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# Numerical Simulation of the Influence of Water Repellent Treatment on Carbonation of Concrete

J. Heinrichs<sup>1</sup>, St. Schmeiser<sup>2</sup> and A. Gerdes<sup>1,2</sup>

<sup>1</sup>Institute for Technical Chemistry, Water- and Geotechnology, Research Centre Karlsruhe, Germany

<sup>2</sup>Faculty of Mechatronics and Science, University of Applied Sciences, Karlsruhe, Germany

## **Abstract**

Chemical and physical processes, e.g. carbonation or penetration of chlorides cause numerous damages of reinforced concrete structures. The durability of these structures can be improved using surface protective systems, e.g. water repellent treatment. But the water repellent treatment alters the drying attitude of concrete. This in turn mainly influences the process of carbonation. For an improved estimation of the corrosion risk for these structures a numerical model has been developed. The model describes the transport, storage and chemical reaction of the main influence variables for carbonation of treated and untreated concrete. The knowledge of these processes is required for the assessment of new water repellent agents and gives information about the complex interrelationship respectively. For the numerical calculation the concrete is considered as a chemical solid-state reactor by using the finite-element-program "FEMLAB".

## 1 Introduction

Nowadays the durability of reinforced concrete becomes more and more important. The term durability comprises the maintenance of load capacity and the functional efficiency of the construction over the whole service life. Most of the damage mechanisms, e.g. sulphate attack or carbonation, are based on a reactive transport. This means that starting from the material surface during the transport of concrete aggressive compounds through material components a chemical reaction takes place. The progress of this reactive transport depends on several factors, such as concetrating moisture distribution of the covercrete quality. Indeed this process needs then a lot of time. For example it can take decades until the carbonation reaches the reinforcement placed in a depth of 30 mm. But the application of preventive surface protection systems, e.g. water repellent treatment can change the rate of carbonation. Therefore, a modification of the moisture distribution of the concrete is responsible which strongly affects the carbonation.

The recent state of knowledge is ambiguous, hence the main focus of this work is on the modelling of the carbonation of concrete treated with water repellent agents. On one hand side there are references that the rate of carbonation is reduced in treated concrete. On the other hand there are experimental investigations which reveal that treated concrete carbonates faster. Therefore this question must be clarified before water repellent treatment can be applied in a common way. A requirement for the application of water repellent treatment in bigger scales is to clarify this question.

In the introduced approach the porous cementious material is considered as a chemical solid-state reactor. For the simulation the especially for modelling of solid-state reactors designed program "FEMLAB" was chosen.

# 2 Numerical investigation

### 2.1 Software

The numerical modelling was performed with the finite-element program "FEMLAB" (Version 3.0) distributed by Comsol. This program offers the opportunity to simulate complex physical and chemical processes which can be described by partial differential equations.

One main advantage of this program is the coupled analysis of different processes by using the option "multiphysics". Here the user has access to an extensive model library with predefined applications which can be adjusted by the input of material parameters. The program also offers in an equation based modus the chance to define partial differential equations (PDE-modus). The numerical simulations can be realised in 1D, 2D or 3D. Furthermore "FEMLAB" offers the solution of linear, non-linear, stationary, time-dependent and Eigenvalue problems.

To simulate carbonation processes in concrete "FEMLAB" provides the "Chemical Engineering" modul. In this modul mass balance like e.g. diffusion, convection, or Navier-Stokes-equations can be solved. In this case only physical and chemical material parameters have to be defined, the corresponding equations are formulated automatically by "FEMLAB".

## 2.2 Modelling

## 2.2.1 Preliminary remarks

Validation of the model can not be shown yet, since by now corresponding experiments are still in the process. Instead well-known models from literature were used to describe transport processes [4 - 10].

For the simulation following assumptions are specified:

Two types of concrete specimens, untreated and treated with a water repellent agent, with a water-cement ratio of 0.5 and a cement content of 350 kg/m³ were investigated. In case of the treated concrete specimen the numerical model contains 2 layers. The assumed properties of these layers are listed in Table 1.

In different parameter studies the penetration depth in treated concrete specimen is varying between 1 and 10 mm and specimen geometry is varying between 4 and 32 cm in length.

All surfaces of the specimens except the front surface have been sealed. In this way unidirectional transport processes like moisture and  $\rm CO_2$  transport was enforced. Hence the model can be reduced to a one dimensional problem.

