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Limitations of FEM modelling of chloride diffusion when considering different parameters of binary and ternary concrete mixtures

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Abstract: The numerical modelling of chloride diffusion in concrete structures requires an appropriate description of input parameters. The main inputs for the model are the diffusion coefficient of concrete and derived aging factor. The model itself can be susceptible to the values of these parameters because of the size of the finite elements and size of the time step. Due to the potential use in probabilistic calculations, which requires millions of simulations, it is desirable to create a highly optimized model. It is important to pay attention to the accuracy of the calculation, but also to its calculation time. The presented results show the possible limits of the finite element model of the diffusion in a concrete structure. This is demonstrated on the reference ordinary Portland cement mixture and 32 various binary and ternary concrete mixtures, which show a significant effect of different diffusion coefficients and aging factors on the overall convergence. This study provides guidance on which extreme material parameters, out of the potential range, may adversely affect model results.

Keywords: numerical analysis, chlorine, concrete, high-performance concrete, binary and ternary mixtures

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Introduction

The durability and sustainability of reinforced concrete structures designed for long-term usages, such as bridges, are a significant issue. The assessment of durability, maintenance and repair of these structures during their lifetime, including demolition, is subsequently assessed based on many aspects (Martín-Pérez et al., 2000; Tikalsky, Pustka & Marek, 2005; Hooton, 2012; Teplý & Vořechovská, 2012; FIB, 2013).

The financial and social impacts are significant problems; therefore, a great deal of emphasis is placed on the design of material parameters. These material parameters enter the numerical calculations and can significantly affect the designing of structures in various ways. It is, therefore, necessary to consider the design of mixture, structural design, statistical evaluation, numerical modelling and all of the associated aspects as a complex problem. Lifetime assessment and relevant test methods are still under development (Glass & Buenfeld, 1997; Han, 2007; Bitaraf & Mohammadi, 2008; Marsavina et al., 2009; Vořechovská et al., 2009; Ghosh, Hammond & Tikalsky, 2011; Yao et al., 2016; Ghosh et al., 2017; Teplý & Podroužek, 2017; Sun et al., 2018).

The estimated lifespan of a reinforced concrete bridge when modelling of the corrosion process can be divided into an initial and a propagation period. This article deals with the first part of the corrosion process. The article is primarily focused on the optimization of the Finite Element Method (FEM) model, considering different input values of material parameters. The discussed 2D FEM model (Lehner & Konečný, 2015) serves to solve the chloride diffusion on the concrete layer using the Fick's second law of diffusion. The model describes the transport of chloride ions across the reinforced concrete bridge deck and estimates the chloride concentration at the reinforcement level. The evaluation of the accuracy of the selected concrete mixtures were discussed in (Lehner, Konečný & Brožovský, 2016; Lehner & Konečný, 2019), where it turned out that it is necessary to take into account the limits for the value of the maturation coefficient, as there is a problem with the convergence of the results.

The results of the 2D numerical model were compared to the 2D analytical equation for time-dependent chloride penetration, including the aging effect. In this study, the new results calculated on a large set of material parameters (Ghosh & Tran, 2015; Lehner, Ghosh & Konečný, 2018) are shown. The maturing of concrete has a significant decreasing effect on the diffusion coefficient over time (Thomas & Bamforth, 1999), which means that the ability of chloride ions to penetrate the concrete decreases in time. Hence, the expected corrosion initiation time can be extended, as theoretically derived from laboratory and numerical experiments (Lehner & Konečnỳ, 2016).

In the case of binary and ternary based high-performance concrete (HPC) mixtures, the concrete maturing process takes longer. Thus, the diffusion parameters and aging factors can be out of the potential range. The diffusion coefficient is a time dependent parameter with a model formulated according to (Mangat & Molloy, 1994; Hooton, 2012) as follows:

$$D_{c,t} = D_{c,28}\left(\frac{t_{28}}{t}\right)^{m} \tag{1}$$

where:

$D_{c,t}$ – the diffusion coefficient for a selected age [m^2/s],
m – the aging factor describing the decrease of diffusion coefficient over the period of measurement for concrete in time t [years],
t_{28} – the age related to the diffusion coefficient [years],
$D_{c,28}$ – diffusion coefficient at a reference period, e.g. 28 days [m^2/s].

