Numerical Analysis of Chloride Ion Penetration in a 2-D Semi-Infinite Solid Exposed to a Saline Environment

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Abstract - The diffusivity equation of time/depth dependent concentration in semi-infinite solid is presented and solved using the Galerkin finite element method. The method formulates a time/depth dependent problem from Fick's second order model and proceeds to calculate the associated vectors from a rectangular shape element with its associated interpolation functions and boundary conditions from which the solutions were obtained with a concrete cube of $150 \times 150 \times 150 mm$ dimension. The numerical result obtained is validated with the result obtained from the cubes immersed in a pond test of Escravos Beach seawater for 28days with percentage concentration of 0.63% by wt of concrete. The results show that numerical solution can predict better results as does experimental, as the both the exact solution and FEA solution tended to the experimental result.

Keyword: Finite element, semi-infinite, concrete cubes, rectangular element, saline

1. Introduction

Concrete is a man-made composite, the major constituent of which is natural aggregate such as gravel and sand or crushed rock. Since concrete is a building and structural material it is composed of three constituents namely: cement, water and aggregate, sometimes additional material known as admixture is added to control certain properties [1]. It is reported that concrete provides physical and chemical protection to the reinforcing steel from penetrating chlorides which may cause steel depassivation leading to increased risk of steel corrosion [2]. The chloride resistance depends on the permeability of the concrete and the thickness of cover to the reinforcement. The integrity of the concrete cover under service load, in terms of cracking and crack width, also influences the resistance to penetrating chlorides. In solving mass transfer cases as it applies to concentration profiles in semi-infinite medium an exemplified method was used [3]. Though rigorous he computed the concentration in the semi-infinite medium as a function of time and distance from the surface assuming no bulk flow. Using the water from the Lagos lagoon in Nigeria, with concrete cubes cast with fresh and salt water [4], they sort to look at the influence of salt water on the compressive strength in concrete with a 150mm by 150mm by 150mm mould and a mix ratio of 1:2.4 by weight of concrete and 0.6 water-cement ratio. It was observed that there was an increase in the compressive strength of concrete in the presence of salt or ocean water in the mixing and curing water. 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 [5]. In determining the fundamental properties of concrete and the diffusion coefficient, electrochemical test and an optimization model was develop. They show 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. The software calculates the penetration profile taking into account parameters such the water-cement ratio, initial as chlorides concentration, and the pozzolan content in the mixture [6]. Some test methods were considered by the Concrete Institute of Australia and they seek to demonstrate the dangers for specifiers in not fully understanding the nature, methodology and purpose of tests chosen for the specification [7]. Chloride profile can be found by the grinding technique of producing the powder samples, the analysis of the chloride contents and the interpretation of the observations. Further, how the chloride profile can be reduced to three parameters was done when chloride ingress is caused by chloride diffusion [8]. Unlike mixture theory, the notion of the representative elementary volume (REV) was introduced, where different parts of the domain are occupied by different phases. Subsequently, the classical balance laws of continuum mechanics are imposed on each phase subject to the requisite interface boundary conditions. This is followed by the derivation of macroscopic balance equations by means of averaging over the REV domain. This approach, while maximally inclusive of the microstructural aspects of the low, requires an inordinate degree of modeling resolution, and is very challenging for computational implementation.

An improved formula for the dependence of diffusivity on pore humidity which give satisfactory diffusion profiles and long term drying predictions and can be suited into the finite element programs for shrinkage

