III European Conference on Computational Mechanics
Solids, Structures and Coupled Problems in Engineering
C.A. Mota Soares et.al. (eds.)
Lisbon, Portugal, 5–8 June 2006

# SOLVING THE CHLORIDE DIFFUSION EQUATION IN CONCRETE STRUCTURES FOR PREDICTION OF INITIATION TIME OF CORROSION USING THE FINITE POINT METHOD

**Maryam Bitaraf[1], Soheil Mohammadi[2]**

School of Civil Engineering, University of Tehran, Tehran, Iran
[1] Graduate Student, mrybitaraf@yahoo.com
[2] Assistant Professor, smoham@ut.ac.ir

**Keywords:** Finite point method, meshless methods, chloride diffusion.

**Abstract.** *In this paper, a finite point method (FPM) is developed and adopted for solving the chloride diffusion equation for prediction of service life of concrete structures and initiation time of corrosion of reinforcement. Diffusion of chloride ions is generally assumed to follow the Fick's second law. FPM is a truly meshless method which uses a moving last square approximation within a collocation strong form for solving the governing differential equation. Several 1D and 2D problems are solved using FPM and the results are compared with the analytical solution, classical finite element and finite difference methods, and weak form meshless based Element Free Galerkin method.*

# 1 INTRODUCTION

Reinforced concrete structures exposed to sea environments suffer from corrosion of steel bars due to the chloride ingress. This corrosion may lead to serious damages to concrete structures and cost of repair, inspection and maintenance activities for these structures could reach a level comparable to the cost of construction of new structures. Therefore, the chloride penetration is a major factor that affects the durability of concrete structures. The durable life (or service life) of a structure is conventionally determined based on the initiation time to corrosion of steel bars, which is caused by penetrated amount of chloride [1]. The initiation period is defined as the time required for sufficient chloride penetration into the concrete cover to initiate corrosion. Diffusion of chloride ions is generally assumed to follow the Fick's second law [2].

In this paper, a meshless finite point method (FPM) is adopted for solving the chloride diffusion problem. Finite point method was first proposed by Onate et al. in 1996 for solving the flow problems [3] using a weighted least square (WLS) scheme for approximating the unknown functions. Onate used FPM for the analysis of compressible and incompressible viscous flows and convective transport [4,5] and elasticity problems [6]. FPM is a truly meshless procedure in which the approximation around a point can be obtained using moving least square (MLS) techniques, similar to the EFG method. The discrete system of equations is obtained by sampling the governing differential equations at each point.

The present paper is organized as follows. First in section 2 the basis of FPM is briefly described. Section 3 deals with the chloride diffusion model while its analytical and FPM solutions are described in section 4. Several numerical examples are then solved, discussed and analytical, FPM, EFG [7], FDM and FEM [8] results are compared in section 5, followed by the concluding remarks.

# 2 FINITE POINT METHOD

Finite point method is a meshless numerical procedure based on the combination of moving least square interpolations on a domain of irregularly distributed points with a point collocation scheme to derive system equations.

## 2.1 Discretization of Governing Equations

Assume a problem governed by the following set of differential equations

$$A(u_j) = 0 \quad in \;\; \Omega \tag{1}$$

with boundary conditions

$$\begin{aligned} u_j - \bar{u}_j &= 0 \quad on \;\; \Gamma_u \\ B(u_j) &= 0 \quad on \;\; \Gamma_t \end{aligned} \tag{2}$$

The discretized system of equations in the FPM is found by collocating the differential equation at each point in the analysis domain. This gives

$$\begin{aligned} \left[A(u_j)\right]_p &= 0 \quad p = 1,2,\ldots,N_r \\ \left[u_j\right]_s - \bar{u}_j &= 0 \quad s = 1,2,\ldots,N_u \\ \left[B(u_j)\right]_r &= 0 \quad r = 1,2,\ldots,N_t \end{aligned} \tag{3}$$

In the above, $N_u$ and $N_t$ are the number of points located on the boundaries $\Gamma_u$ and $\Gamma_t$, respectively, and $N_r$ are the rest of the points in $\Omega$ not belonging to $\Gamma_u$ or $\Gamma_t$.