In the beginning of the investigation concrete specimens are completely saturated by water (100% pore humidity corresponds to  $w_s = 110 \text{ kg/m}^3$ ).

Constant environmental conditions are presumed, i.e. temperature is 20 °C and relative humidity of the surrounding air is 75 %.

 ${\rm CO_2}$  concentration  $c_{max}$  is assumed to be 0.6 g/m³. This value represents the concentration in the atmosphere.

All transport processes are described by Fick's 1. law, which is described in the following chapter.

## 2.2.2 Model formulation of carbonation

Carbonation is based on a sequence of different reactions. Simplified it can be expressed by the following equation:

$$Ca(OH)_2 + CO_2 \xrightarrow{H_2O} CaCO_3 + H_2O$$
 (1)

Carbonation takes place when  $\mathrm{CO}_2$  from the surrounding air migrates through the pores into the concrete and reacts dissolved in the pore solution with the cement  $\mathrm{Ca}(\mathrm{OH})_2$  in the aqueous solutions. Thereby carbon dioxide is only transported via diffusion through air filled pore volume of the concrete. Diffusion of carbon dioxide through aqueous solution can be excluded here. When the carbonation front reaches the reinforcement, where in consequence of the declining pH-value in the carbonated part reinforcement corrosion can occur.

Following conditions affect carbonation:

- carbon dioxide concentration of the surrounding air,
- concrete moisture,
- chemical composition of the concrete,
- concrete quality.

Carbon dioxide transport can be described by Fick's 1. law of diffusion, see below, equation (2).

$$\delta \frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R \tag{2}$$

The driving force for diffusion is the gradient of carbon dioxide concentration c. Parameter D denotes the diffusion coefficient of  $CO_2$  in concrete. The reaction of  $CO_2$  is described by the reaction rate R.

## (a) Determination of diffusion coefficient D

The diffusion coefficient of  $CO_2$  can not be determined experimentally, because of the reaction of cement with  $CO_2$  while carrying out the tests. Therefore the diffusion coefficient is estimated by using the inert gas oxygen. Diffusion coefficient  $D_0$  of oxygen is assumed to be 3.8e-8 m²/s by Bunte [1]. That depends on temperature  $\vartheta$  ( $f_{T,D}$ ), concrete moisture  $\varphi$  ( $f_{H,D}$ ), described by regression parameters  $a_1 - a_4$  (see Figure 1), and structural changes in the pore void due to carbonation ( $f_{KG,D}$ ), equations (4 - 6). The latter is expressed by the carbonation degree KG, equation (11), and depends on the material specific parameter  $m_B$ .

Diffusion coefficient D can be expressed by equation (3) [1, 8]:

$$D = D_0 \cdot f_{T,D} \cdot f_{H,D} \cdot f_{KG,D} \tag{3}$$

$$f_{T,D} = \frac{9 + 273}{293} \tag{4}$$

$$f_{H,D} = a_1 + \frac{a_2}{1 + (a_3 - a_3 \cdot \varphi)^{\alpha_4}}$$
 (5)

$$a_1 = 0.993$$
  $a_2 = -0.974$   $a_3 = 3.621$   $a_3 = 5.75$ 

$$f_{KG,D} = \exp[m_B \cdot KG] \tag{6}$$

## (b) Determination of reaction rate R

The consumption of  $CO_2$  during the reaction with  $Ca(OH)_2$ , equation (1), is characterised by the input of the parameter R. This term is regarded as a "sink term" and describes the reaction rate  $v_r$  of carbonation, which is influenced by temperature  $T(f_{T,R})$ , concrete moisture  $\varphi(f_{H,R})$ , formed by the parameters  $b_1$  -  $b_4$  (see Figure 1), the  $CO_2$  concentration  $c(f_{K,R})$ , carbonation degree  $KG(f_{KG,R})$  as well as by concrete specific parameter, equation (8 - 11).