and creep effects in concrete structures was proposed [9]. Furthermore, the well-known diffusion mechanisms which include the ordinary diffusion, Knudsen diffusion and surface diffusion were analyzed while the diffusion in concrete was treated as a combination of these mechanisms. Also a developed mathematical model which was used to predict experimental absorption isotherms of Portland cement paste at low temperatures was presented [9]. An analysis of chloride profiles obtained from reinforced concrete bridges which was exposed to de-icing salts was presented [10]. Using a diffusion model a number of chloride profiles were analyzed for a diffusion coefficient for a typical Portland cement concrete in wet conditions which is about $3 \times 10^{-12} m^2 / s$, and suggested that there is a need for improved coating (epoxy) for structures of this type to reduce chloride transport. An equation governing drying and wetting of concrete was formulated [11]. This equation is based on the assumption that the diffusivity and other material parameters are dependent on pore humidity, temperature and degree of hydration. It is found that the diffusion coefficient decreases when passed from 0.9 to 0.6 pore humidity resulting from fitting computer solutions for slabs, cylinders and spheres against other test data available. Furthermore, the characterization of moisture diffusion inside early-age concrete slabs subjected to curing was investigated. Time-dependent relative humidity (RH) distributions of three mixture proportions subjected to three different curing methods (i.e., air curing, water curing, and membrane-forming compounds curing) and sealed condition were measured for 28 days [12]. A one-dimensional nonlinear moisture diffusion partial differential equation (PDE) based on Fick's second law, which incorporates the effect of curing in the Dirichlet boundary condition using a concept of curing factor was developed to simulate the diffusion process. Model parameters are calibrated by a genetic algorithm (GA). Experimental results show that the RH reducing rate inside concrete under air curing is greater than the rates under membrane-forming compound curing and water curing. It was also shown that the effect of water-to-cement (w/c) ratio on selfdesiccation is significant. Lower w/c ratio tends to result in larger RH reduction. RH reduction considering both effect of diffusion and self-desiccation in early-age concrete is not sensitive to w/c ratio, but to curing method [12]. A focus on the apparent chloride diffusion

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coefficient derived by evaluating chloride profiles using Fick's 2nd law of diffusion is found to be time dependent and may decrease considerably with increasing age of the concrete. In service life predictions of marine structures this time dependency of the diffusion coefficient is taken into account by an age factor [13]. A finite element method was formulated to solve the 2nd order Fick's model of time/depth dependent concentration of semi-infinite solid in nonhomogeneous materials such as concrete subjected to chloride environment in the 1-D regime [14]. 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.

2. Materials and Methods

A sample of seawater from the Escravos water was collected and measured for its chemical compounds to determine the chloride content. The percentage composition by mass of dissolved compound from laboratory analysis is as presented.

Table 1: % composition of chemical compound inEscravos seawater

Dissolved Compound of seawater	
NaCl	28.97
MgCl ₂	18.48
CaSO ₄	0.57
K ₂ SO ₄	2.35
KBr	2.03
Mg SO ₄	0.46
Other chemical compounds	46.96

From the laboratory analysis, Chloride (Cl) was found to be about 630 mg/l (0.63 kg/m³) and Sodium (Na) 60.3 mg/l (0.0603 kg/m³) respectively of seawater.

2.1 Data used for concrete design

The mix was formed using Portland limestone cement (PLC) as the reference mixture for a grade 30 mix. The rectangular specimen used has the following mix design presented herein:

- a. Estimated w/c ratio = 0.5
- b. Estimated compressive strength F_c at 28 days = $25 \ N/mm^2$
- c. 5% deflection rate (k = 1.64)
- d. Portland limestone Cement (PLC)
- e. Slump required = 10 30 mm
- f. Maximum aggregate size = 20
- g. Minimum cement content = 290 kg/m^3
- h. Maximum cement content = 550 kg/m^3

- i. Coarse aggregate conformity: zone-3 of BS:882
- j. Relative density = 2.7

The rectangular concrete cubes measuring $150 \times 150 \times 150$ mm were formed from the mix above and specimens were coated with epoxy paint on all but two faces to represent the 2-D (in the x-y axis).

2.2 Numerical Analysis

Using Fick's second law of diffusivity equation with necessary boundary conditions for a 2D cube in the x - y plane we have

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y} \right)$$
(1)

Where D_x and D_y are the diffusion coefficient in the *X* and *y* directions, respectively

$$C(x.y,t) = erf\left[\frac{x}{2\sqrt{D_x t}}\right] erf\left[\frac{y}{2\sqrt{D_y t}}\right]$$
(2)

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) \tag{3}$$

$$0 = -\frac{\partial C}{\partial t} + D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)$$
(4)