Equation (3) leads to a system of algebraic equations of the form

$$\mathbf{KU} = \mathbf{f} \tag{4}$$

where **K** is a non-symmetric coefficient matrix which its symmetry is not generally achieved and **U** is a vector collecting the nodal point parameters $u_i^h$ .

## 3 CHLORIDE DIFFUSION MODEL

Diffusion of chloride ions is generally assumed to follow the Fick's second law [2]. The general diffusion equation can be written as :

$$\frac{\partial C}{\partial t} = D(t)\nabla^2 C \tag{5}$$

where C is the chloride content in concrete, D is the chloride diffusion coefficient, and t is the exposure time. The chloride diffusion coefficient is a function of both time and temperature [1]:

$$D(t,T) = D_{ref}\,(\frac{t_{ref}}{t})^m \exp\left[\frac{U}{R}(\frac{1}{T_{ref}} - \frac{1}{T})\right] \tag{6}$$

with :

$D(t,T) =$ diffusion coefficient at time t and temperature T.
$D_{ref} =$ diffusion coefficient at some reference time ($t_{ref}$) and temperature ($T_{ref}$)
$m =$ a constant depending on mix proportions such as water-cementatius material ratio and the type and proportion of cementations materials.
$U =$ activation energy of the diffusion process
$R =$ gas constant
$T =$ absolute temperature

## 4 EXAMPLES

In this section, several 1D and 2D equations for prediction of service life of concrete specimens are solved using FPM. First a special problem of constant diffusion coefficient (D) is assumed. Then some problems are solved assuming D as a function of time and temperature. Finally the results are compared with the analytical solution and EFG, FDM, FEM [9] solutions on the same grid.

For FPM, $m_p=3$ and $m_p=6$ are chosen for 1D and 2D problems, respectively. The radius of support domain is chosen separately for each node from $r_m=1.4\ r_{min}$ where $r_{min}$ is the minimum value for the radius of support domain in order to contain at least 3 or 6 nodes for 1D or 2D problems, respectively. An exponential weight function is also adopted:

$$W(x - x_I) = \begin{cases} e^{(-r/cr_m)^2} & r \le r_m \\ 0 & r > r_m \end{cases}$$

where

$$r = |\mathbf{x} - \mathbf{x}_I| \tag{7}$$

$r_m$ is the radius of support domain

$$\mathrm{c} = 0.3$$

Generally, an optimum value for constant $\alpha$ has to be chosen by a parametric study for each problem. Numerical studies, however, have shown that a value of $\alpha$=1.4 can be efficiently used for all selected problems.

The following parameters required by the chloride diffusion equation are assumed for all numerical examples.

$U = 35000$ j/mol

$R = 8.3143$ jouls per Kelvin per mole.

$t_{ref} = 28$ days

$T_{ref} = 293^{\circ} K \; (20^{\circ} C)$

### 4.1 1D problem

In this example, the chloride content ingress in a concrete slab is investigated. The problem specifications are defined in Table 1; with $C_t$ defined as the required chloride content to initiate the corrosion of concrete.

| Thickness *(mm)* | Cover *(mm)* | D *($m^2$/s)* | m | $C_t$ % |
|---|---|---|---|---|
| 1000 | 50 | $10^{-12}$ | 0 | 0.1 |

Table 1: Specifications of the 1D cross section of concrete slab.

For the first part of analysis, based on a constant diffusion coefficient, the annual temperature is assumed to be a constant 20 $^{o}$C.

To calculate the result at 20 years, half of the slab is modeled by 21 nodes. The curves of chloride content versus depth and time at cover 50 mm are depicted in figures 1 and 2.

