CarboChlorCon 1.0 - software for concrete carbonation and chloride ingress

Vít Šmilauer¹, Karel Pohl¹

¹Czech Technical University in Prague in Prague, Faculty of Civil Engineering, Thákurova 7, 166 29 Prague 6, Czech Republic

Monday 10th November, 2014

Abstract

Carbonation and chloride ingress are the most relevant damaging mechanisms for steel corrosion in reinforced concrete structures. Massive utilization of supplementary cementitious materials in cement binders implies recalibration of existing models for these phenomena. Carbonation model formulated by Papadakis and model for chloride ingress from Kwon are extended for crack effect, which accelerates both damaging mechanisms. Both models were reformulated in an incremental form, allowing a gradual crack growth. It was found that crack width 0.3 mm decreases induction time approximately five times when compared to an uncracked concrete. Validation on in situ samples shows good predictions for chloride profiles.

Keywords: carbonation, chloride ingress, durability, crack, transport, induction period.

1 Introduction

Carbonation and chloride ingress are the most relevant damaging mechanisms for steel corrosion in reinforced concrete structures [1]. Extensive study of Japanese bridges in 1970's revealed serious under-prediction of life expectancy and this fact was reflected in the prescriptive-based codes later [2]. Similar situation exists today for widely used blended cements in concrete production, which were rarely used at those times.

Service life of a structure t_l has generally the form

$$l_t = t_c + t_i + t_p + t_r \tag{1}$$

where t_c is the construction phase, t_i is the initiation period, t_p stands for propagation period and t_r reflects post-repair period [3]. We aim at predicting the initiation period t_i , without going into propagation or post-repair phases. The length of initiation period is the most relevant period in service life. Concrete cover thickness over reinforcement and exposure class are the most sensitive parameters influencing length of initiation period. A new engineering model for carbonation and chloride ingress is presented. The model combines recent results from concretes made from blended cements and includes the effect of cracked concrete on the damage acceleration [4, 5, 6]. Given the cover thickness of concrete, the model predicts the end of initiation period or the beginning of propagation phase [3]. Different boundary conditions reflecting various exposure classes can be set up. The model allows simulating accelerated carbonation tests or to study the effect of early-age cracking due to excessive drying or higher mechanical load.

It is evident that the current practice in designing concrete cover thickness is too conservative. Several examples from partially-cracked concrete structures demonstrate discrepancy between older prescriptive predictions, simulations and measurements [2, 7]. The presented model opens the way to performance-based design and provides input data for more sophisticated life cycle cost analysis.

2 Model for carbonation

Carbonation depth of a sound (macroscopically uncracked) concrete has the form [8]

$$x_c = \sqrt{\frac{2D_{e,CO_2}CO_2}{0.218(C+kP)}}\sqrt{t} = A_1\sqrt{t},$$
(2)

where x_c is the carbonation depth, D_{e,CO_2} is the effective diffusivity for CO₂, C is the Portland cement content in kgm⁻³, $k \in \langle 0.3, 1.0 \rangle$ is the efficiency factor of supplementary cementitious material (SCM-slag, silica, fly ash), P is the amount of SCM in kgm⁻³, CO_2 is the volume fraction of CO₂ in the atmosphere taken as 3.6e-4 and t is the time of exposure.

The effective diffusivity in m^2s^{-1} is given by empirical equation [8]

$$D_{e,CO_2} = 6.1 \cdot 10^{-6} \left(\frac{[W - 0.267(C + kP)]/1000}{\frac{C + kP}{\rho_c} + \frac{W}{\rho_W}} \right)^3 \cdot (1 - RH)^{2.2},$$
(3)

where W is the water content in fresh concrete in kgm⁻³, C is the cement density in kgm⁻³ assumed as 3150 kgm⁻³ and RH is the relative humidity of ambient air. Eqs. (2), (3) allow predicting either carbonation depth, x_c , or induction time, t, of uncracked concrete.

Cracked concrete leads to faster carbonation. This acceleration was quantified [4], which changes Eq. (2) to the form

$$x_c(t) = (2.816\sqrt{w} + 1)A_1\sqrt{t},\tag{4}$$

where w is the crack width in mm and A_1 is the carbonation velocity according to Eq. (2). Eq. (4) allows computing carbonation depth and induction time as well. Note that crack 0.3 mm increases carbonation depth by a factor of 2.54. This also means that induction time is 6.46 times shorter compared to uncracked concrete.

