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Computer-aided modeling of concrete service life

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ABSTRACT

A significant step forward for a thorough durability design process of reinforced concrete structures is the development of software packages, based on predictive models, for the estimation of concrete strength and service life. Such an attempt, in full compliance with the European Standards for cement and concrete, is presented in this study. Upon defining the concrete mix design, the software calculates the main chemical and volumetric characteristics, as well as the compressive strength, of concrete. By taking into account the environmental conditions where the structure will be exposed, concrete service life is predicted, using fundamental mathematical models (based on reaction engineering principles) that simulate the reinforced concrete deterioration mechanisms leading to corrosion of the embedded reinforcement (caused by either carbonation or chloride ingress). A validation process of the yielded results is also presented, and the effectiveness of the simulation tool in designing for durability is illustrated. The goal of this study is to promote wider acceptance in achieving feasible and durable solutions to structural concrete design problems.

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1. Introduction

Given the increased number of premature structural deterioration cases observed on reinforced concrete (RC) structures, a comprehensive design process becomes imperative. Bearing in mind that such deterioration can be caused by mechanical and/or environmental actions, an in-depth understanding and modeling of the physicochemical processes that lead to concrete deterioration (under harmful environmental agents) is the first step for a valid service life estimation. On this note, certain research attempts [1–3] have been proved successful in identifying the service life of a reinforced concrete element under chloride exposure, at a probabilistic manner and also in assessing the carbonation depth in time [4].

What is missing however, is a comprehensive set of tools that will aid the designer in identifying the influence of both the most common harmful environmental agents (carbonation exposure and chloride ingress), by taking under consideration the environmental and mix design particularities of a reinforced concrete structure, in order to take all the appropriate measures (in advance) to mitigate their effect, in safeguarding a prolonged service-life of any type of structure.

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On the European Standard for concrete [5] durability is approached by the definition of limiting parameters on cement and concrete composition (W/C ratio, cement content, etc.), as well as by the development of performance-related methods (PRMs). Such a method (PRM) is necessary when a service life significantly higher of 50 years is required, or when the environmental actions are particularly aggressive [5]. A PRM considers each relevant deterioration mechanism, in addition to the service life of the structure, and the criteria which define the end of this service life, in a quantitative way. It can based on data derived from established performance test methods for each relevant mechanism, or on the use of proven predictive models. Considering that in reinforced concrete the most serious deterioration mechanisms are those leading to reinforcement corrosion, it is therefore necessary, if a long service life is required, the modeling attempts to focus on these types of mechanisms/chemical attack processes. Bearing all of the above in mind, a significant step forward could be the development of appropriate software for the estimation of concrete service life, using reliable mathematical proven models, based on performance-related methods.

In this study, a deterministic simulation tool in full compliance with the European Standards for cement and concrete [5,6], based on proven predictive models developed by Papadakis et al. [7–10], for estimation of concrete service life and strength is briefly presented. Emphasis is given on the concept of service life estimation, on tool validation and utilization schemes. As an illustrative





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example, the effects of cement type and of several supplementary cementing materials on reinforced concrete durability are studied using the simulation tool.

2. Concrete service life estimation tool

The structure and the main outputs of the concrete service life estimation tool are illustrated in Fig. 1. Upon selection of the cement type (based on the full range of cement types defined in the European Standard for cement [6]) and standard strength class, as well as, selection of quantity and type of additives (types I and II), admixtures and aggregates, the concrete mix design is defined and the main chemical and volumetric characteristics of concrete (chemical composition of hydrated cementitious materials, porosity and related characteristics) are calculated. The concrete compressive strength is accurately estimated, introducing a new (recently published) approach [11], based on the cement strength class and on the efficiency factor of SCM [12–16], using a modified version of Feret's formula. By taking into account the environmental conditions where the structure will be exposed (according to the exposure classes defined in EN 206 [5]) the concrete service life is reliably predicted using fundamental mathematical models that simulate the basic deterioration mechanisms of reinforced concrete, such as carbonation and chloride penetration. Principles of chemical and material engineering have been applied to simulate the physicochemical processes [8,9]. In addition, cost and environmental aspects on concrete composition are analyzed. Finally an optimization procedure is taking place, where (if necessary) the mix design is adjusted in order to meet concrete strength and service life requirements.

Furthermore, the software package [7] offers the possibility of investigating the efficiency of various protection measures as water proof sealants, cement–lime mortar coating and inhibitors.

2.1. Service life estimation

As it was previously mentioned, principles of chemical and material engineering have been applied to simulate the physicochemical processes leading to concrete deterioration for carbonation and chloride exposure.