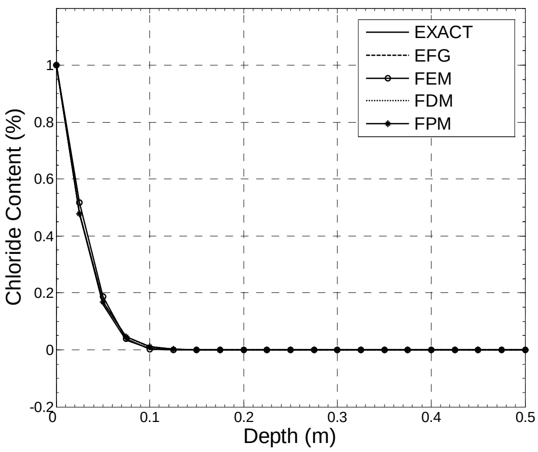



Figure 1: Chloride content-depth at time =20 years(21 nodes)

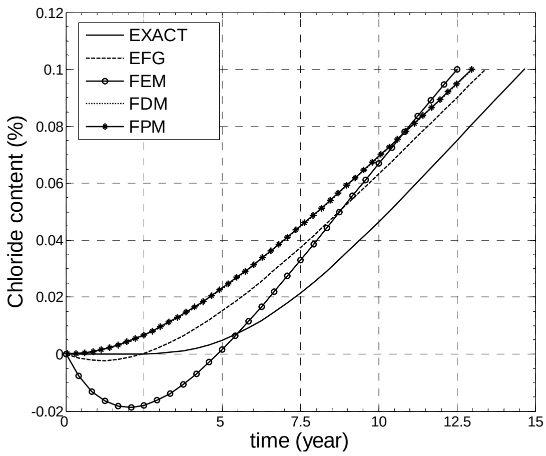



Figure 2: Chloride content-time at cover depth=50mm(21 nodes)

Table 2 compares $L_2$ errors of FPM, EFG, FDM and FEM methods, defined as:

$$L_2 = \left[ \int_{\Omega} (C_{exact} - C^h)^T (C_{exact} - C^h) d\Omega \right]^{1/2} \tag{8}$$

| | Number of nodes | FPM | EFG | FEM | FDM |
|---|---|---|---|---|---|
| $L_2$ error% | 21 | 0.1897 | 0.1678 | 0.4984 | 0.1879 |

Table 2: Chloride content error at time=20 years

Table 3 compares the initiation periods to start corrosion predicted by different methods.

The results also show that for this simple 1D problem, FPM provides very similar results to FDM, both less accurate than EFG.

| | Number of nodes | FPM | Exact | EFG | FEM | FDM |
|---|---|---|---|---|---|---|
| initiation period (year) | 21 | 12.98 | 14.7 | 13.4 | 12.5 | 13 |

Table 3: The initiation period of corrosion for constant diffusion coefficient

For the case of non-constant diffusion coefficient, no analytical solution is available. In order to simulate problems with non-constant diffusion coefficient, the annual average temperature history of Bandar Abbas, Iran, shown in Figure 3, is considered as a practical simulation, and m is set to 0.2.

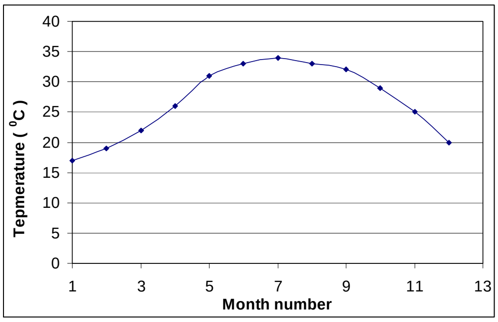



Figure 3: Annual temperature history of Bandar Abbas, Iran[9]

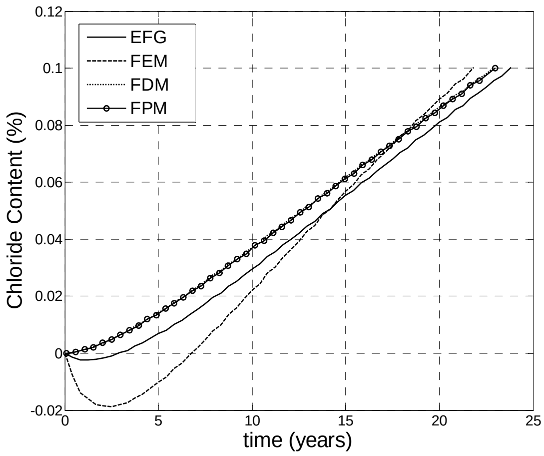



Figure 4: Chloride content-time at cover depth=50mm(21 nodes)