In reality, crack may grow gradually over service time. Thus Eq. (4) needs to be recast into an incremental form. An increment of carbonation depth in a given time step Δt is evaluated from the total derivative of Eq. (4)

$$\Delta x_c(t) = \frac{(2.816\sqrt{w_{i+1}}+1)A_1}{2\sqrt{t_{i+0.5}}}\Delta t + \frac{2.816A_1\sqrt{t_{i+0.5}}}{2\sqrt{w_{i+0.5}}}\Delta w,$$
(5)

where w_{i+1} is the crack width at the end of a time step, $t_{i+0.5}$ is the mid-time during time integration. It is assumed that a nonzero crack increment Δw at integration time $t_{i+0.5}$ has no effect on carbonation depth, thus the term Δw can be left out. Eq. (5) allows predicting either carbonation depth or induction time of gradually cracking concrete.

2.1 Examples on carbonation

Let us consider a regular concrete made from ordinary Portland cement, w/b=0.45, C=400 kgm⁻³, W=202.5 kgm⁻³, P=50 kgm⁻³. Fly ash with almost zero calcium content is considered as a supplementary cementitious material, hence k=0.5 [8]. Let us expose the concrete to relative humidity 0.60. Consider thickness of the cover 30 mm. Assume that a crack of given width is always introduced in the beginning of exposure.

The second concrete has a lower binder content, w/b=0.45, $C=200 \text{ kgm}^{-3}$, $W=90 \text{ kgm}^{-3}$, $P=0 \text{ kgm}^{-3}$. Table 1 compares both concretes in terms of induction time as computed from Eqs. (2)-(5).

Crack width (mm)	Concrete C =400 kgm ⁻³	Concrete $C=200 \text{ kgm}^{-3}$
0.0	246	157
0.1	69.7	44.5
0.2	49.2	31.4
0.3	39.1	24.9

Table 1: Induction time for carbonation in years, two concretes, cover thickness 30 mm.

3 Model for chloride ingress

Implemented model for chloride ingress is based on Kwon et *al.* [5]. Let us consider 1D transient problem of chloride ingress into concrete with an initially zero chloride content

$$C(x,t) = C_s \left[1 - erf\left(\frac{x}{2\sqrt{D_m(t)f(w)t}}\right) \right],\tag{6}$$

where C_s is the chloride content at surface in kgm⁻³, $D_m(t)$ is the mean (averaged) diffusion coefficient at time t in m²s⁻¹, x is the position from the surface in m and f(w) gives acceleration by cracking and equals to one for a crack-free concrete. C_s and C(x,t) can be related to a concrete volume or to a binder volume, however, the units must be kept consistent through the computation.

Instantaneous diffusion coefficient D(t) for chloride ingress is assumed to decrease over time t according to the power law

$$D(t) = D_{ref} \left(\frac{t_{ref}}{t}\right)^m,\tag{7}$$

where m is a decay rate (also called an age factor). The same exponential form was employed in a new fib Model Code 2010 [9]. If m = 0, a constant value of $D(t) = D_{ref}$ is recovered; the model was proposed by Collepardi et al. [10]. Nowadays it became clear that this assumption is too conservative and is not generally recommended.

The mean diffusion coefficient $D_m(t)$ is obtained by averaging D(t) over exposure time

$$D_m(t) = \frac{1}{t} \int_0^t D_{ref} \left(\frac{t_{ref}}{\tau}\right)^m \mathrm{d}\tau = \frac{D_{ref}}{1-m} \left(\frac{t_{ref}}{t}\right)^m, \ t < t_R,$$
(8)

$$D_m(t) = D_{ref} \left[1 + \frac{t_R}{t} \left(\frac{m}{1-m} \right) \right] \left(\frac{t_{ref}}{t_R} \right)^m, \quad t \ge t_R, \tag{9}$$

where t_R is time, within which the diffusion coefficient is assumed to be constant and is generally taken as 30 years. t_{ref} corresponds to time, in which the diffusion coefficient was measured. Figure 1 shows characteristic evolution of a diffusion coefficient during 100 years.



Figure 1: Evolution of actual and mean diffusion coefficients.

The mean diffusion coefficient $D_m(t)$ increases when cracks are present in the concrete. Based on recent results, the following scaling function is proposed [5]

$$f(w) = 31.61w^2 + 4.73w + 1, (10)$$

where w stands for crack width in mm. The crack width 0.3 mm increases mean diffusion coefficient by a factor of 5.26. In reality, crack width evolves and incremental solution needs to be formulated. If crack width is incorporated, the mean coefficient $D_{m,w}(t)$ changes to Eq. (11). It is evaluated from a crack increment by differentiating Eq. (10)

$$D_{m,w}(t) = D_m(t) \int_0^{\overline{w}} 63.22w + 4.73 dw =$$
$$D_m(t) \sum_{i=0}^n \left[63.22 \left(w(t_i) + \frac{w(t_{t+1}) - w(t_i)}{2} + 4.73 \right) \right] [w(t_{i+1}) - w(t_i)].$$
(11)

In practical implementation, the values of f(w) and w are stored and Eq. (11) needs to be evaluated only in the current time step. This speeds up the solution.