	CONCRETE MIX DESIGN (according to EN 197, EN 206)									
		Cement T	ype	Selection between 27 cement types (ENV-197) and of Standard Cement Strength Class. Composition in clinker, other main constituents, minor constituents, gypsum. Cement density and content						
	INDUT	Additions	Additions Ty sil		Type I (filler aggregate and/or pigments), Type II (siliceous/calcareous fly ash, silica fume), additions density and content					
	INFUT	Admixtur	es	Type densi	(retarder, accelera ty, solid content, c	ator, air-entraining, plasticizer, losage. Total admixture conten	superplasticizer), t			
		Water		Water added, water from admixtures and aggregates, water density and content						
		Aggregate	es	Aggr	egate type, aggreg	ate density, maximum nominal	aggregate size			
	OUTDUT	Air		Entra	pped-air content,	entrained-air content, total air c	ontent			
	OUTPUT	Aggregate	content	, fresh	concrete density					
						↓ ↓				
(CHEMICAL	& VOLUM	ETRI	С СН	ARACTERIST	TICS OF CONCRETE				
Ι	NPUT	Cement Cor Oxide Anal	mpositi ysis	ion,	Oxide analysis o constituents of c ash	f clinker, oxide analysis and ac ement, oxide analysis and activ	tivity of other main ity of silica fume and fly			
(OUTPUT	Reaction deg	ree of o	ther m	ain constituents o	f cement and concrete additions	s. Contents of calcium			
		nydroxide, ca	aicium s	sincate	nyurate, chemica	ny-bound water, porosity				
						↓ ↓				
ESTIMATION OF CONCRETE STRENGTH		ESTIMATION OF SERVICE LIFE WITH RESPECT TO CARBONATION INPUT All of the previous, plus		TION OF LIFE WITH TO	ESTIMATION OF SERVICE LIFE WITH RESPECT TO	COST & ENVIRONMENTAL ASPECTS INPUT All of the previous, plus				
I	NPUT All of the previo	ous	CAR INPU All of	BON J T the pr	ATION revious, plus	CHLORIDE PENETRATION INPUT All of the previous, plus	ASTEC 15 INPUT All of the previous, plus			
I	NPUT All of the previo	nus	INPU All of enviro Ex Re CO US co an	BON T the pronument of the prosument elative O_2 -con se of moating (alysis,	ATION evious, plus tal conditions e class humidity, itent in air nortar or other 'type, chemical width)	CHLORIDE PENETRATION INPUT All of the previous, plus environmental conditions • Exposure class • Internal concentration of Cl ⁻ • External source of Cl ⁻ • Cl ⁻ concentration at concrete surface • Degree of exposure • Relative humidity • Use of corrosion inhibitors, coatings, etc.	 AST ECTS INPUT All of the previous, plus Financial input purchase cost of materials, mixing, transport. and delivery cost Environ. input environmental impact from materials production 			
I	NPUT All of the previo	nus	CAR INPU All of enviro E23 Re CC U3 cco an	BON UT The pronument the prosument the prosumen	ATION evious, plus tal conditions e class humidity, itent in air nortar or other (type, chemical , width)	CHLORIDE PENETRATION INPUT All of the previous, plus environmental conditions • Exposure class • Internal concentration of Cl ⁻ • External source of Cl ⁻ • External source of Cl ⁻ • Cl ⁻ concentration at concrete surface • Degree of exposure • Relative humidity • Use of corrosion inhibitors, coatings, etc.	 AST ECTS INPUT All of the previous, plus Financial input purchase cost of materials, mixing, transport, and delivery cost Environ. input environmental impact from materials production OUTPUT 			
	NPUT All of the previo DUTPUT Mean compre strength Strength Class Strength ratio Strength Deve	ssive 2/28 days elopment	 CAR INPP All of enviro Eb R Rc CO Us coordinate Us coordinate OUT Coordinate Coordinate	BON JT f the pr comment co	ATION evious, plus tal conditions e class humidity, tent in air nortar or other (type, chemical .width) n-initiation n-propagation vice life	CHLORIDE PENETRATION INPUT All of the previous, plus environmental conditions • Exposure class • Internal concentration of Cl • External source of Cl • Cl concentration at concrete surface • Degree of exposure • Relative humidity • Use of corrosion inhibitors, coatings, etc. OUTPUT • Adequate concrete cover needed to sustain a corrosion free structure, for a given service life • corrosion-initiation period	 ASTECTS INPUT All of the previous, plus Financial input purchase cost of materials, mixing, transport, and delivery cost Environ. input environmental impact from materials production OUTPUT Concrete production cost Environmental cost 			

TECHNICAL AND ECONOMICAL OPTIMIZATION

Mixture proportions optimization to achieve the specified strength and durability at the lowest cost.

Fig. 1. Logic tree of software for estimation of concrete service life, strength, economical and environmental cost.

2.1.1. Modeling for carbonation exposure

In terms of carbonation exposure, a system of non-linear differential equations, developed by Papadakis et al. [8] models in a quantitative way the physicochemical processes leading to concrete carbonation. These include the diffusion of CO_2 in the gasphase 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 solution of the set of differential equations permits the calculation of the carbonation depth x_c , at a given time t, as well as the estimation of the critical time, $t_{cr,carb}$, required for the carbonation front to reach the reinforcement located at a distance c (concrete cover to reinforcement), for both Portland and blended cements, as well as when additions of supplementary cementing materials (SCM) are used separately in concrete, according to the following equation:

$$x_{c} = \sqrt{\frac{2D_{e,CO_{2}}(CO_{2}/100)t}{0.33CH + 0.214CSH}}, \ t_{cr,carb} = \frac{(0.33CH + 0.214CSH)c^{2}}{2D_{e,CO_{2}}(CO_{2}/100)}$$
(1)

where CO_2 is the CO_2 -content in the ambient air at the concrete surface (%), CH and CSH are the contents of calcium hydroxide and calcium–silicate–hydrate in concrete volume (kg/m³), D_{e,CO_2} the effective diffusivity of CO_2 in carbonated concrete (m²/s), where in an ambient relative humidity, RH (%), is calculated as:

$$D_{e,CO_2} = 6.1 \times 10^{-6} \left(\frac{\varepsilon_c - \varepsilon_{air}}{1 - \frac{A}{d_A} - \varepsilon_{air}} \right)^3 (1 - \text{RH}/100)^{2.2}$$
(2)

where ε_c is the porosity of the carbonated concrete, ε_{air} the volume fraction of entrapped or entrained air in concrete (m³/m³), *A* the aggregate content in concrete volume (kg/m³) and d_A the aggregate density (kg/m³).

