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OPTIMIZATION OF TIME STEP AND FINITE ELEMENTS ON THE MODEL OF DIFFUSION OF CHLORIDES

Petr Lehner, Petr Konečný and Jiří Brožovský
Department of Structural Mechanics, Faculty of Civil Engineering, VSB-Technical University of Ostrava, Czech Republic
E-mail: petr.lehner@vsb.cz

ABSTRACT

The paper deals with model of a reinforced concrete bridge deck loaded with effects of deicing agents. The theoretical 2D example is focused on the optimization of the mesh of finite elements and assessment of size of time stepping. The model uses finite element method based on thermal-diffusion analogy. The algorithm is implemented in Matlab. The original algorithm that is enhanced by optimization criteria is used to evaluate the results. They are compared with an analytic equation for time dependent chloride penetration including the effect of aging. Thus obtained results allow speeding up further calculations.

Keywords: concrete, optimization, finite element method, chlorides, time dependency.

INTRODUCTION

The aim of the authors herein is to briefly introduce possibilities to optimize the numerical finite element chloride diffusion algorithm with respect to the time step size, mesh shape and element size.

The applied 2D FEA model [10] serves to solve Fick's second diffusion law using the computer tool compatible with the Matlab. The model focuses on the transport of chloride ions through a reinforced concrete bridge deck with a transverse crack and on an estimate of the concentration of chlorides at the reinforcement level or in places with damage to the epoxide coating of the reinforcement. The numerical model is extension of [13] and [6].

Due to the enormous development of computer technology in the last decades, which is still ongoing, simulation approaches have gained increased significance. Thus inherited randomness of engineering problems may be described using suitable probabilistic tools ([3], [7], [8], [9] and [14]).

This method uses a large number of simulations, which leads to high computing demands. One option is to reduce the period of one simulation by optimizing the number of finite elements. Since the calculation contains time-dependent diffusion coefficient, it is necessary to optimize the timing step in discretization equation as well. These approaches can help reduce computational difficulty while not sacrificing precision.

METHODOLOGY

Paper shows the results of comparison of the 2D model and the analytical formula for 1D diffusion of chloride ions. This is used with uniform load at surface of cross section and 2D model is using for description of the 1D penetration in case of the square meshed model. First part of paper discusses assessment of size of the mesh and second part of paper focuses on the influence of the time step size.

Furthermore the model is loaded from two orthogonal directions. It is used when searching for the maximum effectiveness ratio of the finite element mesh.

Analytical model

For evaluation of numerical model accuracy the analytical solution is used. Comparison is performed on specific point in the mesh.

The analytical formula capable of aging implementation introduced in [8] is given below:

$$C_{z,t} = C_0 \left[1 - erf\left(\frac{z}{\sqrt{4 \frac{D_{c,t}}{1-m} t^{(1-m)}}} \right) \right] \tag{1}$$

where where is $C_{z,t}$ concentration of chlorides [% by mass of total cementitious materials] at time t [years], C_0 is concentration of chlorides [% by mass of total cementitious materials (%/cem)] at the surface directly inside the concrete, D_c is apparent diffusion coefficient of chloride ions in concrete [m^2/s], t is chloride exposition time [s], z is reinforcement depth [m], $D_{c,i}$ is diffusion coefficient of chloride ions in concrete at reference time one second [m^2/s] a m is aging factor.

Numerical model

The finite element model is capable of modeling concrete aging (reduction of diffusion coefficient in time) and uses 2D isoparametric three nodded finite element. Current study does not include description of the model or the finite element since it focuses on optimization. The numerical model is described in detail in the articles [10] and [11].

It is generally assumed that a small number of finite elements lead to faster calculation. For this reason, optimization is used to find the smallest but effective number of elements. The Matlab program code [10] 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.

