Numerical analysis of chloride diffusion considering time-dependent diffusion coefficient

Petr Lehner, Petr Konečný, Pratanu Ghosh and Quang Tran

***Abstract*—The procedure of 2D chloride ion diffusion modelling is summarized including evaluation of the application of time-dependency on the diffusion coefficient. The effect of the variation of the diffusion coefficient over time is studied. Available established time dependent diffusion coefficient formula is compared between one high performance concrete (HPC) mixture and one ordinary portland cement (OPC) based concrete mixture measured from laboratory investigation.

***Keywords*—**Corrosion, chloride diffusion coefficient, FEM, time-dependency.

I. Introduction

THE paper that is extension of the work presented in [14] and focused on the advancement of the chloride induced corrosion model of reinforced concrete bridge decks [19], [10], [20] with respect to the application of time-dependent diffusion coefficient [4]. The other objective was preparation for simulation speed-up and comparison of data of two types of concrete mixtures. One of the most significant types of distress in many bridge decks is the corrosion of reinforcing steel from the ingress of chloride salts applied to melt snow and ice. The chloride ions penetration process is primarily governed by the diffusion mechanism in case of bridge decks.

In Central Europe, water-proof membrane is the most common practice of construction to protect the steel reinforcement in concrete. The epoxy-coated reinforcement is widely used in Northeastern United States for protection of the steel reinforcement. Both methods significantly delay the corrosion initiation although repair or rehabilitations are necessary within 20-30 years of service life [9], [10], [4].

For this reason, there is a strong need to focus on the development of numerical deterioration models of chloride induced corrosion of reinforced bridge decks.

II. Numerical Solution

A. Probabilistic Assessment

The application of probabilistic assessment with the Monte Carlo simulation and **2-D Finite Element Analysis** is used in the model of reinforced concrete bridge deck with crack and epoxy-coated reinforcement [10]. The model was not able to address the effect of concrete hardening expressed as time-dependent diffusion coefficient increment. The change of the diffusion coefficient over time is significant especially in case of HPC.

B. Non-stationary Model

The problem of chloride diffusion shall be addressed probabilistically (see eg. [19], [10]) due to the large scatter of input parameters. The probabilistic applications (such as e.g. [16], [10], [11], [7], [15], [18]) create a demand for large computing capacity. In this case, the model implemented using scripting language under commercial FEA package [1], [10] runs rather slow. Creation of an executable code is in the process that can speed-up the simulation.

This model is prepared in house software uFem [5] which is faster but it allows modeling only for stationary 2-D diffusion problems. This paper describes non-stationary model prepared under Matlab [17] as a step before the executable form preparation [6].

C. Effect of Transverse Crack

The cracking in structural concrete affects directly the ingress of chlorides in reinforced concrete bridge decks in the Northeastern U.S.A [9], [3], [10]. Figure 1 shows how chloride ions penetrates into the bridge deck and shows 2-D effect of transverse crack. This is the output diagram of the

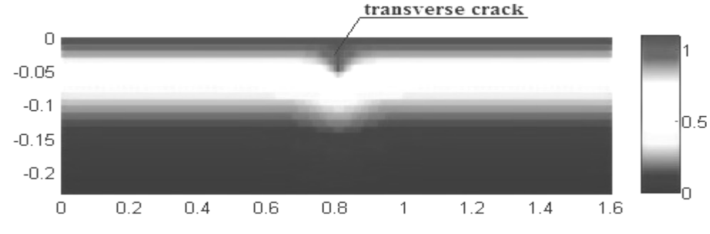

Fig. 1 Effect of transverse crack

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Matlab model [13].

D. *Time-dependent Diffusion Coefficient*

The other part of the paper focuses on the implementation of time-dependent diffusion coefficient based on the model [4] followed by its sample application. The time-dependent effect allows modeling the increase of concrete resistance against the chloride ingress during concrete maturing. The prolonged maturity is significant especially with selected HPC mixtures [12].

III. Problem Solution

A. *Non-stationary diffusion*

The current stage of the work is focused on the numerical implementation of the non-stationary 2-D diffusion problem under MatLab [17]. This implementation follows commercial finite element package [10] that would be gradually replaced by application of in house code [6] in order to obtain better control over the numerical modelling.