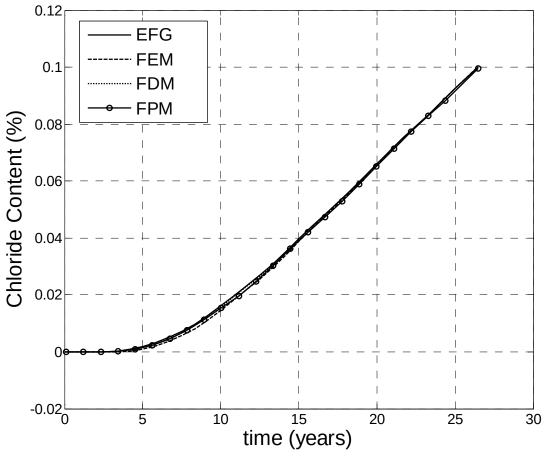



Figure 5: Chloride content-time at cover depth=50mm(101 nodes)

Figures 4 illustrate the chloride content with respect time at the depth of 50 mm for a model of 21 nodes. Similarly, the results obtained from a model of 101 nodes are depicted in figure 5.

The initiation periods obtained with different methods are compared in Table 4. The results show that FPM and FDM provide very close predictions, and both are more accurate than FEM. The EFG outcome is the most accurate between these methods, nevertheless it should be noted that the FPM procedure is more straightforward in comparison to EFG and it doesn’t need any integration procedures, making it a simple approach to implement as well as being computationally inexpensive.

| | Number of nodes | FPM | EFG | FEM | FDM |
|---|---|---|---|---|---|
| initiation period (year) | 21 | 23 | 23.8 | 21.8 | 22.9 |
| | 101 | 26.5 | 26.5 | 26.5 | 26.5 |

Table 4: The initiation period for non-constant diffusion coefficient

## 4.2 2D problems

In this section, chloride ingresses in square and circular columns shown in Figure 6 are investigated. The problem specifications are defined in Table 5:

| Cover *(mm)* | D *($m^2/s$)* | m | $C_t$ % |
|---|---|---|---|
| 50 | $10^{-12}$ | 0 | 0.1 |

Table 5: Problem specifications for the square and circular column sections.

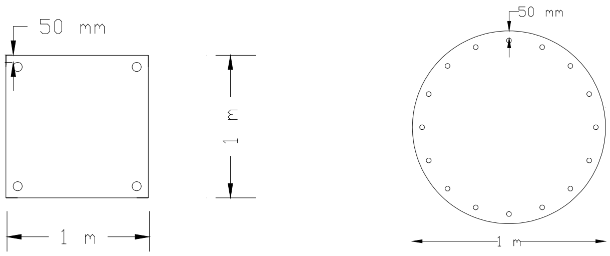



Figure 6: Cross sections of square and circular columns

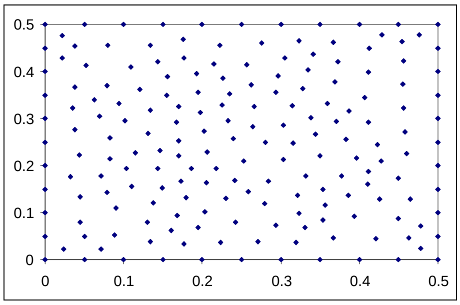
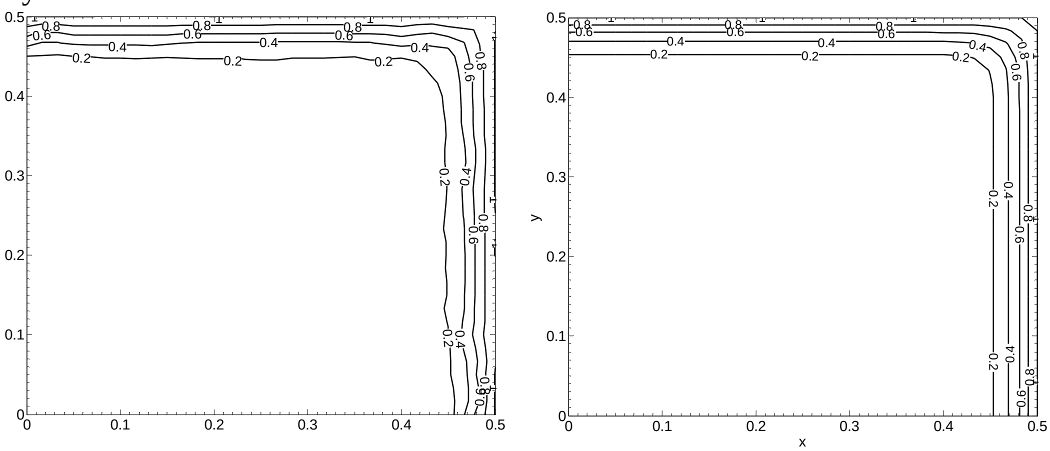