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Discretization equation

The time step is present in equation (2). This is time discretization equation for calculation of unknown values of chloride concentration [10]:

$$r_{(t)}=(K * \tau + C/\Delta t) \backslash (f T + (C/(\Delta t) - K * (1-\tau)) * r_{(t-1)} \quad (2)$$

where $r_{(t)}$ is the desired concentration of chlorides in time, K is conductivity matrix, C is capacity matrix, f, is vector of load and Δt is time step. Values in conductivity matrix are based on material parameters, namely diffusion coefficient $D_{c,t}$ and a curing coefficient m.

There is premise that the value of the time step significantly affects the calculation. On the beginning of the calculation the studied service life period structure is selected. Therefore, the number of steps in the calculation is obtained by simply dividing the service life of the time step size.

Because there is thermal-diffusion analogy used, may be expected, that stability results will be achieved when the time step size according to the equation [1]:

$$\Delta t \leq \frac{\Delta x * \Delta z}{D_{c,ref}} \quad (3)$$

where Δx and Δz are dimensions of finite element [m], $D_{c,ref}$ reference diffusion coefficient [m^2/s].

SQUARE MESH MODEL

First examples present part of reinforced concrete bridge deck with constant thickness and variable width. Width of part is changing because the mesh has square shape and the horizontal number of elements is maintained. It should be noted that there are always two triangular finite elements in one square of the mesh. This ensures the possibility of comparison of a growing number of vertical finite elements. The input parameters for this example are given in Table-1. This presents model with a regular square mesh.

Table-1. The parameters for model example with the square mesh.

Name	Values	Units
Width of investigated bridge deck	variable	m
Thickness of bridge deck	0.25	m
Investigated lifespan period	100	years
Cover depth	0.05	m
Diffusion coefficient at 28 days	5.59×10^{-12}	m^2/s
Aging factor	0.284	-
Surface chloride concentration	0.6	%/cem
Chloride background concentration	0	%/cem

Assessment of accuracy

The values of concentration are investigated in depth of reinforcement, in half the width of cross section. In the example there are selected two output values. It is in two different times from initial operation of chloride ions.

Specifically it is 10 and 100 years from beginning of life time. These times are selected because there is different behavior. In 10 years the concentration rises faster than in 100 years. Different sizes of elements have been entered. The target accuracy was determined by analytical equation (1).

Size of the element

The first version of calculation divides model into the five finite elements over the thickness. The size of the one square of mash was 0.05 m. Width of cross section is 0.10 m. In each new calculation were added five rows of elements in vertical direction. For this example the value of time step Δt is calculated using equation (3).

The Table-2 shows the results of each version. It also contains percentage difference with the analytical equation (1). The value of concentration of chlorides from analytic solution in 10 years is 0.093 %/cem.The value of concentration of chlorides from analytic solution in 100 years is 0.320 %/cem.

Table-2. Effect of element size. The concentration of chlorides from numerical model and difference in comparison with analytic model.

El. size (m)	**Concen.** (%/cem)		**Difference** (%)		**Time** (s)
	10 y.	**100 y.**	**10 y.**	**100 y.**	
0.050	0.154	0.339	63.10	5.25	0.02
0.025	0.107	0.326	13.88	1.22	0.13
0.017	0.098	0.324	4.42	0.47	0.41
0.013	0.096	0.323	1.65	0.22	0.99
0.010	**0.095**	**0.322**	**0.58**	**0.12**	**1.97**
0.008	0.093	0.320	0.06	0.07	3.44

According to the assumptions, larger number of finite elements led to more accurate results. The required boundary is 1% difference from analytic results in 10 and 100 years.

This accuracy was achieved with the 25 finite elements lines so the size of the mesh square is 0.01 m. The Table-2 also shows the computation time for one simulation. This is very important value, because if we know a number of simulations, it indicates how long probabilistic assessment will take. For illustration, the

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graphical results of chloride concentration for chosen variants are given Figure-1.