It is evident from this equation that the aging coefficient has a major effect on the diffusion coefficient values at later times of the structure's service life. Therefore, it is assumed that the extreme values of the m-factor can produce an inaccurate result in the numerical solution of the chloride diffusion process. Thus, evaluating the effect of the diffusion coefficient and the aging factor to the stability and precision of the numerical solution of chloride ion diffusion is an important issue discussed herein, especially with the application of progressive HPC mixtures.

1. Probabilistic assessment of reliability and analytical solution

The parameters of concrete typically show random variability as reported in the studies based on the probabilistic durability prediction (Stewart & Rosowsky, 1998; Janas, Krejsa & Krejsa, 2009; Teplý & Vořechovská, 2012). The basic recommendations for parameters or distribution of the diffusion coefficient with the aging effect are proposed in (FIB, 2013; Ghosh et al., 2017; Lehner, Ghosh & Konečný, 2018). The time dependent variability of the diffusion coefficient is described extensively in (Lehner, Ghosh & Konečný, 2018).

However, the limitations induced by parameters with values extremely out with the average are not considered in the finite element studies. As shown in the article (Lehner & Konečný, 2019), there are certain values of the diffusion coefficient and aging factor that yield significant inaccuracies. In this case, it was necessary to reduce the size of the finite element and the time step of the nonlinear calculation, which resulted in an extreme increase of the calculation time. However, this procedure is unsuitable for the probabilistic calculations because the combination of a large number of simulations and a long calculation time is undesirable. Due to this fact, a study that evaluates an effect of a large value of real parameters would be helpful, because it can carry out the specific limits of calculation. It was necessary to find out at what value the diffusion coefficients and maturation coefficients have a significant effect on the deceleration of the calculation and possibly on the inaccuracy of the results.

2. Analytical solution

The modified 2D analytical model was used to determine the accuracy of the results. The constant diffusion coefficient for concrete applied in (Yao et al., 2016) is modified considering the aging factor (Mangat & Molloy, 1994). The result equation was presented in the conference paper (Lehner & Konečný, 2019):

$$C(x,z,t) = C_0\left\{1-\left(\frac{x}{2\sqrt{\frac{D_{c,i}}{1-m}t^{1-m}}}\right)\left(\frac{z}{2\sqrt{\frac{D_{c,i}}{1-m}t^{1-m}}}\right)\right\} \tag{2}$$

where:

$C_{x,z,t}$ – concentration of chlorides [% by mass of total cementitious materials] at time t [s] and location x, z [m],

C_0 – concentration of chlorides [% by mass of total cementitious materials (%/cem)] at the surfaces (in this case at the two perpendicular adjacent sides),

$D_{c,i}$ – diffusion coefficient of chloride ions in concrete at reference time one second [m^2/s] (the same coefficient in both directions were assumed),

t – chloride exposure time [s],

x, y – locations of investigated point [m],

m – aging factor [–] (the same coefficients in both directions were assumed).

3. Numerical finite element model

The article (Lehner & Konečný, 2019) dealt with two possibilities of optimization of 2D chloride diffusion finite element model. The optimization of the size of finite elements and the size of the time step was introduced. In this article, the basic input parameters of the model are considered the same as in the previous task. The width of the modelled cross section is 25 cm, thickness is 25 cm, the investigation time is 100 years, and the surface chloride concentration is 0.6%. In papers (Lehner, Konečný & Brožovský, 2016; Lehner & Konečný, 2019) the ideal size of element for this example was evaluated as 1 cm. Equally, equation (3) has been shown as ideal for determining the time step in most cases, even though the computation time can be longer:

$$\Delta t \leq \frac{\Delta x \times \Delta z}{D_{c,ref}} \tag{3}$$

where:

Δt – minimum value of time step [–],

Δx, Δz – dimensions of finite element [m],

$D_{c,ref}$ – a reference diffusion coefficient [m^2/s].