Once the carbonation front reaches the embedded bar, corrosion can take place with its known consequences, including concrete cracking. At that point it can be reasonably assumed that major repair will be necessary. Hence the appearance of generalized cracking may be considered to signal the end of the service life of the structure (Z_{carb}). Overall, the time required to crack the concrete cover can be expressed (Fig. 2) as the time required for the carbonation front to reach the bar (initiation period of corrosion, $t_{cr,carb}$, estimated as mentioned above) plus the time necessary for the layer of rust to build up around the bar and split the cover (corrosion propagation period, $t_{pr,carb}$).

However, in certain cases [8,10] and according to Morinaga [17] the corrosion rate in carbonated concrete at high relative humidity values can be of such magnitude, that the arrival of the carbonation front at the bar is followed shortly by splitting of the concrete



Fig. 2. Schematic illustration of initiation and propagation periods of corrosion in a reinforced concrete element.

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 to the service life of reinforced concrete.

If an approximation of the propagation period is required, then a model of the physicochemical processes of corrosion and cracking has to be applied. However, until now there is no a generally accepted fundamental model for corrosion propagation of the concrete reinforcement [7,18], attributed to the complex phenomena of corrosion as well to the definition of detectable effects that define the limit of an acceptable damage, such as the level of cracking.

An alternative approach would be to assume a zero propagation period ensuring at least the lower limit for service life. However, this assumption is not valid, especially for low relative humidity when the propagation period is much higher than the initiation period due to lack of moisture. As a general conclusion from various works [17,18], the propagation period depends strongly on relative humidity. For example 70% RH results in a propagation period almost double of the initiation period, while for 80% RH the propagation period is about half of the initiation period and for 90% RH, the propagation period is about 1/5 of the initiation period.

According to Morinaga [17,19], for usual environmental conditions (20 °C temperature and 55% < RH < 95%) the rate of corrosion q_c (10⁻⁴ g/cm²/yr) of steel bar in concrete, can be approached by the following empirical formula:

$$q_c = 65(\text{RH}/100) - 35 \tag{3}$$

The critical amount of corrosion Q_{cr} (10^{-4} g/cm²) causing cracking and splitting of the concrete cover c (mm), for usual concrete strength and for a reinforcing bar of 10 mm in diameter, can be approached as [17,19]:

$$Q_{\rm cr} = 6(1+0.2c)^{0.85} \tag{4}$$

In this way the propagation period $t_{pr,carb}$ (in years) can be expressed as the ratio of the previously mentioned factors Q_{cr}/q_c :

$$t_{\rm pr,carb} = \left[6(1+0.2c)^{0.85} \right] / \left[65(\rm RH/100) - 35 \right]$$
(5)

Finally, the service life Z_{carb} (in years) regarding carbonation-induced corrosion of concrete reinforcement, is the total sum of the two periods ($Z_{carb} = t_{cr,carb} + t_{pr,carb}$, $t_{cr,carb}$ has to be converted in years dividing by 31,557,600 s/yr).

2.1.2. Modeling for chloride ingress

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.

The physicochemical processes of Cl^- diffusion in the aqueous phase, their adsorption and binding in the solid phase of concrete, and their desorption, are described [9] by a non-linear partial differential equation (Eq. (3)). Solution of Eq. (6), allows the calculation of the Cl^- bound in the solid phase [$Cl^-(s)$].

$$\frac{\partial [\mathsf{CI}^{-}(\mathsf{aq})]}{\partial t} = \frac{D_{e,\mathsf{CI}^{-}}(1 + K_{eq}[\mathsf{CI}^{-}(\mathsf{aq})])^{2}}{K_{eq}[\mathsf{CI}^{-}(s)]_{sat} + \varepsilon (1 + K_{eq}[\mathsf{CI}^{-}(\mathsf{aq})])^{2}} \frac{\partial^{2}[\mathsf{CI}^{-}(\mathsf{aq})]}{\partial x^{2}} \tag{6}$$

$$[Cl^{-}(s)] = \frac{K_{eq}[Cl^{-}(aq)]}{1 + K_{eq}[Cl^{-}(aq)]} [Cl^{-}(s)]_{sat}$$
(7)