Multiplying through by a weight function W(t) and integrating by part

$$0 = -W \frac{\partial C}{\partial t} + DW \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right)$$
(5)
$$0 = -\int_A W \frac{\partial C}{\partial t} dA - DW \frac{\partial c}{\partial x} \Big|_A + D \int_A \frac{\partial W}{\partial x} \frac{\partial C}{\partial x} dA - DW \frac{\partial c}{\partial y} \Big|_A + D \int_A \frac{\partial W}{\partial y} \frac{\partial C}{\partial y} dA$$
(6)
$$0 = -\int_A W \frac{\partial C}{\partial t} dA - D \left(W \frac{\partial c}{\partial x} \Big|_A + W \frac{\partial c}{\partial y} \Big|_A \right) + D \int_A \left(\frac{\partial W}{\partial x} \frac{\partial C}{\partial x} + \frac{\partial W}{\partial y} \frac{\partial C}{\partial y} \right) dA$$
(7)

Eq. (7) is referred to as the weak form

2.2 Finite element formulation

The weak form in eq. (7) requires that the approximation chosen for C be at least linear in both the x and y direction so that there are no terms in it that are identically zero. Since the primary variable is simply the function itself, the Lagrange family of interpolation function is admissible.

Let
$$q = \left(W \frac{\partial c}{\partial x} \Big|_{A} + W \frac{\partial c}{\partial y} \Big|_{A} \right)$$
 and (8)

$$W = \psi_i^e(x, y) \text{ And } C = \sum_i C_j \psi_j(x, y)$$
(9)

Therefore,

$$0 = -\int_{A} \psi_{i}^{e} \frac{\partial \sum_{1}^{n} C_{j} \psi_{j}}{\partial t} dA - Dq + D \int_{A} \left(\frac{\partial \psi_{i}^{e}}{\partial x} \frac{\partial \sum_{1}^{n} C_{j} \psi_{j}}{\partial x} + \frac{\partial \psi_{i}^{e}}{\partial y} \frac{\partial \sum_{1}^{n} C_{j} \psi_{j}}{\partial y} \right) dA$$
(10)

$$D\{C_{j}\}\int_{x_{j}}^{x_{j}}\int_{y_{i}}^{y_{i}}\left(\frac{\partial\psi_{i}^{e}}{\partial x}\frac{\partial\psi_{j}}{\partial x}+\frac{\partial\psi_{i}^{e}}{\partial y}\frac{\partial\psi_{j}}{\partial y}\right)dxdy+\int_{x_{j}}^{x_{j}}\int_{y_{i}}^{y_{j}}\psi_{i}^{e}\psi_{j}^{e}\frac{\partial C_{j}}{\partial t}dxdy=Dq(11)$$

The Coefficient matrix

$$\left[K^{e}\right] = \int_{x_{1}, y_{1}}^{x_{2}, y_{2}} \left(\frac{\partial \psi_{i}^{e}}{\partial x} \frac{\partial \psi_{j}}{\partial x} + \frac{\partial \psi_{i}^{e}}{\partial y} \frac{\partial \psi_{j}}{\partial y}\right) dx dy$$
(12)

The mass matrix
$$\left[M^e\right] = \int_{x_1}^{x_2} \int_{y_1}^{y_2} \psi_i^e \psi_j^e dx dy$$
 (13)

In linear form, the equation becomes $D[K^{e}]\{C_{j}\}+[M^{e}]\{C_{j}\}-Dq=0$ (14)

$$q = \frac{dC}{dx}\Big|_{x=L} + \frac{dC}{dy}\Big|$$
(15)

Simplifying $[K^e]$ and $[M^e]$ matrices, a rectangular linear element interpolation function is used. The concrete cube domain is discretized into four rectangular blocks as shown below:

$$\psi_1 = \left(1 - \frac{x}{X}\right) \left(1 - \frac{y}{Y}\right) \tag{16}$$

$$\psi_2 = \frac{x}{X} \left(1 - \frac{y}{Y} \right) \tag{17}$$

$$\psi_3 = \frac{x}{X} \frac{y}{Y} \tag{18}$$

$$\psi_4 = \frac{y}{Y} \left(1 - \frac{x}{X} \right) \tag{19}$$

2.3 Evaluating the element matrix for 2-D concrete cube

In other to solve $[K^e]$ matrix, we substitute the rectangular interpolation function of eqs. (16)-(19) into eq. (11)