Reaction rate *R* can be expressed by equation (7) [8, 10]:

$$R = v_r = \alpha \cdot f_{T,R} \cdot f_{H,R} \cdot f_{K,R} \cdot f_{KG,R} \tag{7}$$

Saetta [10] derived the reaction rate k of the carbonation from the Arrhenius approach for temperature dependent reactions. A is the frequency factor,  $E_0$  denotes the activation energy for reaction (both are empirical constants),  $R_W$  is the gas constant of water vapour and  $\alpha$  describes the influence of an open system.

$$f_{T,R} = k = A \cdot \exp\left[-\frac{E_0}{R_w T}\right] \tag{8}$$

$$f_{H,R} = b_1 + \frac{b_2}{1 + (b_3 - b_3 \cdot \varphi)^{b_4}} \tag{9}$$

$$b_1 = -0.0066$$
  $b_2 = 1.0066$   $b_3 = 3.50$   $b_3 = 4.00$ 

$$f_{K,R} = \frac{c}{c_{max}} \tag{10}$$

$$f_{KG,R} = 1 - KG$$
, mit  $KG = \frac{g}{g_{\text{max}}}$  (11)

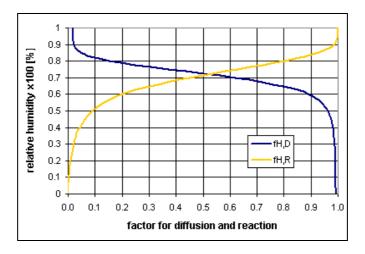
The carbonation degree KG describes the progress of reaction between calcium hydroxide and carbon dioxide and is expressed by the amount of bound carbon dioxide g and the maximum bonding capacity  $g_{max}$  towards  $CO_2$ .

In Figure 1 the influence of moisture on the diffusion of carbon dioxide and the following reaction with calcium hydroxide in concrete is shown.

In both processes a strong moisture dependency is obvious. At a relative humidity higher than 90 %, the reaction rate is high, but no diffusion of  $\rm CO_2$  takes place through the saturated pores. At a relative humidity below 50 % reaction almost stops, whereas here the carbon dioxide is able to migrate unhindered through the dry pore void of the concrete.

## 2.2.3 Model formulation of moisture transport

In porous materials moisture is only transported and stored in the pores. The size and shape of the pores is mainly dependent on the water-cement-ratio. The transport of moisture in concrete is based on several transport mechanism each with different driving forces. Of main importance is the liquid transport, consisting of capillary conduction and surface diffusion, and the



**Figure 1:** Influence of relative humidity on the reaction rate of carbonation (fH,R) and CO<sub>2</sub> diffusion coefficient (fH,D) respectively

water vapour diffusion. The reason for the liquid transport is a capillary pressure gradient. As the distribution of the capillary pressure in porous materials is unknown, *Krischer* [5] uses the liquid water content  $w_f$  as driving potential. The reason for water vapour transport is the water vapour partial pressure p. The balance equation of the moisture content can be expressed by an approach with the 1. diffusion law by *Fick*, equation (12) [6 - 8].

$$\left[\frac{\partial w_f}{\partial t} + \nabla \cdot (-D_f \nabla w_f)\right] + \left[\frac{\partial w_g}{\partial t} + \nabla \cdot (-D_g \nabla p)\right] = R \tag{12}$$

Regarding mono-layered structures, e.g. untreated concrete, the material moisture can be reduced to the liquid water content  $w_{\rm f}$ , because the gaseous fraction  $w_{\rm g}$  is very small compared to the total water quantity.

In multi-layered structures with complex pore-systems, e.g. concrete with water repellent agents, the several layers have different adsorption-desorption isotherms and diffusion coefficients, The morterial moisture for the two layers must also be taken into account. For the mathematical specification the equation (12) must be transformed in a potential dimension. For that the relative humidity  $\varphi$  was selected, equation (13) [2].

$$\delta \frac{\partial \varphi}{\partial t} + \nabla \cdot (-D\nabla \varphi) = R \tag{13}$$

The conversion in this potential dimension was made by the factor  $\delta$ , equation (14). The first term displays the time-dependent alteration of the liquid water and the second term the alteration of water vapour. The value in the brackets displays the volume of the gas-filled pore space. The connection between the content of liquid water  $w_f$  and relative humidity  $\varphi$  is performed by the moisture storage function, equation (15).

$$\delta = c_H^H = \frac{\partial w_f}{\partial \varphi} + \frac{p_s}{R_w T} \left( \psi - \frac{w_f}{\rho w} - \frac{\varphi}{\rho w} \frac{\partial w_f}{\partial \varphi} \right)$$
 (14)

$$w_f = f(\varphi) = w_s \frac{(k-1)\varphi}{k-\varphi} \tag{15}$$

The characterisation of the moisture storage function for the untreated concrete is performed by an approximation function, derived from the BET-theory by  $K\ddot{u}nzel$  [7]. In this approach  $w_s$  is the saturated water content of the concrete and k is an approximated parameter which can be calculated by the equilibrium water content at 80 % relative humidity.

