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NUMERICAL ANALYSIS OF CHLORIDE ION PENETRATION IN SEMI-INFINITE SOLID EXPOSED TO A SALINE ENVIRONMENT: THE 1-D CASE

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Abstract

In this paper, a finite element method is formulated to solve the 2nd order Fick's model of time dependent concentration of semi-infinite solid in non-homogeneous materials such as concrete subjected to chloride environment. The method formulates a time dependent problem from the Fick's model and proceeds to calculate the associated vectors from which the solution can be obtained. The result obtained is highly accurate and when compared with the exact solution and related literature tended fast to the transient state solution.

Keyword: Finite element, semi-infinite, concrete, transient state.

1. Introduction

The deterioration of reinforced structures due to physical and chemical attack has been a major concern to civil engineers; hence the durability of concrete structures exposed to marine environment depends mainly on the ability of concrete to resist chloride ingress [1]. Also a simple model for chloride penetration has been developed to assess the service life of concrete structures exposed to marine environment [2]. The complex phenomenon associated with concrete depends on many parameters related to the concrete properties and to the micro-environmental characteristics. Furthermore, when unprotected concrete is exposed to aggressive substances containing chloride, the chloride will penetrate the concrete. The natural content in the pore liquid and the binder of the near-to-surface layer of the concrete will raise [3]. It is widely known that the ingress of chloride ions constitutes a major source of durability problems affecting reinforced concrete structures which are exposed to marine environments. Once sufficient quantity of chloride has accumulated around the embedded steel, pitting corrosion of the metal is liable to occur unless the environmental conditions are strongly anaerobic [4]. In concrete, the flow rate is very low [5], hence the chemical potential driving the diffusion transfer of moisture may include, temperature, solute concentration giving an osmotic pressure and moisture content giving rise to surface (adsorption) forces and vapor/water interface forces in the capillaries. Amongst the various exposure conditions that concrete and reinforced concrete structures may be subjected to during their service life, chlorides represent one of the most complex and eventually most hazardous attacks [6]. The capacity of any type of concrete to resist chloride penetration is the presence of the diffusion coefficient of the chloride and it is used to predict the service life of reinforced concrete structures [7]. In determining the fundamental properties of concrete and the diffusion coefficient, electrochemical test and an optimization model was developed. The development and implementation of a software that calculate the chloride penetration profile in concrete obtained using traditional Portland cements and cementitious mixtures from the addition of pozzolanic materials such as silica fume, metakaolin, fly ash, etc was brought forth [8]. The software calculates the penetration profile taking into account parameters such as the water-cement ratio, initial chlorides concentration, and the pozzolan content in the mixture. Furthermore, focus on the apparent chloride diffusion coefficient was derived by evaluating chloride profiles using Fick's 2nd law of diffusion and is found to be time dependent and may decrease considerably with increasing age of the concrete [9]. The differences between self-diffusion, tracer diffusion and chemical diffusion was explained and a relationship for the temperature dependence of the diffusion coefficients in terms of the atomic jump mechanism, both for diffusion via interstitial mechanism and for a vacancy mechanism was further derived. [9]. Some of the test methods with real specifications to demonstrate the dangers of specifiers in not fully understanding the nature, methodology and purpose of tests chosen for the specification were examined, and the matter of time is highlighted and the real relevance of the tests to the design life of the structure was looked into [10].

2. Materials and Methods

The equation governing the transient concentration problem in materials is given as:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad (1)$$

Where x is the length of the concrete cube, C is concentration, D is the diffusivity coefficient and t is the time.