The non-stationary diffusion of chloride ions is modeled using thermal diffusion analogy. While the thermal process describes the Fourier equation, the process of non-stationary chloride is determined by Fick's second law [9], as expressed in equation (1):

$$\frac{dC_{x,t}}{dt} = D_c \cdot \frac{d^2 C_{x,t}}{dx^2} \qquad (1)$$

where $C_{x,t}$ is the concentration of chlorides (percent by mass of total cementitious materials) at time t (years) and depth x (meters) and D_c is the apparent diffusion coefficient (m^2/year).

B. *Implementation of the Algorithm*

The Matlab program code [13] itself offers user interface for the computation of chloride concentration in selected point of the bridge deck cross-section and selected age including graphical and text output. Figure 2 shows one of the color charts, which is used for visual display of 2-D concentrations of chloride ions in the construction.

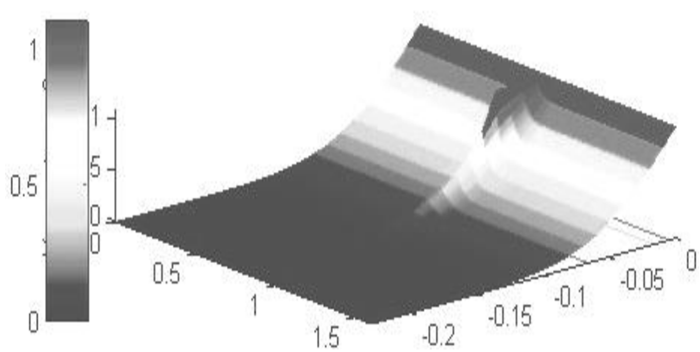

Fig. 2 Example of 3D graphical output

C. *First Numerical Example*

The following example compares results obtained using author's code [13] and commercial FEA package macro [10], [1].

This example represents a model of unprotected concrete deck with transverse crack embedded with epoxy-coated steel reinforcement. Finally, the concentration of chloride ions at three points on the structure was compared.

Table 1 show inputs parameters for first example.

Concentration of chlorides on surface of bridge deck [%]	1,1
Diffusion coefficient D_c, [$10^{-12}m^2/s$]	4,91
Depth of the bridge deck D_{epth} [m]	0,23
Width of the bridge deck B [m]	1,60

Tab. 1 Parameters for first example

In Figure 3, it can be observed that the results of Matlab program [13] and commercial FEA system are almost same.

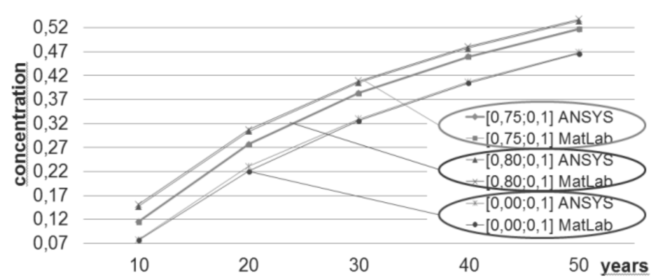

Fig. 3 First example results

D. *Time-dependent Diffusion Coefficient*

The chloride diffusion coefficient D_c is a function of both time and temperature se discussed e.g. in [4]. The relationship that is adopted in the paper uses the following relationship to account for time-dependent changes in the diffusion coefficient [4], see equation (2):

$$D_c(t) = D_{c,ref} \cdot \left(\frac{t_{ref}}{t}\right)^m , \qquad (2)$$

where $D_{c(t)}$ is diffusion coefficient at time t, $D_{c,ref}$ is the diffusion coefficient at some reference time t_{ref} (e.g. 28 days), m is a constant (aging factor) depending on mix proportions. The following equation (3) is used to modify m based on the level of fly ash (%FA) or slag (%SG) in the mix-design. Following relationship is only valid up to replacement levels of 50% fly ash or 70% slag [3]:

$$m = 0.2 + 0.4(\%FA/50 + \%SG/70). \qquad (3)$$

The Equation (3) is current enhancement of the program [13]. In this case, 1-D behavior was tested on the 2-D model.