The presented article does not contain a description of the model or a derivation of the finite element, but further information can be found for example in (Konecny & Lehner, 2017). The model can be exposed to a given chloride concentration loading from the top and the side surfaces (Fig. 1).

When using the model, the chloride concentration value can be determined anywhere in the structure. The example of a graphical output of the node mesh and chloride concentration at a specific time is given in Figure 1.

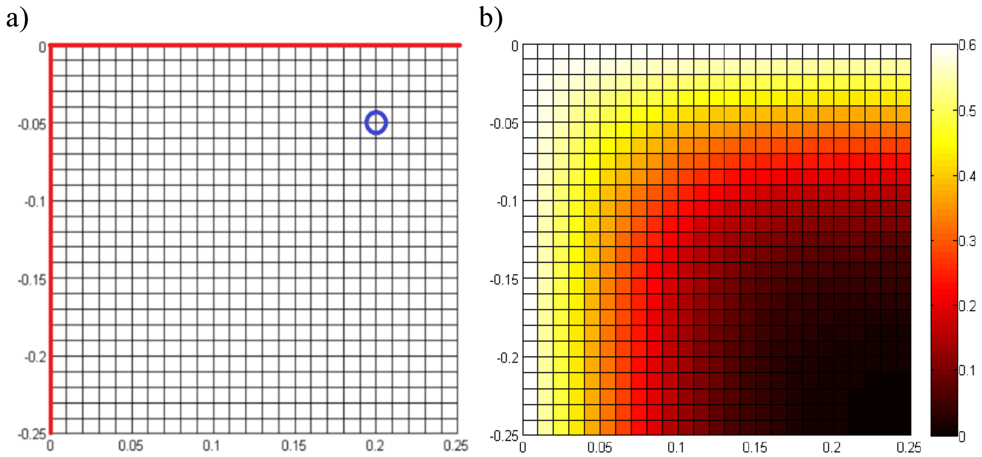

Fig. 1. The mesh of nodes with chloride loading (red lines) and the point of interest (a), Example of graphic output of the concentration of the chlorides on the selected concrete cross section from the FEM model (b) (*own study*)

4. Material properties and parametric study

Thirty-three different mixtures from the series of laboratory tests (Ghosh & Tran, 2015) were selected for numerical testing. For these mixtures, different behaviour can be expected, due to the larger differences between the reference diffusion parameter and the aging factor.

The reference mixture was made of ordinary Portland cement (OPC), and 32 mixtures were prepared as high-performance binary and ternary concretes (HPC). The basic parameters of all considered mixtures are shown in Figure 3 (Lehner, Ghosh & Konečný, 2018; Konečný et al., 2020).

In the first phase of the analysis, the minimum and maximum values for the diffusion parameters and the m-factor were taken from the set of values. These values were used for a parametric study to determine the effect of input parameters on concentration results obtained from the FEM model (Fig. 2). The values of concentration were investigated in the depth of reinforcement (0.05 m) and at the distance of 0.20 m from sideloading (Fig. 1).

The classification of $D_{c,(28)}$ and m-factor is related to the relationship with the ability to resist chloride penetration. A high value of $D_{c,(28)}$ means low resistance at the age of 28 days. High m-factor means a big increase of resistance over time. The name of the mixture (ID) is derived from the amount of cementitious material.