2.1 Finite element formulation

The variational form of the Fick's 2nd equation above is

$$0 = \int_{\Omega} W(t)\left[-\frac{\partial C}{\partial t} + D\frac{\partial^2 C}{\partial x^2}\right]dx \qquad (2)$$

Where t is time, Ω is domain of interest, dx is the differential element and ∂C is the incremental change in concentration

Expanding the above integral by means of integration by parts yields:

$$\begin{aligned} 0 = &-\int_x^{x+h} W(t)\frac{\partial C}{\partial t}dx - D\int_x^{x+h}\frac{\partial W_{(t)}}{\partial x}\frac{\partial C}{\partial x}dx \\ &+W(t)\left[D\frac{\partial C}{\partial x}\right]\Bigg|_{x+h} - W(t)\left[D\frac{\partial C}{\partial x}\right]\Bigg|_{x} \end{aligned} \qquad (3)$$

Let

$$Q_a = \left[D\frac{\partial C}{\partial x}\right]\Bigg|_{x+h} \text{ and } -Q_b = \left[D\frac{\partial C}{\partial x}\right]\Bigg|_{x} \qquad (4)$$

Eq. 4 represent the value of the secondary variables at the boundary $x+h$ and x respectively

$$\begin{aligned} 0 = &-\int_x^{x+h} W(t)\frac{\partial C}{\partial t}dx - D\int_x^{x+h}\frac{\partial W_{(t)}}{\partial x}\frac{\partial C}{\partial x}dx \\ &+W(t)Q(t_{x+h}) + W(t)Q(t_x) \end{aligned} \qquad (5)$$

Since the primary variable is the function itself, the Lagrange interpolation family functions is admissible. It is proposed that C is the approximation over a typical finite element domain by the expression below

$$\text{If } C = \partial\sum_{j=1}^{n}\psi_j(x)C_j(x) \text{ and } w = \psi_i(x) \qquad (6)$$

$$\int_x^{x+h}\psi_i\psi_j\frac{\partial C_j}{\partial t}dx + D\int_x^{x+h}\frac{\partial \psi_i}{\partial x}\frac{\partial \psi_j}{\partial x}C_j dx = \{Q_i\} \qquad (7)$$

where

$$K_{ij}^{e}=\int_{x}^{x+h}\frac{\partial\psi_i}{\partial x}\frac{\partial\psi_j}{\partial x}dx \quad M_{ij}^{e}=\int_{x}^{x+h}\psi_i\psi_j dx \tag{8}$$

Let the space around the solid be divided into a finite number of elements interconnected at the nodes. The concentration must then be expressed in terms of the values at the nodes thus; the finite element model becomes:

$$\left[M_{ij}^{e}\right]\left\{\dot{C}_j\right\}+D\left[K_{ij}^{e}\right]\left\{C_j\right\}=\left\{Q_i^{e}\right\} \tag{9}$$

Expanding eq. 7 for one quadratic element we have

For i = 1 and j = 1 to 3

$$\left\{Q^{e}\right\}=D\begin{pmatrix}\int_{x}^{x+h}\frac{\partial\psi_1}{\partial x}\frac{\partial\psi_1}{\partial x}dx & \int_{x}^{x+h}\frac{\partial\psi_1}{dx}\frac{\partial\psi_2}{dx}dx & \int_{x}^{x+h}\frac{\partial\psi_1}{\partial x}\frac{\partial\psi_3}{\partial x}dx\\ \int_{x}^{x+h}\frac{\partial\psi_2}{\partial x}\frac{\partial\psi_1}{\partial x}dx & \int_{x}^{x+h}\frac{\partial\psi_2}{\partial x}\frac{\partial\psi_2}{\partial x}dx & \int_{x}^{x+h}\frac{\partial\psi_2}{\partial x}\frac{\partial\psi_3}{\partial x}dx\\ \int_{x}^{x+h}\frac{\partial\psi_3}{\partial x}\frac{\partial\psi_1}{\partial x}dx & \int_{x}^{x+h}\frac{\partial\psi_3}{\partial x}\frac{\partial\psi_2}{\partial x}dx & \int_{x}^{x+h}\frac{\partial\psi_3}{\partial x}\frac{\partial\psi_3}{\partial x}dx\end{pmatrix}\begin{Bmatrix}C_1\\C_2\\C_3\end{Bmatrix}+\begin{pmatrix}\int_{x}^{x+h}\psi_1\psi_1dx & \int_{x}^{x+h}\psi_1\psi_2dx & \int_{x}^{x+h}\psi_1\psi_3dx\\ \int_{x}^{x+h}\psi_2\psi_1dx & \int_{x}^{x+h}\psi_2\psi_2dx & \int_{x}^{x+h}\psi_2\psi_3dx\\ \int_{x}^{x+h}\psi_3\psi_1dx & \int_{x}^{x+h}\psi_3\psi_2dx & \int_{x}^{x+h}\psi_3\psi_3dx\end{pmatrix}\begin{Bmatrix}\dot{C}_1\\\dot{C}_2\\\dot{C}_3\end{Bmatrix} \tag{10}$$