For the
$$\begin{bmatrix} K^e \end{bmatrix}$$
 matrix
 $\begin{bmatrix} K^e \end{bmatrix} = \int_{x_1 y_1}^{x_2 y_2} \left(\frac{\partial \psi_i^e}{\partial x} \frac{\partial \psi_j}{\partial x} + \frac{\partial \psi_i^e}{\partial y} \frac{\partial \psi_j}{\partial y} \right) dx dy$ (20)
 $\begin{bmatrix} K_{11}^1 \end{bmatrix} = \int_{0}^{x_1} \int_{0}^{x_2} \left[\left(\left(-\frac{1}{X} \right) \left(1 - \frac{y}{Y} \right) \right)^2 + \left(\left(-\frac{1}{Y} \right) \left(1 - \frac{x}{X} \right) \right)^2 \right] dy dx$ (21)
 $\begin{bmatrix} K_{11}^1 \end{bmatrix} = -\frac{Y}{3X} + \frac{X}{3Y}$ (22)
But $\begin{bmatrix} K^1 \end{bmatrix} = \begin{bmatrix} K^2 \end{bmatrix} = \begin{bmatrix} K^3 \end{bmatrix} = \begin{bmatrix} K^4 \end{bmatrix}$, the assembled $\begin{bmatrix} K^e \end{bmatrix}$
matrix is thus given in eq. (23) for a single element.
 $\begin{bmatrix} \frac{Y}{3X} + \frac{X}{3Y} & -\frac{Y}{3X} + \frac{X}{6Y} & \frac{Y}{6X} - \frac{X}{6Y} & \frac{Y}{6X} - \frac{X}{3Y} \\ -\frac{Y}{3X} + \frac{K}{6Y} & \frac{Y}{3X} + \frac{X}{3Y} & \frac{Y}{6X} - \frac{X}{6Y} & -\frac{Y}{6X} - \frac{X}{6Y} \\ \end{bmatrix}$

$$\begin{bmatrix} P & Y \\ -\frac{Y}{6X} - \frac{X}{6Y} & \frac{Y}{6X} - \frac{X}{3Y} & \frac{Y}{3X} + \frac{X}{3Y} & -\frac{Y}{3X} + \frac{X}{6Y} \\ \frac{Y}{6X} - \frac{X}{3Y} & -\frac{Y}{6X} - \frac{X}{6Y} & -\frac{Y}{3X} + \frac{X}{6Y} & \frac{Y}{3X} + \frac{X}{3Y} \end{bmatrix}$$
(23)
For the $\begin{bmatrix} M^e \end{bmatrix}$ matrix

Recall eq.(13) above. Substitute the interpolation functions of eqs. (11) to (16) into it will yield the following:

$$\begin{bmatrix} M^{e} \end{bmatrix} = \int_{x_{1}}^{x_{2}} \int_{y_{1}}^{y_{2}} \psi^{e}_{i} \psi^{e}_{j} dx dy$$

$$\begin{bmatrix} M_{11}^{1} \end{bmatrix} = \int_{0}^{X} \int_{0}^{Y} \left[\left(1 - \frac{x}{X} \right) \left(1 - \frac{y}{Y} \right) \right]^{2} dy dx$$

$$\begin{bmatrix} M_{11}^{1} \end{bmatrix} = \frac{XY}{9}$$
But $\begin{bmatrix} M^{1} \end{bmatrix} = \begin{bmatrix} M^{2} \end{bmatrix} = \begin{bmatrix} M^{3} \end{bmatrix} = \begin{bmatrix} M^{4} \end{bmatrix}$,
the assembled $\begin{bmatrix} M^{e} \end{bmatrix}$ matrix is thus given below as (25)

$$\left[M^{e}\right] = \begin{bmatrix} \frac{XY}{9} & \frac{XY}{18} & \frac{XY}{36} & \frac{XY}{18} \\ \frac{XY}{18} & \frac{XY}{9} & \frac{XY}{18} & \frac{XY}{36} \\ \frac{XY}{36} & \frac{XY}{18} & \frac{XY}{9} & \frac{XY}{18} \\ \frac{XY}{18} & \frac{XY}{36} & \frac{XY}{18} & \frac{XY}{9} \end{bmatrix}$$
(25)

For the flux matrix $\left[q^{e}\right]$

eq

2.4 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)

2.5 Assembling of the elemental equation for 2-D concrete cube

The assembly of the finite element equations is based on two basic principles.