## (a) Determination of moisture diffusion coefficient D

For the untreated concrete the moisture diffusion coefficient D consists the coefficients of the gaseous water  $D_g$  and liquid water  $D_f$ , equation (16) [8]. For the treated concrete only the moisture vapour diffusion coefficient  $D_g$  is essential, see Table 1.

$$D = D_f + D_g \tag{16}$$

The moisture vapour diffusion coefficient  $D_g$  is shown in equation (17):

$$D_{g} = D_{g0} \cdot p_{s} \tag{17}$$

It has to be mentioned that  $D_g$  is constant for the whole drying period which means it is independent from the material moisture content. The determination of this coefficient is based on the ideal gas equation, water vapour diffusion resistance index  $\mu$  and the water vapour saturation pressure  $p_s$ , which is temperature g dependent, equations (18 - 20) [4].

$$p_s = 610.78 \cdot \exp\left[\frac{a\,\mathcal{G}}{b+\mathcal{G}}\right] \tag{18}$$

a = 17.08 b = 234.18°C für  $\theta \ge 0$ °C

$$D_{g0} = \frac{D_D}{\mu R_w T} \tag{19}$$

$$D_D = 2.3 \cdot 10^{-5} \frac{P_0}{P} \left(\frac{T}{273}\right)^{1.81}$$
 (20)

The calculation of liquid transport coefficient  $D_f$  is demonstrated in equation (21) [4]:

$$D_f = D_{wf} \frac{\partial w_f}{\partial \varphi} \tag{21}$$

Thereby  $\partial_{W_f}/\partial \varphi$  is the derivation of the moisture storage function. The liquid transport coefficient is mainly influenced by the material moisture and the temperature  $\mathcal{G}$ . *KiessI* [4] developed an exponential function, which can be described by the moisture conducting parameter of the dry concrete  $D_{f,tr}$  (for w=0) and the water saturated concrete  $D_{f,s}$  (for  $w=w_s$ ), equation (22).

$$D_{wf} = D_{f,tr} \exp \left[ \frac{w}{w_s} \ln \frac{D_{f,s}}{D_{f,tr}} \right] \left( \frac{9}{40} + 0.5 \right)$$
 (22)

Because of the moisture balance that has to be equilibrated with the hygric environmental conditions, on the material surface exchange processes with the environment take place. This is also taken into account in the numerical

model. The exchange of the moisture amount  $q_H$  normal to the surface follows as described in equation (23) [8]:

$$q_H = k_c \left( c_b - \varphi_O \right) \tag{23}$$

In this equation  $k_c$  is the moisture transfer parameter and  $c_b$  is the relative humidity of the ambient air, being dependent on temperature and pressure.

# (b) Determination of parameter R

The water produced due to the process of carbonation is an additional water source R within the concrete. Indeed this is not considered in the numerical model, this means R = 0 (Table 1). In a fully with water repellent treated layer no carbonation does appear and therefore R is also 0.

## 2.2.4 Model formulation of water repellent treatment

The water repellent agent penetrates by capillary transport into the concrete boundary layer. A hydrophobic silicon film is then formed by a chemical reaction. In the hydrophobic zone moisture transport takes place only via diffusion. It is further assumed that in this area no carbonation takes place [3]. A list of the assumed parameters for the specific transport processes, described by *Fick's* law, is given in Table 1. The list is subdivided regarding the water repellent treated part and the untreated part of the concrete.

Since there is no reaction of the  $CO_2$  in the treated section, R is equal zero. The  $CO_2$  diffusion coefficient depends on temperature  $(f_{T,D})$  and a factor which describes the alteration of the pore void due to water repellent treatment  $(f_{B,D})$ . This factor attenuates the diffusion coefficient value of the water vapour,  $D_g$ , as well. Since numerical modelling uses the relative air humidity as the driving potential, the parameter  $\delta$  is introduced. The value  $\psi$  denotes the pore volume.

On the basis of these parameters the numerical model for carbonation inside a water repellent treated concrete can be simulated.