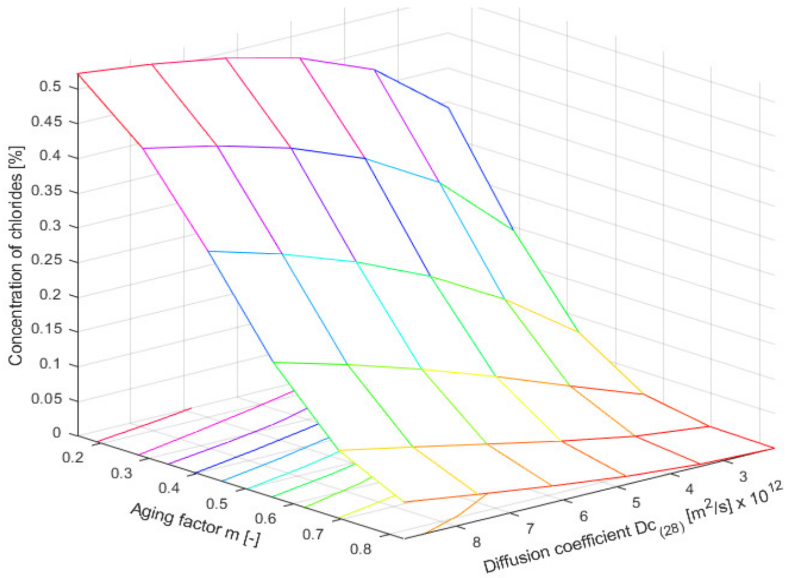

Fig. 2. Results of parametric study of influence of diffusion coefficient and aging factor to the concentration of chlorides

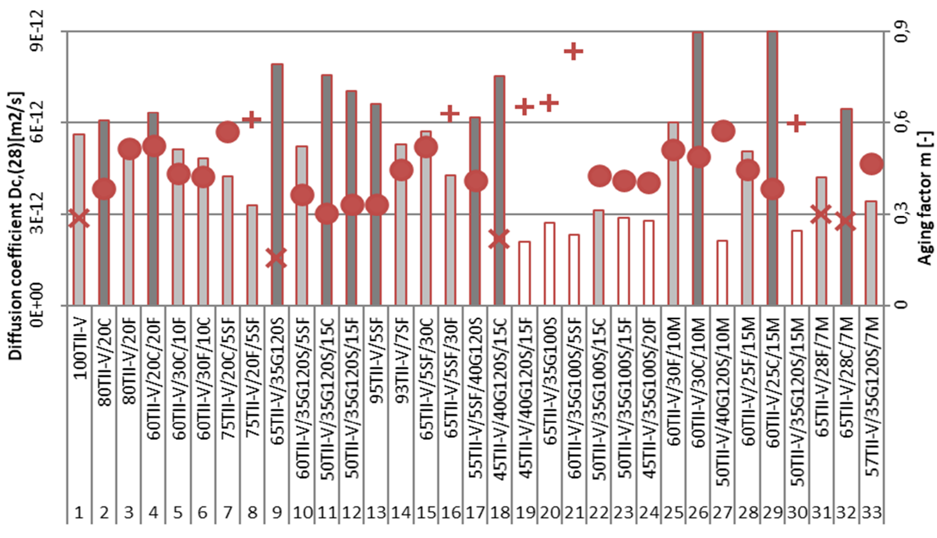

Fig. 3. Diffusion coefficient $D_{c,(28)}$ [m^2/s] (high = white bars = $0 - 3\times10^{-12}$, moderate = grey bars = $3 - 6\times10^{-12}$, low = black bars = $6 - 9\times10^{-12}$), Aging factor m [–] (low = cross = = 0.0 – 0.3, moderate = point = 0.3 – 0.6, high = plus = 0.6 – 0.9) (*own study*)

5. Result of the analysis

The results from the calculations using the analytical equation and the FEM model are shown in Table 1. The table also shows the differences in the individual mixtures where the analytical model is considered as reference.