Using one-dimension Lagrange Quadratic Interpolation function of $\left\{\psi_i^{e}\right\}$ for a linear quadratic element,

$$\psi_1=\left(1-\frac{x}{h}\right)\left(1-\frac{2x}{h}\right) \quad \psi_2=\left(\frac{4x}{h}\right)\left(1-\frac{x}{h}\right)$$

$$\psi_3=\left(-\frac{x}{h}\right)\left(1-\frac{2x}{h}\right) \tag{11}$$

Evaluating the $\left[K_{ij}\right]$ and $\left[M_{ij}\right]$ matrices for a Concrete Cube using eq.8 and eq, 11

$$K^{e}=\frac{D}{3h^3}\begin{bmatrix}7h^2-24hx+48x^2 & -8\left(h^2-3hx+12x^2\right) & h^2+48x^2\\ -8\left(h^2-3hx+12x^2\right) & 16\left(h^2+12x^2\right) & -8\left(h^2+3hx+12x^2\right)\\ h^2+48x^2 & -8\left(h^2+3hx+12x^2\right) & 7h^2+24hx+48x^2\end{bmatrix} \tag{12}$$

$$M^{e}=\begin{bmatrix}\dfrac{\frac{2h^4}{15}-h^3x+3h^2x^2-4hx^3+4x^4}{h^3} & \dfrac{h^4-30h^2x^2+60hx^3-120x^4}{15h^3} & \dfrac{30h^2x^2-h^4+120x^4}{30h^3}\\ \dfrac{h^4-30h^2x^2+60hx^3-120x^4}{15h^3} & \dfrac{8h}{15}+\dfrac{16x^4}{h^3} & -\dfrac{30h^2x^2-h^4+60hx^3+120x^4}{15h^3}\\ \dfrac{30h^2x^2-h^4+120x^4}{30h^3} & -\dfrac{30h^2x^2-h^4+60hx^3+120x^4}{15h^3} & \dfrac{\frac{2h^4}{15}+h^3x+3h^2x^2+4hx^3+4x^4}{h^3}\end{bmatrix} \tag{13}$$

Analyzing the cube element by element we take elements at $x=0,h,2h,3h$ for both K^{e} and M^{e} matrices [11], the matrix can be assembled as shown in Fig1.

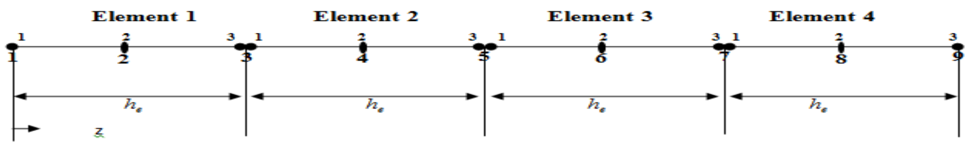

Figure 1: Four quadratic element mesh

For a four quadratic element mesh, the assembled $\left[K^e\right]$ matrix is presented thus:

$$\left[K^e\right]=\frac{D}{3h_e}\begin{bmatrix} k_{11}^1 & k_{12}^1 & k_{13}^1 & 0 & 0 & 0 & 0 & 0 & 0 \\ k_{21}^1 & k_{22}^1 & k_{23}^1 & 0 & 0 & 0 & 0 & 0 & 0 \\ k_{31}^1 & k_{32}^1 & k_{33}^1+k_{11}^2 & k_{12}^2 & k_{13}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & k_{21}^2 & k_{22}^2 & k_{23}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & k_{31}^2 & k_{32}^2 & k_{33}^2+k_{11}^3 & k_{12}^3 & k_{13}^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & k_{21}^3 & k_{22}^3 & k_{23}^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & k_{31}^3 & k_{32}^3 & k_{33}^3+k_{11}^4 & k_{12}^4 & k_{13}^4 \\ 0 & 0 & 0 & 0 & 0 & 0 & k_{21}^4 & k_{22}^4 & k_{23}^4 \\ 0 & 0 & 0 & 0 & 0 & 0 & k_{31}^4 & k_{32}^4 & k_{33}^4 \end{bmatrix} \quad (14)$$

Substituting the values obtained from eq. 12 into eq. 14 yielded the global system of matrix as shown below.

$$\left[K^e\right]=\frac{D}{3h_e}\begin{bmatrix} 7 & -8 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -8 & 16 & -8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -8 & 38 & -80 & 49 & 0 & 0 & 0 & 0 \\ 0 & 0 & -80 & 208 & -128 & 0 & 0 & 0 & 0 \\ 0 & 0 & 49 & -128 & 230 & -344 & 193 & 0 & 0 \\ 0 & 0 & 0 & 0 & -344 & 784 & -440 & 0 & 0 \\ 0 & 0 & 0 & 0 & 193 & -440 & 614 & -800 & 433 \\ 0 & 0 & 0 & 0 & 0 & 0 & -800 & 1744 & -944 \\ 0 & 0 & 0 & 0 & 0 & 0 & 433 & -944 & 511 \end{bmatrix} \quad (15)$$

For a four quadratic element mesh, the assembled M^e matrices are as presented thus:

$$\left[M^e\right]=\frac{h}{30}\begin{bmatrix} M_{11}^1 & M_{12}^1 & M_{13}^1 & 0 & 0 & 0 & 0 & 0 & 0 \\ M_{21}^1 & M_{22}^1 & M_{23}^1 & 0 & 0 & 0 & 0 & 0 & 0 \\ M_{31}^1 & M_{32}^1 & M_{33}^1+M_{11}^2 & M_{12}^2 & M_{13}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & M_{21}^2 & M_{22}^2 & M_{23}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & M_{31}^2 & M_{32}^2 & M_{33}^2+M_{11}^3 & M_{12}^3 & M_{13}^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & M_{21}^3 & M_{22}^3 & M_{23}^3 & 0 & 0 \\ 0 & 0 & 0 & 0 & M_{31}^3 & M_{32}^3 & M_{33}^3+M_{11}^4 & M_{12}^4 & M_{13}^4 \\ 0 & 0 & 0 & 0 & 0 & 0 & M_{21}^4 & M_{22}^4 & M_{23}^4 \\ 0 & 0 & 0 & 0 & 0 & 0 & M_{31}^4 & M_{32}^4 & M_{33}^4 \end{bmatrix} \quad (16)$$

Substituting the values obtained from eq. 12 into eq. 16 yielded the global system of matrix as shown below.

$$\left[M^e\right]=\frac{h}{30}\begin{bmatrix} 4 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 68 & -178 & 149 & 0 & 0 & 0 & 0 \\ 0 & 0 & -178 & 496 & -418 & 0 & 0 & 0 & 0 \\ 0 & 0 & 149 & -418 & 1628 & -3118 & 2039 & 0 & 0 \\ 0 & 0 & 0 & 0 & -3118 & 7696 & -5038 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2039 & -5038 & 10508 & -16738 & 9989 \\ 0 & 0 & 0 & 0 & 0 & 0 & -16738 & 38896 & -23218 \\ 0 & 0 & 0 & 0 & 0 & 0 & 9989 & -23218 & 13864 \end{bmatrix} \quad (17)$$

but $\overline{Q}_i^e = \left(Q_i^1\right)_{s+1} + \left(Q_i^1\right)_s$ and

$$\bar{Q}_i^e = \frac{1}{2}\left(Q_i^1\right)_{s+1} + \frac{1}{2}\left(Q_i^1\right)_s \tag{18}$$