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

boundary conditions : $[Cl^{-}(aq)] = [Cl^{-}(aq)]_{0}$ at x = 0 (concrete surface), $\partial [Cl^{-}(aq)]/\partial x = 0$ at x = M (axis of symmetry)

where *x* is the distance from the concrete surface (m), *t* is the time (s), K_{eq} the equilibrium constant for Cl⁻ binding (m³ of pore volume/kg), [Cl⁻(s)]_{sat} the saturation concentration of Cl⁻ in the solid phase (kg/m³ concrete), [Cl⁻(aq)] the concentration of Cl⁻ in the aqueous phase, D_{e,Cl^-} is the intrinsic effective diffusivity of Cl⁻ in concrete (m²/s), calculated as:

$$D_{e,Cl^{-}} = \frac{2.4 \times 10^{-10}}{\left(\frac{C + \sum (kP_{ACT})}{d_c} + \frac{W}{d_W}\right)^2} (\varepsilon_{eff})^{3.5},$$
(8)

with ε_{eff} being the effective (for diffusion) concrete porosity (m³ pore volume/m³ concrete), calculated as:

$$\varepsilon_{\rm eff} = W/d_W - 0.226 \times 10^{-3} \left\{ C + \sum (kP_{\rm ACT}) \right\} \tag{9}$$

where *C* cement content (kg cement/m³ of concrete), P_{ACT} the active content of each SCM added either as cement constituent or as concrete addition, having an efficiency factor *k*, and d_c , d_w , cement and water densities, respectively,

Furthermore, the solution of Eq. (3) allows the calculation of the adequate (minimum) concrete cover needed in order to sustain a chloride-induced corrosion free structure for a given service life, as well as the 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. Afterwards, the propagation of corrosion process takes place at a rate that depends strongly on the availability of both oxygen and water. The service lifetime of a structure, regarding chloride penetration, can be considered to be least $t_{cr,chlor}$.

In the case of an RC structure where the concrete cover is not crack free, the model can be adjusted accordingly. It is widely understood that cracks increase the transport properties of concrete, creating perfect pathways for gas and liquid transportation, thus, facilitating the ingress of deleterious species such as CO₂ or chlorides into concrete and accelerating the initiation time for the corrosion of the steel reinforcement. The estimation of the life span of reinforced concrete structures having cracks is influenced by characteristics, such as crack width and length, in addition to the concrete properties and the environmental exposure conditions. The models developed by the authors to estimate the service life of reinforced concrete structures (as far as chloride ingress and the action of carbon dioxide from the atmosphere is concerned), presented briefly in the current study, take under consideration parameters influenced by the appearance of cracks on the concrete cover. Research has shown that the presence of cracks increases the diffusion coefficient of both chloride ions and carbon dioxide. A comparison of chloride diffusion coefficients for cracked and uncracked concrete showed an increase in the diffusion coefficient for cracked concrete by one or two orders of magnitude [20,21], while a crack width of 0.2 mm was found to increase the carbon dioxide diffusion coefficient about three orders of magnitude compared to an average quality crack-free concrete [22]. In the model, by adjusting the values of the effective chloride and/or carbon dioxide diffusion coefficients and by taking under consideration the initial conditions (Cl⁻ concentration of the surface, environmental exposure, etc.), an initial profile corresponding to a cracked concrete surface is created, which will be used by the model as a starting point on the calculation of the service life estimation parameters.

2.2. Cost and environmental aspects

Cost and environmental aspect regarding concrete composition are also addressed. Although it is not the aim of the current study to elaborate in detail on these two features of the model, for reasons of completeness a very brief introduction is given.

In terms of economic cost [7], the concrete production cost KT (ϵ/m^3) is calculated (per volume unit of 1 m³ of fresh concrete) by taking into account factors as materials purchasing cost $(K_P, \epsilon/m^3)$, mixing cost for concrete production $(K_M, \epsilon/m^3)$, cost of transportation and delivery $(K_B, \epsilon/m^3)$, and other operational costs $(K_G, \epsilon/m^3)$, as it shown in the following equation.

$$KT = K_p + K_M + K_B + K_G = (CU_C + SU_S + FU_F + AU_A + WU_W + DU_D)$$
$$+ (P_M t_M U_E) + \left(K_T + \frac{P_B}{Q}U_E\right) + K_G$$
(10)

where $U_{C,S,F,A,W,D}$, are the cement, silica fume, fly ash, aggregate, water, admixtures values, ϵ/kg . *C*, *S*, *F*, *A*, *W*, *D*, are the cement, silica fume, fly ash, aggregate, water, admixtures content (kg/m³ of concrete), P_M the mixing power/m³ of concrete (J/s m³), U_E the cost of energy (ϵ/J), t_M the mixing time (s), K_T the cost of transportation (ϵ/m^3), P_B the pumping power (J/s), *Q* the concrete flow (m³/s).

It should be noted that on the calculation of the concrete mixing cost, the parameters P_M and t_M depend on concrete workability and density and, therefore, on concrete composition parameters. The cost of transportation K_T depends on the distance between project location and plant, hence is independent of concrete compositional parameters. At the project location, the cost is burdened with pumping and application expenses. Fixed and operational costs include the fixed cost of purchase and establishment of equipment (depreciation values), labor and administration costs and general operational costs.

In terms of environmental cost [7,23], the CO₂ emissions from concrete production can be expressed as the summation of the emissions from, the chemical conversion process in clinker production (during cement manufacturing), from the energy consumption due to fossil fuel combustion (also during cement manufacturing), from the electrical energy required for the grinding of any additive materials and from the energy required (in terms of fuel consumption) for the transportation of the raw materials and of the final product. A more precise estimation of the environmental footprint of concrete E_{conc} , taking under consideration the environmental factors of each individual concrete component, based on a large set of concrete production data (from the literature and from cement production companies) can be expressed as:

$$E_{\text{conc}} = CE_c + SE_S + FE_F + AE_A + WE_W + DE_D$$
(11)

where *C*, *S*, *F*, *A*, *W*, *D* are the cement, silica fume, fly ash, aggregate, water and admixtures content (kg of cement/m³ of concrete), E_C , E_S , E_F , E_A , E_W , E_D , are the environmental costs of cement, silica fume, fly ash, aggregates, water and admixtures respectively (kg of CO₂/kg of cement).