Table 1. Results of computed concentration of chlorides from FEM model, analytic model, differences and calculation time (*own study*)

Mix. No.	**Aging factor m [–]**	**Time step size [yrs.]**	**FEM model [%/cem]**	**Analytic model [%/cem]**	**Difference [%]**	**Computation time [s]**
1	0.284	0.14	0.3237	0.3231	0.19	53.34
2	0.382	0.13	0.2587	0.2578	0.33	58.96
3	0.514	0.15	0.1399	0.1391	0.55	52.08
4	0.524	0.13	0.1550	0.1545	0.37	62.65
5	0.432	0.16	0.1950	0.1938	0.61	50.43
6	0.422	0.17	0.1939	0.1926	0.65	48.68
7	0.571	0.19	0.0721	0.0724	0.42	41.46
8	**0.607**	**0.24**	**0.0310**	**0.0327**	**5.21**	**31.27**
9	0.152	0.10	0.4655	0.4593	1.36	76.32
10	0.363	0.15	0.2519	0.2509	0.39	50.22
11	0.301	0.11	0.3503	0.3497	0.17	72.46
12	0.331	0.11	0.3181	0.3176	0.18	67.84
13	0.330	0.12	0.3110	0.3104	0.20	62.99
14	0.446	0.15	0.1885	0.1873	0.61	50.24
15	0.520	0.14	0.1434	0.1428	0.47	62.13
16	**0.625**	**0.19**	**0.0452**	**0.0471**	**3.97**	**43.25**
17	0.408	0.13	0.2402	0.2393	0.39	61.91
18	0.216	0.11	0.4131	0.4112	0.47	77.67
19	**0.650**	**0.38**	**0.0018**	**0.0045**	**61.32**	**22.61**
20	**0.663**	**0.30**	**0.0065**	**0.0097**	**32.43**	**30.64**
21	**0.832**	**0.34**	**0.0002**	**0.0005**	**178.01**	**25.74**
22	0.427	0.25	0.1293	0.1277	1.26	30.98
23	0.409	0.28	0.1305	0.1288	1.33	28.04
24	0.404	0.29	0.1289	0.1272	1.37	27.40
25	0.512	0.13	0.1567	0.1560	0.46	60.15
26	0.487	0.09	0.2333	0.2328	0.22	85.01
27	**0.573**	**0.38**	**0.0144**	**0.0162**	**11.14**	**20.31**
28	0.444	0.16	0.1836	0.1824	0.65	48.02
29	0.383	0.09	0.3120	0.3115	0.16	80.15
30	**0.595**	**0.33**	**0.0157**	**0.0177**	**11.28**	**20.80**
31	0.298	0.19	0.2733	0.2724	0.33	36.10
32	0.274	0.12	0.3505	0.3499	0.17	56.06
33	0.464	0.23	0.1135	0.1122	1.21	29.52

Conclusions

The article deals with the investigation of the 2D chloride diffusion model considering different values of material parameters. The comparison of results given by 2D analytical formula and 2D finite element model is presented. Firstly, it is shown that there is a large difference in inaccuracy related to the different mixture properties. The results of mixtures no. 8, 16, 19, 20, 21, 27 and 30 are not sufficiently accurate. These mixtures have a high m-factor, which is shown in Figure 3. Mixture 27 and 30 are classified as highly resistant to chloride penetration. Furthermore, these mixtures have an m-factor at a moderate level. However, it does not mean that the level of a diffusion coefficient will have the same effect on the results as the level of the m-factor. The analysis shows that the reference diffusion coefficient has not that significant effect on accuracy except for two mixtures. The major factor affecting the stability and the precision of calculation is the m-factor, regarding whether it is lower or higher than value 0.57. It was observed that all mixtures with higher m-parameter show inaccurate results. The presented model was relatively simple and idealized with respect to the bridge deck and considered many simplifications. The accuracy of the results can be affected by many factors. It should be noted that the comparison with the analytical solution process assumes that the analytical formula gives accurate results irrespective of the material parameters. This assumption could be evaluated by comparison with long-term diffusion tests. It would be useful to examine how the calculation would behave if the model was prepared for a larger cross-section. However, authors consider available results of the stability of the numerical solution of chloride ingress as sufficient with respect to indicate the significance of the aging factor value.

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