# 3 Results and discussion

## 3.1 Preliminary remarks

As already mentioned in chapter 2.2.2, essentially the progress of carbonation depends on the moisture distribution of concrete. For that reason at first, the drying of concrete has to be simulated in some investigations at first. In

**Table 1:** Compilation of assumed parameter R, D, and  $\delta$  for the two transport processes in each concrete layer, i.e. the water repellent treated part and the untreated part

|                                | treated                               | untreated  |
|--------------------------------|---------------------------------------|--|
| CO <sub>2</sub> -<br>transport | R = 0                                 | $R = -\alpha \cdot f_{T,R} \cdot f_{H,R} \cdot f_{K,R} \cdot f_{KG,R}$ |
|                                | $D = D_0 \cdot f_{T,D} \cdot f_{B,D}$ | $D = D_0 \cdot f_{T,D} \cdot f_{H,D} \cdot f_{KG,D}$                   |
|                                | $\delta = 1$                          | $\delta = 1$   |
| moisture<br>transport          | R = 0                                 | R = 0  |
|                                | $D = D_g \cdot f_{B,D}$               | $D = (D_g + D_f) \cdot f_{KG,D}$                                       |
|                                | $\delta = \frac{p_s}{RT} \psi$        | $\delta = c_H^H$   |

parameter studies the penetration depth of the treated layer and specimen length is varying, respectively. On the basis of these investigations the calculation of the carbonation progress has to be made.

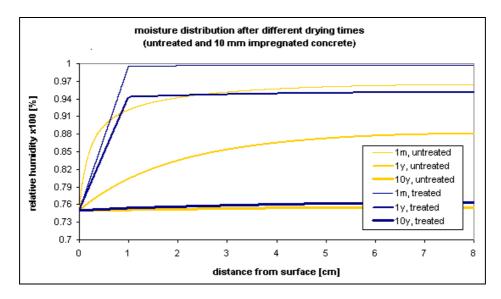
## 3.2 Moisture transfer

# 3.2.1 Introduction

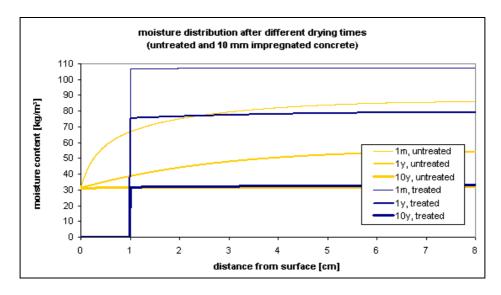
By means of the diffusion coefficients (liquid and water vapour) defined in equation (16), the moisture profile as function of drying time can be calculated.

Figure 2 and Figure 3 show the moisture distribution of an untreated concrete and a treated concrete with a 10 mm penetration depth (w/c = 0.5 and  $w_{\rm S}$  = 110 kg/m³) after different drying times (1 month, 1 year and 10 years). As described in chapter 2.2.3 the driving potential by the capillary transport and the water vapour diffusion can be calculated by the relative humidity  $\varphi$ . The result is a moisture distribution beyond the specimens length in percent, Figure 2. An important fact in this case is the existence of vapour water, only. In contrast to liquid water, the amount of water as water vapour is very low. That means the water content of the untreated and the treated concrete is uncomparable to each other in the first 10 mm. Therefore the moisture has to be denoted in kg/m³, Figure 3.

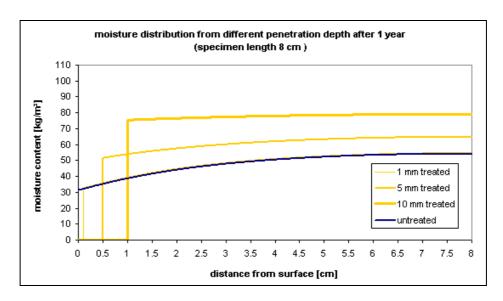
Water vapour transport proceeds only in the impregnation layer, which has an important influence on drying of concrete. That's why Figure 2 and Figure 3 show a clear difference between the untreated and the treated concrete.



**Figure 2:** Moisture distribution of an untreated concrete specimen and a treated concrete specimen with 10 mm penetration depth after different drying times, referred to the relative humidity in %.



**Figure 3:** Moisture distribution of an untreated concrete specimen and a treated concrete specimen with 10 mm penetration depth after different drying times, referred to the material moisture in kg/m³.