Finally, the previous results were compared with the new ones.

In first example, concentration of chlorides was used in depth 0.09 m under surface of concrete deck. The first step was to compare two diffusion coefficients in time. It is shown in figure 4. The black color indicates coefficient with no slag and grey color shows coefficient with %50 of slag.

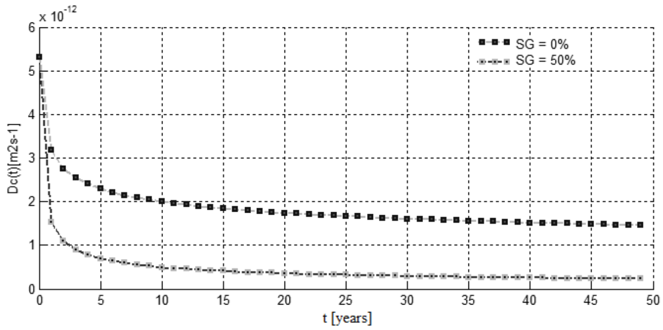

Fig. 4 Value of time-dependent diffusion coefficient over time

This model represents an unprotected concrete bridge deck as an example. The input parameters are: diffusion coefficient $D_c = 5.3\times10^{-12}$ m^2/s, surface chloride concentration $C_0 = 0.63$ %, slab depth is 0.23 m, model width is 0.6 m, investigated depth x = 0.09 m. The same inputs were used in our program as well as commercial FEA system.

In example, the diffusion coefficient decay constant m was used from relationship (3). Table 2 shows comparison of time independent (constant) and time dependent diffusion coefficient results from Matlab program and commercial FEA system.

Time [years]		10	20	30	40	50
Constant Dc	Ansys	0,0773	0,1769	0,2398	0,2833	0,3165
	MatLab	0.0772	0,1763	0,2314	0,2828	0,3104
Time depen. Dc	Ansys	0,0004	0,0023	0,0080	0,0112	0,0160
	MatLab	0,0003	0,0022	0,0069	0,0106	0,0157

Tab. 2 Concentration of chloride ions [%]
0.09 m under surface

Satisfying compliance of results can be easily observed in graphical outputs in Figure 5.

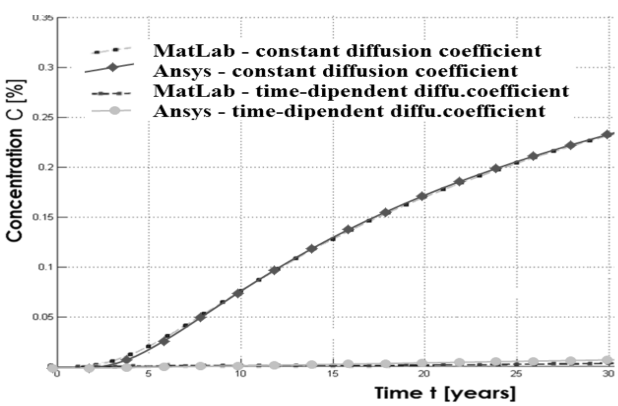

Fig. 5 Graphical results of concentration of chloride ions
0.09 m under surface

E. Comparison with Laboratory Results

There are results from laboratory measurements [8] to compare the values obtained according to equations (2) and (3). Results were prepared for two concrete mixtures.

The first case was mixture labeled as 100TII - V, which is concrete with Type II-V ordinary portland cement [8]. The second case was mixture 45TII-V/35G100S/20F [8]. It is a HPC mixture that contains 35% of slag and 20% of fly ash. This diffusion coefficient was computed using fundamental of electrochemistry as described in [2].

There were 32 laboratory results available at several maturity ages (7, 14, 28, 56, 91 and 161 days) for each of the mixtures.

Influnece of the diffusion coefficient over extended time period is expressed in Figures 6 and 7 based on the type of concrete and three selected computational procedures. These computation procedures are explained below in details.