3.1 Diffusion coefficients for chlorides

Proper determination of diffusion coefficients is not a trivial problem, considering various concretes, cements, inverse models and exposure conditions. Papadakis [11] presented a model for estimating intrinsic effective diffusivity for concretes made from blended cements, however, recalculation to $D_m(t)$ is not straightforward.

Our formulation allows incorporating DuraCrete model [3]. It provides usable data for estimating apparent diffusion coefficient in the form

$$D_a(t) = D_m(t) = k_e k_c D_{Cl}(t_0) \left(\frac{t_0}{t}\right)^m \gamma_{Da},$$
(12)

where $k_e \in \langle 0.27, 3.88 \rangle$ is the environment factor, $k_c \in \langle 0.79, 2.08 \rangle$ is the curing factor, $D_{Cl}(t_0)$ is the measured diffusion coefficient determined at time t_0 , $m \in \langle 0.2, 0.93 \rangle$ is the decay rate factor and $\gamma_{Da} \in \langle 1.25, 3.25 \rangle$ is the partial factor. In our notation, $D_a(t) = D_m(t)$ and $t_0 = t_{ref}$.

To our opinion, the most relevant and well documented field data come from 10year spray/splash exposure tests carried out by Luping and Utgennant [7]. Conclusions from their work state that DuraCrete model strongly underestimates long-term profile, leading to under-designed life of structure [7, pp. 50]. For this reason, we rely more on values determined on 10-year exposure under real conditions [7], which are combined with physical model according to Eqs. (6)-(10).

Table 2 summarizes the decay rate factors for concrete in a splash zone based on DuraCrete model [3, Tab. 8.6]. The chloride content at surface can be taken as 1% of a binder for the majority of cement types [7, pp. 45]. Blended cement with slag rises

the value to 2%, limestone replacement in cement as 10-15% drops the value to 0.6% [7, pp. 45].

Results from the 10-year exposure are summarized in Figure 2, which shows the apparent diffusion coefficient in dependence of water-binder ratio. In this particular case, $t_{ref} = 10$ years, m is unknown, $D_{ref} = (1 - m)D_a$, t_R can be assumed as 30 years.

Binder type	Decay rate factor m	
Ordinary Portland Cement (OPC)	0.37	
OPC + silica fume	0.39	
OPC + slag	0.60	
OPC + fly ash	0.93	

Table 2: Decay rate factor for different binder compositions in a spray/splash zone [3, Tab. 8.6].

3.2 Validation of chloride ingress in a spray zone

Validation relies on data gathered in Swedish de-icing highway environment [7]. Various concrete compositions were exposed to spray/splash environment. First, let us take an ordinary Portland cement OPC I with w/b=0.4. The reference diffusion coefficient is calculated from Figure 2 and yields the value D_{ref} =0.427e-12 m²/s. Figure 3 shows measured concentration of Cl in a binder from the two samples, demonstrating also significant variation after 1.5-year exposure.

Second, the same location and exposure was tested with concrete 95% CEM I + 5% SF, w/b=0.4. The reference diffusion coefficient from Figure 2 yields the value D_{ref} =0.325e-12 m²/s. Apparently, silica fume addition decreased D_{ref} by 24% when compared to previous concrete. Figure 4 shows reasonable predictions of profiles.

Critical chloride content for initiation of the reinforcement corrosion can be taken as 0.6% by weight of a binder [12, pp. 72]. A consistent range 0.5–0.9% is reported [3, Tab 8.7].

3.3 Example on chloride ingress in salt water

Let us consider regular concrete made from ordinary Portland cement, w/b=0.55. According to Figure 2, D_a is $2.0 \cdot 10^{-12}$ m²s⁻¹ at t_{ref} =10 years. According to DuraCrete model [3, Tab 8.6], the decay rate factor for concrete submerged in salt water corresponds to m = 0.30. In such particular case, $D_{ref} = (1 - m)D_a = 1.4 \cdot 10^{-12}$ m²s⁻¹. Figure 5 shows evolution of diffusion coefficients for this particular case.

Let us assume characteristic value $C_s = 10.3\%$ of chlorides per binder for submerged concrete without further reductions [3, Tab 8.5]. The critical level for corrosion is 1.85% per binder [3, Tab 8.7]. The concrete cover is taken as 100 mm.