Figure 7: Distribution of nodes(185nodes) for a quarter of the square column.

### 4.2.1 Square column

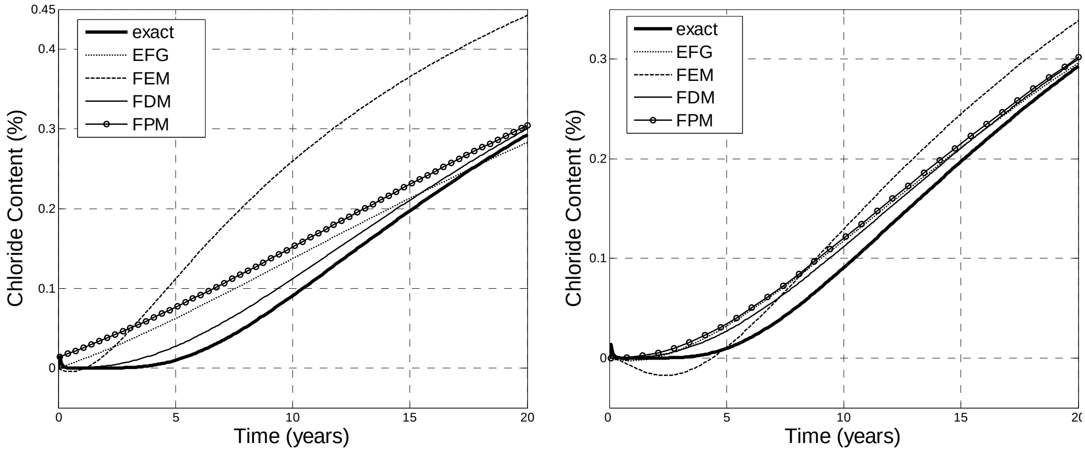
The results at 20 years are calculated assuming constant diffusion coefficient (m=0,T=20). In order to compare the present algorithm with the available FEM and EFG results [9], which were based on 185 nodes for EFG and 328 triangular elements for FEM, similar grid of 185 nodes are used, as depicted in Figure 7. A structured grid is also used for the finite difference approximation. The exact solution is obtained from the analytical solution. Except for the finite element solution, other methods remain close to the exact solution at the final stages of the analysis.




a) FPM method b) exact method

Figure 8: Chloride content contours for a constant diffusion condition at time=20 years for different methods, m=0.

In order to further investigate the effect of number of nodal points, and compare them with refined finite element and element free Galerkin methods, the same problem is simulated by 697 nodes. The equivalent finite elements were 1312, while a 25*25 structured grid was used for the finite difference approximation.
Again, except for the FE solution, all numerical methods converge to the analytical solution as shown in Figure 9.




a) 185 nodes b) 697 nodes
Figure 9: Chloride content-time at cover=50 mm for constant diffusion coefficient.

$L_2$ error of the proposed FPM method, are compared to FDM, FEM and EFG as given in Table 6.

| | Number of nodes | FPM | EFG | FEM | FDM |
|---|---|---|---|---|---|
| $L_2$ error% | 185 | 0.46 | 0.73 | 1.42 | 0.73 |
| | 697 | 0.11 | 0.27 | 0.46 | 0.086 |

Table 6: $L_2$ error at time=20 years for constant D in a square column

Figure 9 and Table 6 illustrate that the FPM error is less than the other methods when 185 nodes are used for solving the problem. By increasing the number of nodes, all methods converge to the exact solution.