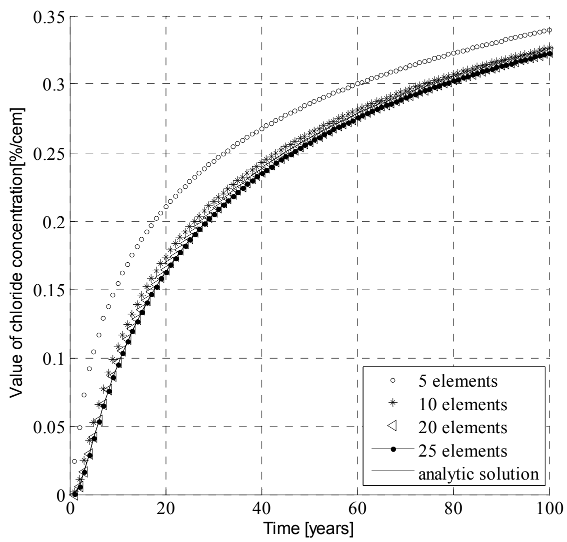

Figure-1. Shape of chloride ion concentration computed for time dependent diffusion coefficient with different number of finite elements in vertical direction.

Size of the time step

Another part of the research is focused on changing the size of the time step. There is the question if it is possible to use a larger time step and thus a smaller number of steps in one simulation. This may lead to faster computation. Standard determination of size of time step uses equation (3). The theoretical time step for studied example shall be 0.14 years. The effect of time step change is studied next.

Table-3. Effect of time step size. The concentration of chlorides from numerical model and difference in comparison with model with a recommended size of time step 0.14 years.

Time step size (y.)	Concen. (%/cem)		Difference (%)		Time (s)
	10 y.	100 y.	10 y.	100 y.	
1.00	0.0855	0.3204	10.19	0.77	0.29
0.50	0.0903	0.3217	5.14	0.37	0.55
0.33	0.0924	0.3222	2.94	0.22	0.88
0.25	0.0935	0.3225	1.78	0.12	1.12
0.20	0.0943	0.3226	0.95	0.09	1.39
0.17	0.0948	0.3228	0.42	0.03	1.70
0.14	0.095	0.322	0.00	0.00	1.97

For model example were chosen 25 x 25 finite elements. In first calculation there was use 110 number of time steps, and size of time step was 1 year. Each new calculation used shorter time step (Table-3). As well as in previous example, there were searched accurate results. There is percentage difference with the results with a recommended size of time step 0.14 years.

Variation of mesh aspect ratio

Equally important part of the paper is preparation of non-symmetrical mesh of finite elements. There is possibility to implement many variants of different mesh aspect ratio. It is very important if we want to implement cracks in concrete bridge deck in the form of finite elements with high penetrability [14].

Model parameters

The dimension of model of cross section is 0.10 × 0.10 m. It is very important to distinguish between the mesh elements and finite elements herein. The mesh is made up of rectangles (Figure-3) and the final elements are triangular (Figure-2).

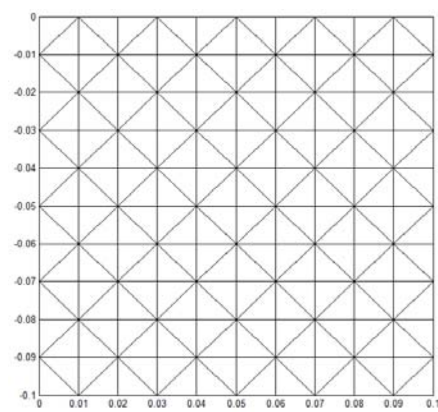

Figure-2. Triangular finite elements are applied on the rectangular mesh.