3. Time Approximation for 1-D Diffusivity Equation

For a given time step s, equation 9 becomes

$$D\left[K_{ij}^e\right]\{C\}_s + \left[M_{ij}^e\right]\left\{\dot{C}_j\right\}_s = \left\{Q_i^e\right\}_s \tag{19}$$

For the next time step $s+1$, eq. 9 becomes

$$D\left[K^e\right]\{C\}_{s+1} + \left[M_{ij}^e\right]\left\{\dot{C}_j\right\}_s = \left\{Q^e\right\}_{s+1} \tag{20}$$

and α family of interpolation for time consideration is given by

$$(1-\alpha)\left\{\dot{C}_j\right\}_s + \alpha\left\{\dot{C}_j\right\}_{s+1} = \frac{\{C_j\}_{s+1} - \{C_j\}_s}{\Delta t_{s+1}} \tag{21}$$

Multiply eq. 20 by $\{1-\alpha\}$ and eq. 21 by α the resulting equations will yield:

$$\begin{aligned}&\left[M_{ij}^e\right]\left[(1-\alpha)\left\{\dot{C}_j\right\}_s + \alpha\left\{\dot{C}_j\right\}_{s+1}\right] \\ &+D\left[K_{ij}^e\right]\left[(1-\alpha)\left\{C_j\right\}_s + \alpha\left\{C_j\right\}_{s+1}\right] \\ &= (1-\alpha)\left\{Q_i^e\right\}_s + \alpha\left\{Q_i^e\right\}_{s+1}\end{aligned} \tag{22}$$

$$\begin{aligned}&\left[\left[M_{ij}^e\right] + \alpha D\Delta t_{s+1}\left[K_{ij}^e\right]\right]\left\{C_j\right\}_{s+1} \\ &= \left[\left[M_{ij}^e\right] - (1-\alpha)D\Delta t_{s+1}\left[K_{ij}^e\right]\right]\left\{C_j\right\}_s \\ &+\alpha D\Delta t_{s+1}\left[\left\{Q_i^e\right\}_s + \left\{Q_i^e\right\}_{s+1}\right]\end{aligned} \tag{23}$$

Taking the initial condition given for chloride diffusion in solid, at $x = 0, C_o = 0,\ s = 0,$ that is initial time $t = 0$ which implies that $\left\{Q_i^e\right\}_s = 0$ and the rate of diffusion was constant with a constant diffusion coefficient (D) and $\alpha = 0.5$ as the Crank Nicholson scheme factor Hence eq. 23 becomes eq. 26

$$\left\{Q_j\right\}_1 = D\Delta t_{s+1}\begin{Bmatrix} Q_1^1 \\ Q_2^1 \\ Q_3^1 + Q_1^2 \\ Q_2^2 \\ Q_3^2 + Q_1^3 \\ Q_2^3 \\ Q_3^3 + Q_1^4 \\ Q_2^4 \\ Q_3^4 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{24}$$

$$\begin{aligned}\left\{C_j\right\}_1 &= \left[\left[M_{ij}^e\right] + D\frac{\Delta t_1}{2}\left[K_{ij}^e\right]\right]^{-1} \\ &\left[\begin{aligned}&\left[\left[M_{ij}^e\right] - D\frac{\Delta t_1}{2}\left[K_{ij}^e\right]\right]\left\{C_j\right\}_0 \\ &+\frac{\Delta t_{s+1}}{2}\left\{Q_i^e\right\}_{s+1}\end{aligned}\right]\end{aligned} \tag{25}$$

3.1 Boundary condition

For a semi-infinite medium, with the following initial and boundary conditions apply:

- C = 0 at x > 0 at time t = 0 (initial)
- C = Cs at x = 0 at time t > 0 (boundary)

$$\left\{C_j\right\} = \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \end{Bmatrix} = \begin{Bmatrix} C_s \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{26}$$

4. Results and Discussion

In other to determine the diffusion of chloride ions (ingress) at different nodes in the concrete discretized, we substitute the various parameters in Table 1 and Eq. 26 into eq. 25. The result obtained from the finite element solution is a presented in Table 2.