1. Continuity of primary variables

2. Equilibrium or balance of secondary variables. In this case a quadrilateral element (or a rectangular element) is used to analyze the domain. It is divided into four different elements as shown in Figure 2

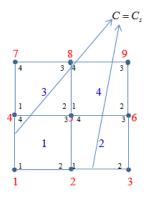


Figure 1: Four rectangular element mesh

The numbers at the vertices outside $(1, 2, 3 \dots 9)$ represent the global nodes, while the numbers in the vertices (1, 2, 3, 4), inside the rectangle represent the local nodes while the numbers (1, 2, 3 and 4) inside each rectangle is used to indicate the elements.

From Figure 1, the assemble K^e matrix is given in below

 k_{11}^1 k_{12}^1 0 k_{21}^1 $k_{22}^1 + k_{11}^2$ k_{12}^2 k_{24}^1 $k_{23}^1 + k_{14}^2$ k_{ij}^2 k_{22}^2 0 k_{21}^2 0 k_{u}^{2} k_{23}^2 0 0 0 k_{41}^{1} 0 k_{42}^2 $k_{43}^1 + k_{11}^4$ $k_{42}^1 + k_{12}^4$ k_{14}^4 $\begin{bmatrix} K^e \end{bmatrix} = \begin{bmatrix} k_{31}^1 & k_{32}^1 + k_{41}^2 & k_{42}^2 \end{bmatrix}$ k_{24}^4 $k_{23}^4 + k_{14}^3$ $k_{24}^1 + k_{24}^2$ $+k_{m}^{4}$ $k_{42}^2 + k_{12}^3$ $k_{44}^2 + k_{11}^3$ 0 k_{31}^2 k_{32}^2 $k_{24}^2 + k_{24}^3$ $k_{22}^2 + k_{22}^3$ 0 k_{u}^{3} k_{44}^{4} 0 0 0 k_{41}^4 k_{42}^4 k_{43}^4 0 0 0 0 0 k_{31}^{4} k_{42}^3 k_{34}^4 $k_{22}^4 + k_{41}^3$ $k_{33}^4 + k_{44}^3$ k_{Λ}^{3} 0 0 0 k^3 0 k_{34}^{3} k^3 (28)

The dimension of the elemental slab is X = 0.75 and

Y = 0.75

$$\begin{bmatrix} X^{e} \end{bmatrix} = \frac{Y}{6X} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{X}{6Y} \begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix}$$
(29)

From Figure 1, the assemble M^{e} matrix is given in below

M_{11}^{1}	M_{12}^{1}	0	M_{14}^{1}	M_{13}^1	0	0	0	0]	
M_{21}^{1}	$M_{22}^1 + M_{11}^2$	M_{12}^{2}	M_{24}^{1}	$M_{23}^1 + M_{14}^2$	M_{13}^2	0	0	0	
0	M_{21}^2	M_{22}^{2}	0	M_{24}^2	M_{23}^2	0	0	0	
M_{41}^{1}	M_{42}^{2}	0	$M_{44}^1 + M_{11}^4$	$M_{43}^1 + M_{12}^4$	0	M_{14}^{4}	M_{13}^{4}	0	
$M^e = M^1_{31}$	$M_{32}^1 + M_{41}^2$	M_{42}^{2}	$M_{34}^1 + M_{21}^2$	$M_{33}^1 + M_{44}^2 + M_{11}^3 + M_{22}^4$	$M_{43}^2 + M_{12}^3$	M_{24}^{4}	$M_{23}^4 + M_{14}^3$	M ³ ₁₃	
0	M_{31}^2	M_{32}^2	0	$M_{34}^2 + M_{21}^3$	$M_{33}^2 + M_{22}^3$	0	M_{24}^{3}	M ³ ₂₃	
0	0	0	M_{41}^{4}	M_{42}^{4}	0	M_{44}^{4}	M_{43}^{4}	0	
0	0	0	M_{31}^{4}	$M_{32}^4 + M_{41}^3$	M_{42}^{3}	M_{34}^{4}	$M_{33}^4 + M_{44}^3$	M_{43}^{3}	
0	0	0	0	M_{31}^{3}	M_{32}^{3}	0	M_{34}^{3}	M_{33}^{3}	(30)

