ (years) for c = 35 mm	100	50	48	78	20	59
$t_{cr,chlor}$ (years) for c = 40 mm	>100	67	60	>100	28	78
$t_{cr,chlor}$ (years) for c = 45 mm	>100	84	75	>100	37	>100
$t_{cr,chlor}$ (years) for c = 50 mm	>100	100	95	>100	46	>100

W/C: water to cement ratio by weight, C: cement content in concrete, c: concrete cover to reinforcement, $t_{cr,chlor}$: initiation period for chloride-induced corrosion of reinforcement.

CONCLUSIONS

A computer software [8], based on proven predictive models, is presented 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.). It also 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 the recommendations of EN 206 for common exposure classes, a general agreement is observed, but also several adjustments are required.

The introduction of performance-related design methods, such as proven predictive models in a form of a user-friendly software, is absolutely necessary when [6]:

- 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 or similar structures, or elements, are to be built;
- new or different constituent materials are to be used;
- a method based on limiting values for concrete composition has been used in design, but there has been a failure to conform.

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