3. Validation and verification

Having presented the structure and the concept behind the modeling of the physicochemical processes leading to concrete deterioration, the results of a wide validation study [24], in terms of carbonation exposure, are given in this section.

A comparison between experimental measurements and model predictions of chloride concentration for various concrete specimens has been presented elsewhere [9,14]. Currently, an ongoing field study is taking place, for a thorough validation based on data derived from structures showing signs of chloride induced corrosion. In the case of carbonation exposure, such a study has

been completed and the validation results are briefly presented bellow.

Carbonation depth results were collected from the recent published literature, under either accelerated conditioning or natural ageing, for different exposure times. Parameters as cement type, mix design characteristics, chemical composition of the clinker and pozzolanic materials, levels of relative humidity and carbon dioxide concentration (where the reinforced concrete element was exposed) were recorded and inserted into the model. The calculated carbonation depth values were compared with the corresponding values taken from the literature (Fig. 3). A very good correlation was observed (an average variation of 7.6% was calculated).

From the characteristic data given in Table 1 it can be seen that the model yields very accurate predictions for a range of both accelerated (up to 1 year) and natural exposure times (up to 18 years, where considering the experimental value of 11.62 mm with a standard deviation of 2.45, the 8.3 mm calculated is a very good approximation) and for different cement and concrete compositions. In Fig. 4, just as a representative example, an excellent agreement between calculated and experimental values is observed, for a longer natural exposure time (up to 4.5 years) and for different W/C ratios.

In addition, data from a set of characteristic structures showings signs of carbonation-induced deterioration were derived. Using the simulation tool, based on information as, the age they were erected, their environmental exposure, the type of cement used and the concrete compressive strength measured, the carbonation depth was estimated and a very good correlation (average variation of 7.2%) was observed (Fig. 5 and Table 2).

4. Utilization of service life estimation tool

Having briefly presented the structure of the concrete service life estimation tool, the concept behind the modeling of the physicochemical processes leading to concrete deterioration (for carbonation and chloride ingress) and its validation actions (up-to-date, since its an on-going process), its utilization will be illustrated in designing for durability by evaluating the effect of every supplementary cementing material defined in EN 197 [6].

The scope behind this task is that even though there is a shift on European level [36] in producing such types of cements (55.5% production of CEM II,) their utilization and manufacture is not yet uniform (possibly due to the availability of raw materials, or



Fig. 3. Comparison of calculated to experimental carbonation depth values. (See above-mentioned references for further information.)

due to issues of economical nature), hence it is difficult to have on overall assessment of the effects of SCM incorporation on concrete durability. However, the service life estimation tool can aid in this direction. On that note, a comparative assessment of the effect of SCM on concrete durability (as type II additives) and of every cement type defined in the European Standard [6] is briefly presented and discussed. The service life evaluation was made in terms of their performance in carbonation and chloride exposure, for a service life of 50 years.

4.1. Effect of type II additives on concrete durability

Supplementary cementing materials (SCM) were evaluated as type II additives as aggregate and as cement replacements. A constant volume unit (1 m³) of concrete was chosen as a common basis. When an SCM was added to this unit, then an equal volume of another component, either cement or aggregate, was removed in order to keep the same total volume and the common comparison basis. A typical CEM I 42.5 mix, water cured for 28 days was selected as the reference type of cement (W/C 0.5, cement content 300 kg/m³, 31.5 mm crushed aggregates, no additives, no admixtures). In the case of fly ash 10%, 20% and 30% replacement levels of the control cement mass were chosen, while in the case of silica fume, since it is a more reactive pozzolanic material than fly ash (and hence the rate of pozzolanic reactions drops below one for lesser quantities than fly ash) 5%, 10% and 15% replacement levels were used. The water content (kg/m^3) was kept constant for all specimens.

Overall it was seen that when SCM were used for aggregate replacement, the carbonation depth was decreased compared to the control mix (Fig. 6a and Table 3).

Incorporation of calcareous fly ash (C-FA) in CEM I type of cement produced a better performance for carbonation exposure than siliceous fly ash (S-FA) (Fig. 6a). Silica fume (SF) did not prove to be as effective as fly ash (FA), in inhibiting carbonation exposure. To draw a comparison between results, 10% addition of SF reduced the carbonation depth by 9.7%, compared to the 17.3% and 18.7% reductions observed when 10% of siliceous and calcareous fly ash was added. In the case where SCM were used as cement replacement materials, the carbonation depth was increased, with the increasing content of every type of SCM used. The explanation for such behavior lays in the way these materials were incorporated into the mix. For aggregate replacement by an SCM the total amount of carbonatable materials remains almost the same and moreover the porosity decreases (and the diffusivity of carbon dioxide, see Table 3) resulting in lower carbonation rates [14].