**Figure 4:** Moisture distribution of an 8 cm concrete specimen with different penetration depths of the water repellent layer after one year (w/c = 0.5).

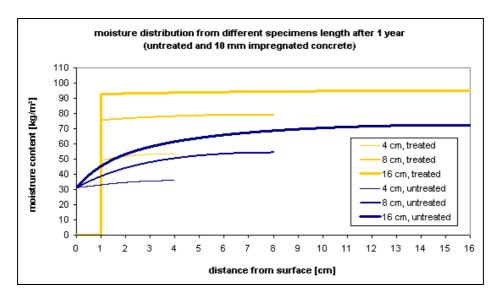
While the treated concrete specimen is showing nearly 100 % of moisture content in a depth of 10 mm after one month, the untreated specimen dried already out to a value of 92 %. That corresponds to a moisture content of approximately 67 kg/m³. Even after one year there is a big difference between the specimens. After 10 years both specimens reach the moisture balance of 75 % ( $w_f = 31 \text{ kg/m}^3$ ).

Furthermore, the treated concrete specimen is forming a horizontal plateau directed to the water repellent layer, which will be kept until the moisture balance is reached. The water content in the water repellent layer is nearly zero. The untreated concrete shows on the other hand a steady developed moisture profile.

Because of the different moisture profiles it is presumed, that this fact has a strong influence to the carbonation, which is even influenced by the moisture content.

# 3.2.2 Different penetration depth of the water repellent layer

The thickness of the water repellent layer can be controlled and depends on different products of water repellent treatment that is used. That's the reason why it is necessary to take a statement about the drying behaviour of treated concrete with different penetration depths.



**Figure 5:** Moisture distribution of an untreated and a water repellent treated concrete specimen with a penetration depth of 10 mm with different specimen lengths after one year (w/c = 0.5).

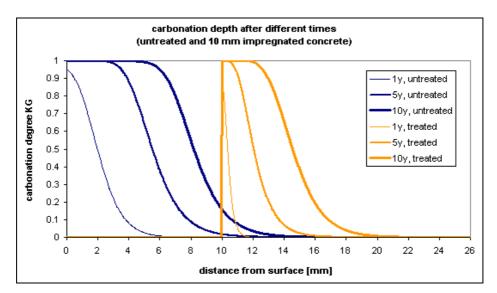
The results are represented in Figure 4 after a drying time of one year. Penetration depths of 1 mm (corresponding to an emulsion), 5 mm and 10 mm (for example with an Octyltriethoxysilan) were surveyed. The total length of the concrete specimens is 8 cm.

Figure 4 shows that a reduction of the penetration depth of the impregnation effects a faster drying. Then the moisture profile is approaching to an untreated concrete. With a penetration depth of 1 mm the treated concrete specimen corresponds to the drying behaviour of an untreated concrete. Experiments of *Gerdes* [3] supporting this result.

# 3.2.3 Different specimen length

Another parameter, which could influence the drying process is the specimen length. For this reason a moisture distribution profile for 4 cm, 8 cm and 16 cm concrete specimens (w/c 0.5) has been calulated for a duration of drying of one year. Now an untreated and a water repellent treated concrete with a penetration depth of 10 mm are surveyed. The results are compiled in Figure 5.

Figure 5 shows, that the drying process depends strongly on the specimen length. With an increasing length of the concrete specimen increased the time which is needed to reach the balance in moisture content. The reason



**Figure 6:** Temporal distribution of the carbonation of an untreated and a water repellent treated concrete specimen with a penetration depth of 10 mm (8 cm concrete specimen, w/c = 0.5).

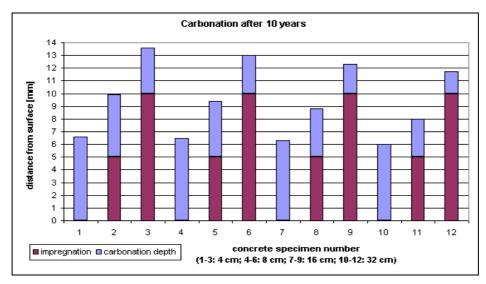
is the higher volume of the water reservoir. This provides the capillary transport of water from the interior of the specimen to the covercrete.

Furthermore, the length of the specimen has a stronger influence to the moisture content of a treated concrete specimen than of an untreated concrete specimen. In that way it can be expected that the progress of carbonation will be change significantly.