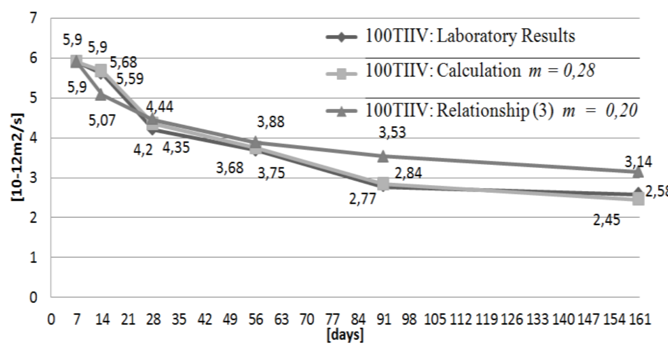

Fig. 6 Diffusion coefficient results for
mixture 100TIIV [$10^{-12}m^2/s$]

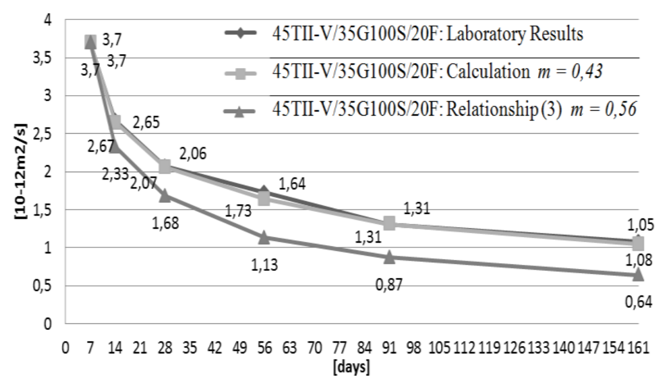

Fig. 7 Diffusion coefficient results for
mixture 45TII-V/35G100S/20F [$10^{-12}m^2/s$]

Laboratory Results represent average value of the actual measurements. The reference value D_{c0} is selected herein as average from the measurements at the age of 7 days even though it would be better to use 28 days value. Most of the concrete takes at least 28 days to achieve its desired compressive strength and hydration to complete. The least-squares curve fitting method was used to determine the coefficient m for the second results obtained with equation (2) noted as **Calculation.** The **Relationship (3)** calculation is based on the reference value D_{c0} and the m parameter computed according to (3) based on the percentage of fly ash and slag.

Comparison between laboratory results and **Relationship (3)** showed similar trend however some differences are observed. Values called **Calculation** with least-squares method curve fitting show good agreement. It can be assumed that 28 days reference value and the aging coefficient computed using curve-fitting of the laboratory data would be more logical for future chloride diffusion analysis.

IV. CONCLUSION

This paper demonstrates implementation of the 2-D diffusion problem related to chloride ion ingress into bridge deck. Special attention is paid to the application of time-dependent diffusion coefficient on two different types of concrete mixtures.

The first part of the paper describes the introductory numerical solution of 2-D chloride diffusion problem using FEA package. The derived algorithm was implemented using MatLab software [17]. The results were compared with commercial FEA package.

This software is suitable for the understanding of the numerical background, but the speed of calculation is unfortunately slow. The algorithm is being currently recoded under the C++ and translated to the in-house software uFEM for better performance.

There were given overview of the application of time-dependency in case of the diffusion coefficient for the analysis of chloride ion ingress into concrete bridge decks.

Comparison of laboratory data for the development of the diffusion coefficient overtime was evaluated with respect to applied equation (3) and the aging coefficient based on the actual measurements. Further comparison between applied equation (3) and available laboratory data including the diffusion analysis is necessary as a next step.

REFERENCES

[1] Ansys 12.0 Release Documentation, 2009.

[2] V. Barde, A. Radlinska, M.Cohen, W.J. Weiss "Relating Material Properties to Exposure Conditions for Predicting Service Life in Concrete Bridge Decks in Indiana", Publication FHWA/IN/JTRP-2007/27., Indiana Department of Transportation and Purdue University, West Lafayette, Indiana, 2009. doi:10.5703/1288284313444.

[3] D.P. Bentz, E. J. Garboczi, Y. Martys, A.R. Sakulich, W.J. Weiss, Modeling of the Influence of Transverse Cracking on Chloride Penetration into Concrete, Cement and Concrete Composites, Vol. 38, 2013, pp. 65-74, April 2013.