The experimentally determined chloride along the diffusion path is also presented in table 2, where each depth represents the distance of the middle of the disc from the exposed surface. The result shows a gradual penetration chloride ion into the block to the measured distance of 9 mm.

Table 1: Parameters for calculating for concrete in Saline Environment [10]

Diffusion Coefficient (D)	5.61E-12 mm^2/s
Chloride Content at Surface (C_s)	0.66% mass of Cement
Background Chloride Content (C_o)	0.001% mass of Cement
Exposure time in Saline Environment (t)	28 days

Table 2: Ionic quantities of chloride at various depth in the concrete cube

Depth (mm)	**Merretz et al (2003) % mass of chloride**	**FEA % mass of chloride**	**Exact % mass of chloride**
0	0.66	0.66	0.66
0.25	0.625	0.637	0.637
0.75	0.562	0.589	0.589
1.5	0.499	0.521	0.521
2.5	0.439	0.433	0.433
3	0.355	0.391	0.391
5	0.246	0.245	0.245
7	0.127	0.139	0.139
9	0.022	0.072	0.072

In Figs. 2 and 3 the plots of the two results completely converged due to the high accuracy of the results. To ascertain the accuracy of the analysis the same problem was analyzed using the exact solution differential equation method. It was realized that the two results obtained converged.

Fig. 3 is a graph of concentration against time in days and it shows that the diffusion of chloride ion will begin just after 5days along the outer surface of the concrete cube. Also the figure shows that at 28days of penetration only about 19% (just over 0.12% by wt) of the concentration by mass of chloride ion had diffused into the concrete at a depth of 75mm. To allow for penetration the diffusion coefficient must be high enough to a maximum of 10^{-7} mm^2/s being the least else penetration cannot begin.

Fig. 4 shows the plots of this work and that of Merretz [10]. This work tends better to the exact differential equation and completely converged due to the high accuracy of the results but the work of Merretz et al [10] shows a little variation due to measurement. However the results are in agreement as shown.