The dimension of the elemental slab is X = 0.75 and Y = 0.75

2.6 Time approximation for 2-D Diffusivity Equation

Following the basic steps outlined [14, 16], the time approximation for a 2-D flow was solved and a model developed as shown below:

$$\{C_s\}_1 = \left[\left[M_{ij}^e\right] + D\frac{\Delta t_1}{2} \left[K_{ij}^e\right] \right]^{-1} \left[\left[\left[M_{ij}^e\right] - D\frac{\Delta t_1}{2} \left[K_{ij}^e\right] \right] \left\{C_j\}_0 + \frac{\Delta t_{s+1}}{2} \left\{q_i^e\right\}_{s+1} \right] \right]$$
(32)

3. Results and Discussion

Using the parameters presented in table 2 the quantity of 2-D chloride ion ingress is as presented in table 3.

in Saline Environment [15]				
Diffusion Coefficient (D)	2.12E-7mm ² /s			
Chloride Content at Surface (C _s)	0.6302% mass of Cement			
Background Chloride Content (C _o)	0.001% mass of Cement			
Exposure time in Saline Environment (t)	28days			

Table 2: Parameters for calculating for concret	e
in Saline Environment [15]	

The results obtained from the analysis as presented in table 3 was plotted as shown in Figure 2. It reveals that the chloride profile predicted by the model almost converge to that of the measured (experimental) profile.

DEPTH	FEA	EXACT SOLUTION	EXP		
(mm)	(% by wt of cement)	(% by wt of cement)	(% by wt of cement)		
0	0.6302	0.6302	0.6302		
1.25	0.4610	0.4610	0.4795		
2.50	0.3112	0.3112	0.3700		
3.75	0.1939	0.1939	0.2320		
5.00	0.1128	0.1128	0.1500		
6.25	0.0638	0.0638	0.0751		
7.50	0.0379	0.0379	0.0632		

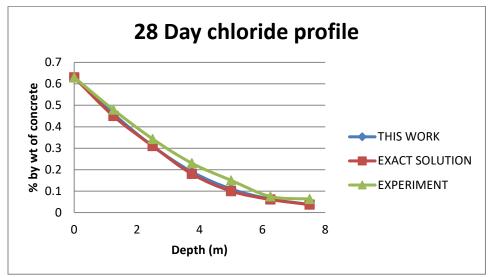


Figure 2: Chloride ion penetration in 2-D

It was observed that the model fits in well with a coefficient of determination (R^2) of 99.7%. This shows that the direction of flow in the 2D-direction was able to account for 99.2% of the variation in the given period of 28days. The estimated standard deviation of the error is found to be 0.0137804. The Degree of Freedom (DF) which indicates the number of independent pieces of information involving the response data needed to calculate the sum of squares for the regression was calculated to be 1 while that of the error was calculated to be 5 with a total DF of 6. Also the total sum of squared (SS) distance was calculated to be approximately 0.274932. From this, the SS Regression which was a portion of the variation explained by the model, was estimated to be 0.273982 while the SS Error which was the portion not explained by the model and was therefore attributed to the errors, was estimated to be 0.000949. The Mean Square Regression (MSR) of the model was estimated to be 0.273982 while the Mean Square of the Error (MSE) also known as Mean Squared Deviation (MSD) which is a risk function was estimated to be 0.000190.

4. Conclusion

Chloride penetration profiles in 2-D experimentally may seem more cumbersome, however, numerically with the appropriate boundary conditions as presented the profiles can be predicted better. Furthermore, numerical solution is not particularly influenced by the concrete quality. Although the Fick's second equation simulated for a particular time step can be used for long term prediction as computed using the FEA method with constant C_s and D which are very important parameters.

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