# 3.3 Carbonation

Basis to the calculation of carbonation constitutes on one hand the approach of the diffusion coefficient for carbon dioxide in concrete with equation (3) and on the other hand on the reaction rate, equation (7). Both parameters depend on the moisture distribution in concrete, Figure 1. So the drying has to be taken into account. On this condition a time-dependent carbonation profile can be calculated. Further factors influence the carbonation. But these are not taken into account in the computer model, for example the liberated water of carbonation (hence simplified stoichiometric calculation follow: by 1 g CO<sub>2</sub> result to 0.41 g H<sub>2</sub>O), equation (1). This is an additional water source in the interior of concrete.

Figure 6 shows the results of an untreated and treated concrete specimen with a penetration depth of 10 mm after 1, 5 and 10 years drying. Carbona-



**Figure 7:** Carbonation depths of different concrete specimens after 10 years (untreated, 5 mm and 10 mm water repellent treated layer, specimen lengths of 4, 8, 16 and 32 cm)

tion will be expressed with the carbonation degree *KG*. The specimen length is 8 cm and the w/c is 0.5.

The carbon dioxide migrates through the impregnated layer easily without any chemical reaction. Hence the carbonation process starts behind the water repellent layer. This should lead to a higher carbonation depth compared to untreated concrete under the same conditions.

Figure 7 shows the calculated carbonation depths for several concrete specimens, depending on different specimen lengths (specimen 1 - 3: 4 cm, specimen 4 - 6: 8 cm, specimen 7 - 9: 16 cm and specimen 10 - 12: 32 cm) and on different penetration depths of the water repellent layer. The carbonation depth is defined for a carbonation degree of 0.9.

The unambiguous trend is obvious: the carbonation depth for the untreated concrete is sligthly reduces with an increasing specimen length. For the treated concrete the following can be mentioned. The carbonation depth of these specimens is significantly higher compared to the untreated specimens. With increasing length of the treated specimen the carbonation depth decreases. This goes along with an reduction of the thickness of the carbonated layer. Furthermore, carbonation is significantly lower in a treated concrete. But then the carbonation front is deeper as a result of th non-carbonable impregnated layer, Figure 6.

Out from that in the follwoing an example is given to show the influence of water repellent treatments on the carbonation rate. For example, if the carbonation front reaches the reinforcement, which is located in a depth of 30 mm, the corrosion risk increase. Assuming a length of 32 cm for the concrete member Starting from this point of view for the concrete member with a length of 32 cm the carbonation front will reach the reinforcement after 145 years. In comparision to that for the treated concrete specimens the carbonation front reach the reinforcement earlier (5 mm penetration depth – approximately 125 years and 10 mm penetration depth – approximately 120 years). The dimensions of the concrete specimens (9 - 11) corresponds more to a real building as the specimens 1 - 9 and therefore, they are more realisitc.

Further decisive factors for the carbonation progress are the seasonal change of relative humidity and the temperature. Likewise rain and drying periods influences the carbonation. If these factors are considered, eventually the carbonation would continue slowly as shown. So the calculation demonstrates only a labour test, i.e. with constant surrounding conditions (drying to 75 % relative humidity). Experiments should validate the existing numerical model.

## 4 Conclusions

From the results the following conclusions can be drawn:

- The interaction of chemical and physical processes, i.e. drying and carbonation of untreated and treated concrete specimens, was realised in a numerical model to investigate the corrosion risk of reinforced concrete structures. FEMLAB is a suitable program for the simulation of reactive transports. The results of these investigations are important for the application in practice and for further development of water repellent systems.
- It is shown, that the drying behaviour of treated and untreated concrete specimens is quite different. This shows the results of a parameter study varying penetration depth and geometry of the specimens. Both parameters have a strong influence on drying and out of it on the carbonation. This could be an explanation for the different results in literature about the carbonation of water repellent treated concrete. In these studies the geometry of the test specimens was not taken into consideration. For example, the carbonation process is delayed with an increasing specimen length because the drying rate is lowered and consequently liquid water in the pores hinders the carbon dioxide to migrate into the concrete.

- For the realistic simulation of the carbonation process of treated concrete other factors such as the climatic conditions, liberating of water due to the carbonation process or the influence of cracks must be taken into account.
- The results of the simulation indicate that for concrete members with a thickness of 32 cm the carbonation front do not reach the reinforcement during a typical servce life of 100 years.

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