In the case of cement replacement by SCM, by reducing the cement and clinker content, the amount of carbonatable materials is also reduced (due to the decrease in total CaO), resulting in higher carbonation rates [28]. In general SCM materials (as cement replacements) proved to be less resistant to carbonation, mainly due to their low binding capacity of CO_2 , caused by their smaller concentrations of Ca(OH)₂, compared to control (due to the consumption by pozzolanic reaction, and lower cement content). However, considering that for reasons of comparison certain parameters were kept unchanged (*W*/*C* ratio, cement content) better performances in carbonation exposure (than control) can be achieved by altering these parameters.

Under chloride exposure (Fig. 6b), specimens incorporating SCM as either aggregate or cement replacement, produced smaller adequate concrete cover values (needed to sustain chloride exposure for a service life of 50 years), compared to control. Silica fume proved to inhibit chloride diffusion more efficiently than FA. A 62.1% reduction of the adequate concrete cover was noticed, compared to 41.1% and 34.5% reductions when siliceous or calcareous fly ash were respectively used (for 10% content of SCM). It has been

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aracteristic estimated carbonation depth values.								
References	Cement type	W/C	RH (%)	CO ₂ (%)				
[25]	Cem I	0.67	72.5	0.0625				
[30]	CEM I + fa	0.68	65.0	3				
[30]	CEM I + fa	0.68	65.0	3				

					Experimental	Calculated	
[25]	Cem I	0.67	72.5	0.0625	5.68	5.30	2 years
[30]	CEM I + fa	0.68	65.0	3	7.50	7.80	4 weeks ^a
[30]	CEM I + fa	0.68	65.0	3	11.0	11.7	9 weeks ^a
[33]	CEM I	0.45	60.0	0.08	11.62 (2.45)	8.30	18 years
[28]	CEM II/B-M	0.55	60.8	0.035	3.50	3.80	9 months
[28]	CEM II/B-M	0.55	60.8	0.035	8.40	8.30	42.5 months
[29]	CEM II/B-L	0.48	60.8	0.035	3.00	2.60	6 months
[29]	CEM II/B-L	0.48	60.8	0.035	3.50	3.70	12 months
[29]	CEM II/B-L	0.48	60.8	0.035	4.00	4.60	18 months
[32]	CEM II/A-l	0.60	65.0	5	15.0	15.9	42 days ^a
[35]	CEM II/A-V	0.54	65.0	5.0	5.71	5.6	1 year ^a
[30]	CEM III/B	0.60	65.0	3	16.00	15.0	9 weeks ^a
[32]	CEM IV/B	0.55	65.0	5	19.50	18.4	42 days ^a

^a Denotes accelerated exposure.



Fig. 4. Calculated and experimental carbonation depth values for different W/C ratios of a CEM II/B-M type of cement.



Fig. 5. Comparison of calculated to measured carbonation depth values from field studies (see Table 2).

noticed that specimens incorporating an SCM, whether it substitutes aggregate or cement, exhibit significantly lower total chloride content for all depths from the surface [37-39]. Rapid chloride permeability results, undertaken by the authors at a previous time [14] on samples incorporating SCM, indicated that they all exhibited lower electrical charge than the control sample (OPC), with silica fume producing the best performance. Such a trend was clearly visible on this evaluation, in which silica fume, proved to be most efficient SCM in inhibiting chloride ingress.

Table 2						
Characteristic estimated carbonatio	n depth	values	from	field	studies	

Carbonation depth (mm)

Exposure time

St	ructure	Age (years)	Carbonation depth (mm)		
			Measured	Calculated	
1	Industrial facility, Patras, Greece (mortar coating)	70	8	6	
1	Industrial facility, Patras, Greece (no mortar coating)	70	20	19	
2	School, Mesologi, Greece	66	45	43	
3	Hospital, Lixouri, Greece	51	43	41	
4	Town Hall, Voia, Greece	38	35	32	
5	Cooling Tower, Megalopolis, Greece (internal)	25	2	2	
5	Cooling Tower, Megalopolis, Greece (external)	25	18	16.9	
6	School, Nafpaktos, Greece	30	52	50.5	
7	Hotel, Galatas, Greece	37	30	32	
8	City Hall, Sami, Greece	40	55	50	

4.2. Effect of CEM II type of cement on concrete durability

On evaluating the different types of CEM II cements, a standard CEM I mix of 0.45 water-cement ratio was selected as the reference type of cement (cement content 300 kg/m³, 31.5 mm crushed aggregates, no additives, no admixtures). On each type of SCM used, three different content levels were considered (minimum, medium and high as explained in Fig. 6). An initial observation is that carbonation depth was increased (Fig. 7) and the critical time for initiation of corrosion (for a 30 mm concrete cover, indicated with *italics* in Fig. 6) was reduced, compared to the control values, for every type of CEM II cement. However, closer inspection reveals that certain types of cements, with low content of SCM (6%) produced a more suitable behavior. More specific:

- Portland-composite cements incorporating 6% artificial pozzolana (Q) and/or blast furnace slag (S), gave the less severe behavior in carbonation (4.1% increase of carbonation depth) followed by cement incorporating 6% burnt shale (T, 4.7% increase of carbonation depth), compared to the rest.
- Cements incorporating pozzolanic materials with hydraulic properties (W, S, and T), behaved much better (4.7% deviation from control) than those containing normal pozzolanic materials (V, P, Q, M, 8.3% deviation from control).
- Cements incorporating silica fume (D) produced a similar performance (11.5% increase of the carbonation depth), regardless of the SCM percentage (6%, 8%, and 10%).