### 4.2.2 Circular column

A circular column, depicted in Figure 6, is studied in this section. Specifications of the problem are the same as the square column. The distribution of nodes is shown in Figure 10. The chloride diffusion problem is solved by FPM for constant diffusion coefficients. The results of FPM and the exact solution for constant diffusion coefficient are compared in Table 7.

| | $L_2$ error% | initiation period (year) |
|---|---|---|
| FPM (585 nodes) | 0.0039 | 12.15 |
| exact | --------- | 14.2 |

Table 7: The initiation period and $L_2$ error for the circular column with constant D

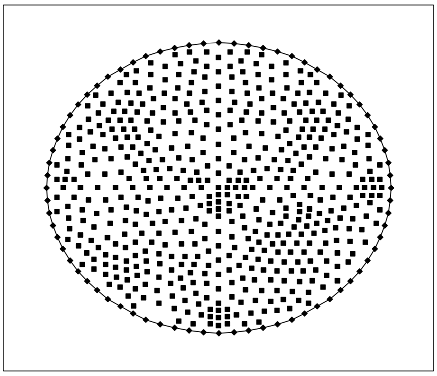


Figure 10: Distribution of nodes for the circular column(585 nodes)

## 5 CONCLUSIONS

A truly meshless finite point approach has been presented for solving the chloride diffusion equation and prediction of service life of concrete structures. FPM is a strong form solution for the diffusion problem using the moving least square approximation for the chloride content field variable. A variety of 1D and 2D simulations were carried out to compare the new approach with analytical and other numerical EFG, FEM, FDM methods.1D tests demonstrated that FPM and FDM provide very close predictions whereas for 2D problems, if regular distribution of nodes are used, the FPM and FDM remain close, while FPM can also be efficiently used for accurate simulation using irregular distribution of nodes.

## ACKNOWLEDGMENT

The authors would like to gratefully acknowledge H. Taghaddos and F. Mahmoudzadeh for providing the required data for EFG and FE solutions.

## REFERENCES

[1] B.H. Oh and B.S. Jnag, Chloride diffusion analysis of concrete structures considering the effects of reinforcements, *ACI Material Journal*,100: 2 ,143-149, 2003.

[2] P. Goltermann, Chloride ingress in concrete structures; Exptrapolation of Observations, *ACI Material Journal*, 100: 2, 114-119, 2003.

[3] E. Onate, S. Idelson, O.C. Zienkiewicz, R.L. Taylor, A stabilized finite point method for analysis of fluid mechanics's problems, *Comp. Meth. In Appl. Engng*, 139: 1-4: 315-347, 1996b.

[4] E. Onate, S. Idelson, O.C. Zienkiewicz and R.L. Taylor. A finite Point Method in computational mechanics. Application to convective transport and fluid flow. *Int. J. Num. Meth. Engng.*, 39: 3839-3866, 1996.

[5] E. Onate, S. Idelson, O.C. Zienkiewicz, R.L. Taylor and C. Sacco, A stabilized finite point method for analysis of convective transport and compressible flows, *Research report* , CIMNE ,1996.

[6] E. Onate, F. Perazzo, J. Miquel. A finite Point Method for elasticity problems. *Computer and Sructue*, 70: 2151-263, 2000.

[7] T. Belytschko, Y. LU and L. GU. Element free Galerkin methods. *Int. J. Num. Meth. Engng.*, 37: 229-56, 1994.

[8] O.C. Zienkiewicz and R.L. Taylor. *The finite element method.* 4th Edition, McGraw Hill, 1989.

[9] H. Taghaddos, F. Mahmoodzadeh, S. Mohammadi, Prediction of service life of concrete structures using mesh free and conventional methods, submitted for publication (2005)

[10] M. Bitaraf , S. Mohammadi, Solving Partial Differential Equations for Plate Bending Problems using Finite Point Method, *Proc. Eccomas Thematic Conference on Meshless Method*, Lisbon, D25, July 2005.