Figure 2: Fitted reference diffusion coefficients for different cement types, 10-year exposure of concrete [7].

Computed induction time according to Eq. (6) is summarized in Table 3. Crack is considered since the beginning of exposure. It is apparent that a macrocrack 0.3 mm decreases induction time by an order of magnitude.

3.4 Applications

The model CarboChlorCon was used for performance-based design of concrete column elements which are located in the vicinity of a highway. This study was initiated and used by companies Eurovia CS, a.s. and Pontex, s.r.o. Carbonation was not an issue, however, chloride ingress plays a significant role. The following Table 4 shows the effect of crack widths and required induction time. It was decided to use concrete



Figure 3: Validation of chloride ingress on OPC I, w/b=0.4 [7].



Figure 4: Validation of chloride ingress on OPC I, w/b=0.4 [7].

Crack width (mm)	Induction time (years)	
0.0	74.58	
0.1	36.02	
0.2	15.70	
0.3	7.76	

Table 3: Induction time for chloride corrosion of submerged concrete, in dependence on original crack width. Cover thickness 100 mm.

cover 50 mm for expected lifetime 100 years and crack width 0.1 mm.



Figure 5: Evolution of diffusion coefficients for chlorides, w/b=0.55.

Crack width (mm)	Induction time (years)		
	30	60	100
0.0	26	31	36
0.1	35	42	49
0.2	47	56	65
0.3	60	71	83

Table 4: Required concrete cover in mm for various crack widths and induction times.

4 Conclusion

A more accurate model for carbonation and chloride ingress has been presented. It was demonstrated that a crack 0.3 mm decreases induction time $6.46 \times$ for carbonation and $5.26 \times$ for chloride ingress at least. For this reason, avoiding macrocracks is one of the most critical factors for durable structures. This can be facilitated by proper curing and suitable mix composition.

Significant scatter in short-term experimental data renders short-term diffusion coefficient questionable. Proper determination for longer exposures presents a challenging experimental task which can be circumvented by using collected chloride profiles from 10 year exposure time.

Acknowledgement

The support from Competence Centres of the Technology Agency of the Czech Republic (TACR) under the project "CESTI - Centre for Effective and Sustainable Transport Infrastructure" TE01020168 is greatly acknowledged.

References

- P. Basheer, S. Chidiact, A. Long, "Predictive models for deterioration of concrete structures", *Construction and Building Materials*, 10(1): 27 – 37, 1996.
- [2] PWRI, "Nationwide survey on airborne chloride", PWRI Technical Memorandum No. 2687 (in Japanese), Public Works Research Institute, 1988.
- [3] A. Muthena, C. Andrade, L.O. Nilsson, C. Edvardsen, et al., "DuraCrete, Final Technical Report", Technical report, , 2000.
- [4] S.J. Kwon, U.J. Na, "Prediction of Durability for RC Columns with Crack and Joint under Carbonation Based on Probabilistic Approach", *International Journal of Concrete Structures and Materials*, 5(1): 11 – 18, 2011.
- [5] S.J. Kwon, U.J. Na, S.S. Park, S.H. Jung, "Service life prediction of concrete wharves with early-aged crack: Probabilistic approach for chloride diffusion", *Structural Safety*, 31(1): 75 – 83, 2009.
- [6] H.W. Song, S.J. Kwon, K.J. Byun, C.K. Park, "Predicting carbonation in earlyaged cracked concrete", *Cement and Concrete Research*, 36(5): 979–989, 2006.
- [7] T. Luping, P. Utgennant, "Chloride Ingress and Reinforcement Corrosion in Concrete under De-Icing Highway Environment – A Study after 10 Years' Field Exposure", Sp report 2007:76, SP Sveriges Tekniska Forskningsinstitut, 2007.
- [8] V.G. Papadakis, S. Tsimas, "Supplementary cementing materials in concrete. Part I: efficiency and design", *Cem. Concr. Res.*, 32(10): 1525–1532, 2002.
- [9] J. Walraven, et al., "Model Code 2010", Technical report, Fib, 2010.
- [10] M. Collepardi, A. Marcialis, R. Turriziani, "Penetration of chloride ions into cement pastes and concrete", *Journal of the American Ceramic Society*, 55(10): 534–535, 1972.
- [11] V.G. Papadakis, "Effect of supplementary cementing materials on concrete resistance against carbonation and chloride ingress", *Cement and Concrete Research*, 30(2): 291 – 299, 2000.
- [12] P. Schiessel, et al., "Model Code 2006", Bulletin no. 34, Fib, 2006.