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Fig. 6. Carbonation depth and sufficient concrete cover for chloride exposure of CEM I with Type II additives (A silica fume, Siliceous fly ash, calcareous fly ash).

 Table 3

 Durability indicators of Type II additives.

SCM type	SCM (%)	$x_c (\mathrm{mm})$	Δx_{c} (%)	$t_{\rm cr,CO_2}$ (years)	$\Delta t_{ m cr}$ (%)	D_{e,CO_2} (m ² /s)	$\Delta D_{e, \mathrm{CO}_2}$ (%)	c ₅₀ (mm)	Δc_{50} (%)	$D_{e,Cl} (m^2/s)$	$\Delta D_{e,\mathrm{Cl}}$ (%)
Control	0	19.6	-	116.9	-	0.927	-	29	-	0.149	-
S-FA	10	16.2	-17.3	172	47.1	0.598	-35.5	17	-41.4	0.047	-68.7
Aggr.	20	13.3	-32.1	200	71.1	0.380	-59.0	7	-75.9	0.011	-93.0
Repl.	30	12.0	-38.8	200	71.1	0.311	-66.4	7	-75.9	0.009	-94.0
Cem.	-10	21.7	-	95.4	-18.4	0.965	4.1	23	-20.7	0.071	-52.1
Repl.	-20	25.1	_	71.3	-39.0	1.089	17.4	21	-27.6	0.046	-68.9
	-30	31.8	-	44.6	-61.8	1.522	64.2	31	-	0.086	-42.2
C-FA	10	15.9	-18.9	177.2	51.6	0.615	-33.7	19	-34.5	0.067	-54.9
Aggr.	20	12.4	-36.7	200	71.1	0.376	-59.4	11	-62.1	0.025	-83.2
Repl.	30	9.8	-50.0	200	71.1	0.235	-74.6	5	-82.8	0.073	-95.1
Cem.	-10	21.3	-	99.3	-15.1	0.988	6.5	25	-13.8	0.096	-35.7
Repl.	-20	23.3	_	83.2	-28.8	1.055	13.8	21	-27.6	0.060	-60.1
	-30	25.5	-	69.2	-40.8	1.119	20.7	17	-41.4	0.033	-77.6
SF	5	18.4	-6.1	132.2	13.2	0.819	-11.6	19	-34.5	0.057	-62.0
Aggr.	10	17.7	-9.7	143.5	22.8	0.755	-18.6	11	-62.1	0.019	-87.5
Repl.	15	16.7	-14.8	161.9	38.4	0.670	-27.8	7	-75.9	0.005	-96.7
Cem.	-5	21.2	-	99.9	-14.5	1.031	11.2	23	-20.7	0.072	-52.0
Repl.	-10	23.4	-	82.2	-29.7	1.187	28.0	17	-41.4	0.029	-80.5
	-15	25.7	-	67.9	-41.9	1.355	46.2	15	-48.3	0.022	-85.4

Where: x_c , Δx_c Carbonation depth and its change as compared to control.

 $t_{\rm cr,CO_2}$, $\Delta t_{\rm cr}$ Critical time for corrosion initiation and its change as compared to control.

 D_{e,CO_2} , $\Delta D_{e,CO_2}$ Effective diffusivity of CO₂ in carbonated concrete and its change as compared to control.

 c_{50} , Δc_{50} Adequate concrete cover to sustain chloride induced free corrosion and its change as compared to control.

 $D_{e,Cl}$, $\Delta D_{e,Cl}$ Effective diffusivity of Cl^{-} in concrete and its change as compared to control.

 The worst performance in carbonation exposure was produced by cements incorporating limestone powder.

The overall behavior of CEM II type of cements in carbonation exposure produced from the simulation tool, has observed by other researchers [30,40], mainly attributed to their low portlandite content and the subsequent reduction of $Ca(OH)_2$ from the pozzolanic activity. However, certain types of cement (6% artificial pozzolana, 6% fly ash, 6% blast furnace slag) produced a more tolerable behavior. It has been stated that in certain cases at low SCM concentration, the pozzolanic action and the filling properties of the SCM afford certain changes in porosity which predominate over the reduction in carbonatable materials leading to a less severe carbonation effect [25,28].

Under chloride exposure every different type of Portland-composite cement used (except the one with limestone, CEM II/B-LL) behaved in an extraordinary way (Fig. 8). Cement incorporating 15% artificial pozzolana (CEM II/A-Q) produced the best performance (reductions of up to 62.2% on the concrete cover and 92.9% reduction of the chloride ions diffusivity) followed by cements incorporating silica fume (CEM II/A-D, 57.8% decrease). Overall the following observations were made:

- Cements containing pozzolanic materials with hydraulic properties, calcareous fly ash (*W*), blast furnace slag (*S*) and burnt shale (*T*), behaved in a similar manner, producing the best performance, overall, at low (6–15%) and high (21–30%) quantities of SCMs. The concrete cover values kept reducing with increasing SCM content (up to 44.4% reduction, for 30% SCM).
- Cements containing siliceous fly ash (*V*) and other composite materials (*M*) produced reduced concrete cover values (35.6% reduction) up to a certain SCM percentage (15% and 21% respectively). At larger SCM quantities an increase in the concrete cover was noted.
- Incorporation of natural pozzolana (CEM II/A,B-P) gave increased concrete cover values (up to 22%).
- Addition of 15% of limestone increased the concrete cover by 26.7% (compared to control) but most important the chloride diffusivity by 67% (Fig. 6).