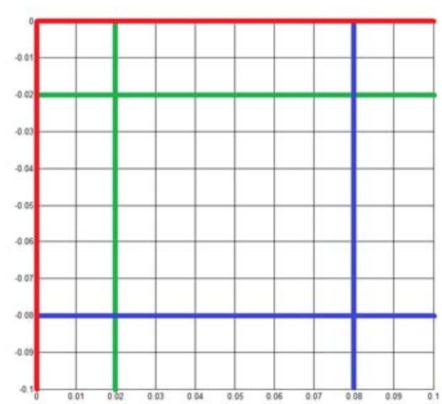

Figure-3. Schema of the mesh. Red lines represent location of load. Green lines show distance 0.02 m from surface and from the left edge and blue lines show distance 0.08 m, respectively.

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In any rectangle there are two finite elements. The main difference from previous examples is the way the load is applied. In this case it is the same load from surface and also from left edge. Location of the result levels and location of chloride load are shown in Figure-3.

This causes diffusion in diagonal direction. The curve of the values in distance of 0.02 m from the surface and from the left edge was compared. Subsequently values of concentration in distance of 0.08 from the surface and from the left edge were evaluated too.

Numerical computation

There are used ratios of sizes of finite elements from 1:1 to 1:16. Value of time step was prepared from equation (3). On the beginning there were 10 x 10 elements of mesh (see in Figure-4).

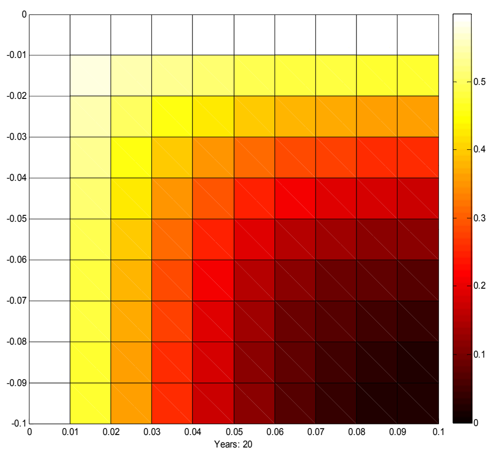

Figure-4. Diffusion of chloride ions in the structure loaded from the surface and from the left edge. Number of mesh elements is 10 × 10. Penetration time is 10 years.

Each new calculation divided width to double number of mesh elements until there were 160. The Figure-5 shows graphic output from the last calculation.

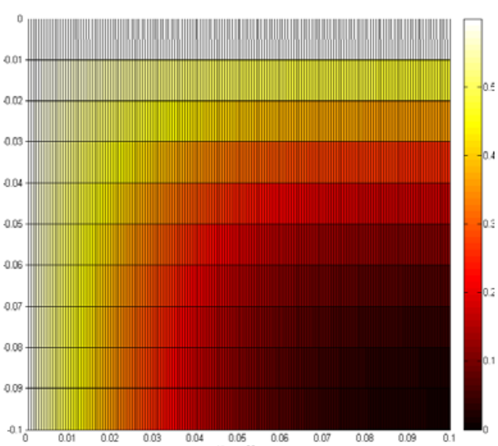

Figure-4. Chloride ion concentration in the structure loaded from the surface and from the left edge. Number of mesh elements is 160 × 10. Penetration time is 20 years.

It is evident that the symmetry between the penetration from surface and from edge is still maintained. Thus it is similar to Figure-4.

Graphical comparison is not sufficient in this case. Thus we need to compare the numerical results. Reference model was divided on elements with size 0.01 × 0.01 m. In Table-4 there are shown values on level 0.02 m from surface. In this example are shown only results in 100 years of service life because results at age 10 years of have minor deviations. It also contains maximum percentage difference with reference model.