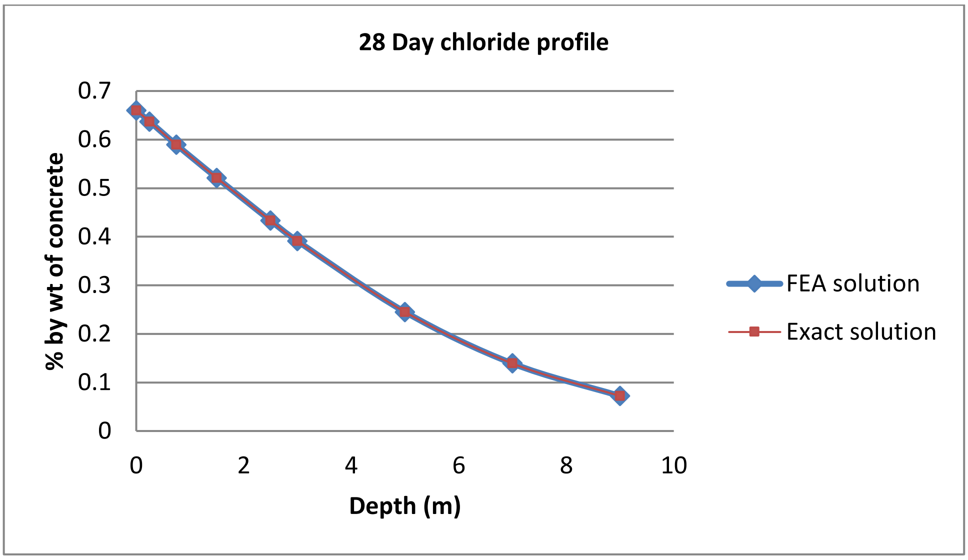

Fig. 2: Concentration against depth

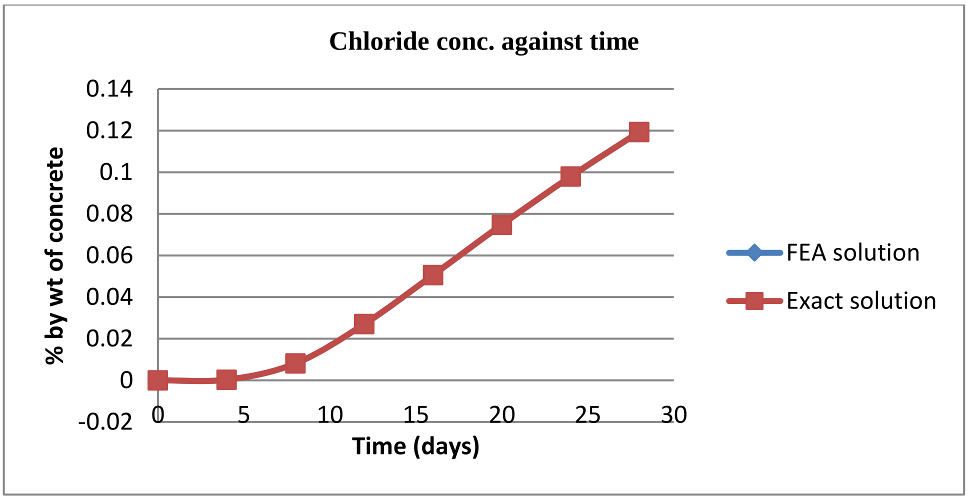

Fig. 3: Concentration against time (days)

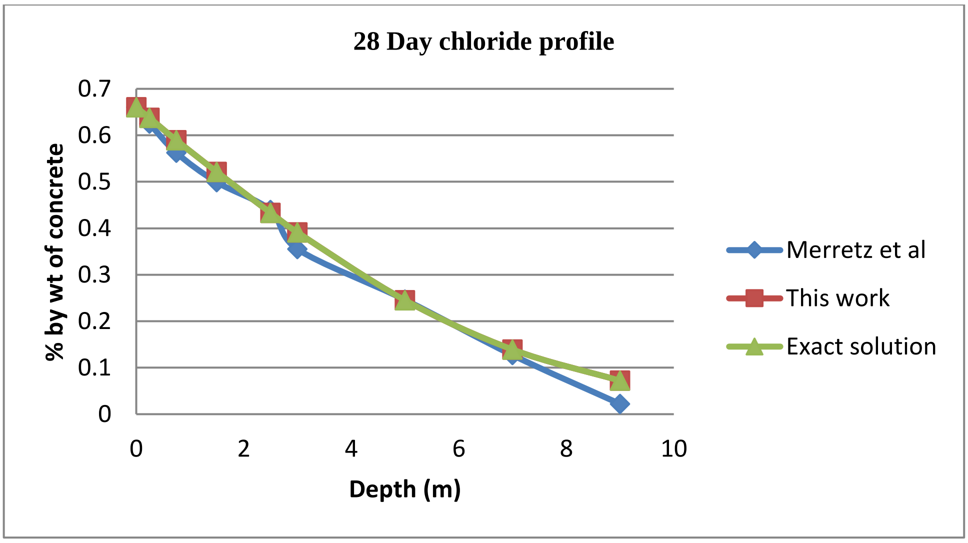

Fig. 4: A graph of concentration against depth

5. Conclusion

Due to the semi-infinite and non-homogeneity of the properties of concrete, it is often difficult to obtain solutions in arithmetic order that can characterize the amount of chloride ion into the concrete, hence the need to analyze numerically to obtain solutions that are accurate as possible. In this work a finite element method was discussed, analyzed and used to solve the 1-D Fick's 2^{nd} order differential equation. The scheme developed is simple and finds its basis on the Galerkin method and the time approximation scheme which was employed. Hence numerical method can predict chloride ion penetration profile as does experimental.

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