[4] E. Bentz, M.D.A Thomas. Life-365 Service Life Prediction Model, Computer Program for Predicting the Service Life and Life-Cycle Costs of Reinforced Concrete Exposed to Chlorides, 2001.

[5] J. Brozovsky, uFEM finite element method program, 2010,

[6] J. Brozovsky and P. Konecny, Reliability of Reinforced Concrete Bridge Decks with Respect to Ingress of Chlorides, in Proceedings of the Third International Conference on Parallel, Distributed, Grid and Cloud Computing for Engineering, B.H.V. Topping, P. Iványi, (Editors), Civil-Comp Press, Stirlingshire, United Kingdom, paper 46, 2013. doi:10.4203/ccp.101.46

[7] R. Čajka, P. Matečková, M. Stará, L. Mynarzová, Probability Assessment of Compressive Strength as a Basis for Post Tensioned Masonry Testing, Recent Researches in Environmental and Geological Sciences, WSEAS Press, ISBN: 978-1-61804-110-4.

[8] GHOSH, P. a TRAN, Q. Long Term Variation and Correlation between Bulk and Surface Resistivity for Different Cementitious mixtures. (under preparation).

[9] R.D. Hooton, M.D.A. Thomas, K. Standish (2001); Prediction of Chloride Penetration in Concrete, Federal Highway Administration, Washington, D.C., No. FHWA-RD-00-142, pp. 405.
http://fast10.vsb.cz/brozovsky/ufem_en.html
July 22-24, 2010, ISBN: 978-960-474-203-5.

[10] P. Konecny, P. J. Tikalsky D. G. Tepke, Performance Evaluation of Concrete Bridge Deck Affected by Chloride Ingress: Simulation-Based Reliability Assessment and Finite Element Modeling, In journal: Transportation Research Record, vol. 2020/2007, Transportation Research Board of the National Academies, ISSN: 0361-1981, Washington, DC, U.S.A.

[11] M. Krejsa, P. Janas, V. Krejsa, Direct Optimized Probabilistic Calculation, Recent Advances in Systems Science and Mathematical Modelling, WSEAS Press, ISBN: 978-1-61804-141-8.

[12] G. J. Kurgan, Comparison of Chloride Penetrability, Porosity, and Resistivity for High Performance Concrete, Master of Science Thesis, Department of Civil and Environmental Engineering, Pennsylvania State University, State College, PA, U.S.A., 2003.

[13] P. Lehner.: Numerical solution 2-D chloride diffusion problem using FEA, Bachelor thesis, 2012. Faculty of Civil Engineering, VŠB – Technical University Ostrava.

[14] P. Lehner, P. Konečný, P. Ghosh Finite Element Analysis of 2-D Chloride Diffusion Problem Considering Time-dependent Diffusion Coefficient Model, Recent Advances in Applied and Theoretical Mathematics, Budapest, WSEAS Press, 2013.

[15] A. Omishore, Advanced Modeling Approaches for Reliability Analysis of Steel Structures. Latest Trends on Engineering Mechanics, Structures, Engineering Geology, WSEAS Press, Corfu Island, Greece,

[16] P. Marek, M. Gustar, T. Anagnos, Simulation-Based Reliability Assessment for Structural Engineers, CRC Press, Inc., Boca Raton, Florida, 1995.

[17] MatLab 7.10.0.854 (R2010b), numerical computing environment, developed by MathWorks 2010

[18] M.M.A. Moghaddam, Analysis of Beam Failure Based on Reliability System Theory Using Monte Carlo Simulation Method, Proceedings of the International Conference on Applied Computer Science, Malta, September 15-17, 2010, WSEAS Press, ISBN: 978-960-474-225-7.

[19] P. J. Tikalsky, D. Pustka, and P. Marek, Statistical Variations in Chloride Diffusion in Concrete, ACI Structural Journal, Vol. 102, No.3, 2005, pp.481-486.

[20] Vořechovská, D., Podroužek, J., Chromá, M., Rovnaníková, P., Teplý, B. Modelling of Chloride Concentration Effect of Reinforcement Corrosion. Computer-Aided Civil and Infrastructure Engineering, 24, 446-458., 2009.