Table-4. The values of concentration of chlorides in distance 0.02 m from surface in 100 years of service life.

z (m)	**Number of elements**				
	10x10	**10x20**	**10x40**	**10x80**	**10x160**
0.00	0.600	0.600	0.600	0.600	0.600
-0.01	0.580	0.580	0.580	0.580	0.580
-0.02	0.561	0.561	0.561	0.561	0.561
-0.03	0.543	0.543	0.543	0.543	0.543
-0.04	0.527	0.527	0.527	0.527	0.527
-0.05	0.512	0.513	0.513	0.513	0.513
-0.06	0.501	0.501	0.501	0.501	0.501
-0.07	0.491	0.491	0.491	0.491	0.491
-0.08	0.484	0.484	0.484	0.484	0.485
-0.09	0.480	0.480	0.480	0.480	0.480
-0.10	0.479	0.479	0.479	0.479	0.479
Max diff.		**0.08%**	**0.10%**	**0.15%**	**0.17%**

There are not showed the results from the horizontal direction because no value is exceeded boundary of 0.10%.

The results are showing that increasing the ratio leads to increased deviation. The Table-5 shows values on level 0.08 from surface. The results again show an increasing trend.

Table-5. The values of concentration of chlorides in distance 0.08 m from surface in 100 years.

z (m)	Number of elements				
	10x10	**10x20**	**10x40**	**10x80**	**10x160**
0.00	0.600	0.600	0.600	0.600	0.600
-0.01	0.541	0.541	0.541	0.541	0.541
-0.02	0.484	0.484	0.484	0.484	0.484
-0.03	0.430	0.430	0.430	0.430	0.431
-0.04	0.382	0.381	0.381	0.382	0.382
-0.05	0.338	0.338	0.338	0.339	0.339
-0.06	0.303	0.302	0.302	0.303	0.303
-0.07	0.273	0.273	0.274	0.274	0.274
-0.08	0.253	0.253	0.253	0.253	0.254
-0.09	0.239	0.240	0.240	0.241	0.241
-0.10	0.236	0.236	0.236	0.237	0.237
Max diff.		**0.42%**	**0.50%**	**0.66%**	**0.83%**

It would be useful to know how much deviation would bring the ratio as 1:100. However in this case it can lead to time consuming calculation. Differences of values are the most important result. It may seem there are low numbers, but in model with crack in bridge deck there can be large range of differences. This can lead to large inaccuracies.

CONCLUSIONS AND DISCUSSIONS

The aim of paper is evaluation of numerical parameters of chloride ion penetration finite element model with respect to quality of results and reasonable speed. The effect of the size of finite elements is compared with analytic formula on specific example of reinforced concrete bridge deck. It is shown that sufficient size of finite element is 0.01 m for given inputs.

The equation for the size of time step from commercial software was also evaluated. The applicability of this formula was confirmed. The results from a second example show that it is appropriate to use the equation for calculation of the size of time step. It would be useful to investigate how the calculation would behave if the model was prepared for larger cross section.

The last part of the paper was focused on comparison of results of finite elements with different aspect ratio. Reference model was divided by elements with size 0.01 x 0.01 m. Each new calculation divided width to double the number of finite elements until there were 160 of these. The structure was loaded from surface and left side.

The results were compared in horizontal and vertical direction in the two levels. Here it can be seen that the difference does not exceed 0.10%. The most important results are differences against symmetrically model. This shows that increasing the aspect ratio of the finite elements brings growing deviation. Also there is seen the difference between result at a depth of 0.02 m and 0.08 m. The maximal deviation on the level 0.02 m is 0.17%. On level 0.08 m the maximal deviation 0.83% at the same aspect ratio. These results can be useful in the reinforcement bridge deck model with crack. In that case, there is large aspect ratio of finite element.

Another question might arise, how will behave elements on border between crack and structure. Certainly it would be useful to apply the chloride load in different location of the cross section and also comparison with 2D analytical equation.

It should be noted that results are related to the discussed model of reinforced concrete bridge deck without cracks. This model is ideal and uses the inputs values of the standard concrete. Accuracy of results can be affected by many factors.

The presented results allow reducing the computation time for the probabilistic Monte Carlo based numerical simulation of chloride ion penetration. The investigation of size of elements, time step and mesh aspect ratio helps to save compute time in case of probabilistic assessment where are hundreds of thousands simulations and time of calculation is essential.

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