The steady performance of the increasing slag content on CEM II/S type of cement, was investigated further, by evaluating

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Fig. 7. Best carbonation depth values for a service life of 50 years of CEM II cement types (with *italics*: the critical time, years, for initiation of corrosion, for a 30 mm concrete cover).



Type of Cement

Fig. 8. Best adequate concrete cover values calculated to sustain a service life of 50 years under chloride exposure, for every type of CEM II cements.

Table 4	
Performance of CEM III type of cements.	

	CEM I (control)	CEM III/A		
SCM (%)	0	36	43	51
$x_c (mm)$	14.8	18.4	19.1	22.3
t _{cr} (years)	200	133.4	123.1	90.3
c ₅₀ (mm)	45	21	15	17
Δc_{50} (%)	-	-53.3	-66.7	-62.2

cements with higher quantities of slag (CEM III), where at 43% of SCM a 66.7% reduction of the adequate concrete cover needed to sustain a chloride free reinforced concrete structure for 50 years was noticed (Table 4). Overall blast furnace cements (CEM III)

performed extremely well under chloride exposure (in contrast to their carbonation behavior).

Comparing the best behavior of CEM II and CEM III type of cements it can be seen that a 43% blast furnace cement (CEM III) produced the best performance in designing for chloride exposure (at 50 years) than any other CEM II type of cement (Fig. 9).

Overall, the ability of concrete to resist a chloride induced attack is mainly related to its microstructures and the chloride binding capacity of the formed hydration products. Recent results indicate that very good resistance to chloride penetration and considerable decreases of the diffusion coefficients were noticed on cements containing pozzolans [39], blast furnace slag [40,41] and silica fume (incorporation of 7.5% of silica fume reduced the diffusion coefficient of chlorides three times compared to a simple OPC



Type of Cement

Fig. 9. Comparative performance of SCMs in chloride diffusion.

mix [42]). On the effect of slag in particular, replacement levels of up to 40% have been known to reduce drastically the chloride penetrability of concrete [41], mainly due to the binding characteristics of the SCM. CEM III type of cement have a very high Al₂O₃/ SO₃ ratio, leading to the formation of more AFm phases (and less AFt phases), increasing in this way the formation of Friedel's salt and the chemical binding of chloride ions [43]. The "not efficient" behavior of cements containing limestone, observed, is not surprising due to the very low aluminum concentration (hence reduced ability to form Friedel's salt). In general CEM II/A-L type of cements have the lowest chloride resistance [44] leading to increased penetration of chloride ions at quantities of limestone above 15% [45] and increased risk of corrosion [46].

5. Conclusions

In this study, the concept and the main principles of a software tool (based on deterministic proven predictive models) for the estimation of concrete service life, have been presented. Its structure is in full compliance with the European Standards for cement [6] and concrete [5]. Emphasis was given on the mathematical modeling of the physicochemical processes leading to concrete deterioration (due to carbonation and chloride ingress) and their outputs. In addition the results of a wide validation scheme implemented were presented, to further reinforce the effectiveness of the mathematical models used.

The tool presented offers a comprehensive approach on concrete service life estimation, in terms of:

- Defining the concrete mix design and the main chemical/volumetric characteristics of concrete.
- Estimating the compressive strength class.
- Accurately predicting the concrete service life, for carbonation and chloride exposure, by taking under consideration the relative exposure classes and by utilizing proven predictive mathematical models of the physicochemical processes leading to such deterioration.

It should also be noted that even though service life predictions are usually made in a probabilistic framework [1-3] (to account for the many uncertainties associated with the composition, processing, construction, curing/maintenance of reinforced concrete, etc.), based on the validity of the results presented in this study, this particular deterministic model can serve as a basis for modeling within such probabilistic frameworks.

By utilizing the software tool, a comparative assessment of all the SCM incorporated cement types (categorized according to [6]), also took place. The main conclusions derived from this effort are in line with other research and experimental studies and the current literature.

Overall it was shown, that specimens incorporating an SCM, whether it substitutes aggregate or cement, exhibit significantly lower total chloride content for all depths from the surface. Under carbonation exposure even though CEM II type of cements produced larger carbonation depths compared to control, certain types of CEM II cement produced a "less severe" behavior, at low quantities of SCM. A possible explanation is that at these low quantities the pore structure refinement predominates over the reduction of the carbonatable materials. Utilization of blastfurnace slag, artificial pozzolana and silica fume proved to be the most effective SCMs. The effect of slag proved to be beneficial even at larger quantities (43%, CEM III). Taking into account the reduction in clinker achieved when an SCM is utilized and the overall performance of these materials presented in this study, utilization of these types of cement not only can guarantee a durable solution (under harmful environmental agents) but they also provide a sustainable solution, by reducing the CO₂ emissions associated with the clinker burning process during cement manufacturing.

It is hoped that the results of this study will promote:

- A wider acceptance of software based predictive models in achieving feasible and durable solutions in reinforced concrete design.
- Further research on the beneficial effects of SCMs on concrete durability to foster their large-scale utilization.

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