Chloride diffusion study in different types of concrete using finite element method (FEM)

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Abstract. Corrosion in RCC structures is one of the most important factors that affects the structure's durability and subsequently causes reduction of serviceability. The most severe cause of this corrosion is chloride attack. Hence, to prevent this to happen proper understanding of the chloride penetration into concrete structures is necessary. In this study, first the mechanism of this chloride attack is understood and various parameters affecting the process are identified. Then an FEM modelling is carried out for the chloride diffusion process. The effects of fly ash and slag on the diffusion coefficient and chloride penetration depth in various mixes of concretes are also analyzed through integrating Virtual RCPT Lab and FEM.

Keywords: concrete; chloride diffusion; rapid chloride permeability test; FEM simulation

1. Introduction

Corrosion of reinforcement has been established as the predominant factor causing widespread deterioration of concrete construction worldwide, especially of the structures located in the coastal marine environment. The most important reason of this kind of corrosion attack on concrete is chloride ingress. It causes corrosion in the steel reinforcements embedded in the concrete. The hydration products of cement provide a high alkaline environment in concrete which will activate a passivating film of iron oxide on the embedded steel bars. The passivating film can keep its chemical stability on the steel surface and protect the steel from being corroded. However, when the chloride concentration in concrete reaches a threshold value, the protective film on the steel bars is destroyed (at pH level below 11), and the reinforcement corrosion starts. As a result effective cross sectional area of reinforcements gets reduced and it is replaced with corrosion products. Hence, the ultimate strength of reinforcement surface tensile stress is generated in concrete, which causes cracking and premature loss of service life of concrete. So, chloride ion ingression and thereby induced reinforcement corrosion in steel-reinforced concretes have

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attracted much research interest. Now, to prevent this kind of loss in serviceability of concrete and also to predict the life time of a concrete structure in a marine environment, a detailed knowledge of the of the whole procedure, starting right from the chloride penetration to the occurring of corrosion damage in concrete is to be understood.

Stanish et al. (2000) stated capillary absorption, hydrostatic pressure, and diffusion are the means by which chloride ions can penetrate concrete. In the bulk of the concrete, the chloride ion movement is controlled by mainly concentration gradients through the pore solution. Therefore, among the three transport mechanisms described above that can bring chlorides into the concrete and to the level of the rebar, the principal method is diffusion. Many studies have been conducted so far to analyze and model this chloride diffusivity in concrete. Suwito et al. (2006) presented this chloride penetration as a coupled diffusion procedure of moisture and chloride ions. Ishida et al. (2009) formulated and modelled this chloride diffusivity for both sound and cracked concrete considering the chloride binding capacity, tortuosity and constrictivity of porous network. Ismail et al. (2004) did some experimental tests on an inert material i.e. brick to study chloride ion diffusion through various width of crack openings ranging from 21 to 128 μ m. Zeng et al. (2007) carried out some FEM analysis of chloride penetration in concrete considering concrete as a heterogeneous structure consisting of two different domains of cement matrix and aggregates. After that, Fu et al. (2010) carried out some studies on numerical modelling of chloride diffusion in cracked concrete specimens. Then Conciatori et al. (2010) built a numerical model based on the FEM and FDM taking into account the capillary suction of water vapour and convection of chloride ions along with diffusion of carbon dioxide. Wang et al. (2011) performed numerical modelling of chloride penetration through various sizes of cracks. They used Vornoi diagram technique for discretization of the domain in to reduce the mesh bias. Thomas et al. (1998) presented some experimental test results to study the diffusivity of chloride ions in different concrete mixes with varying fly ash and slag contents. Yang and Weng (2013) developed a multiphase model for predicting the effective chloride migration coefficient of ITZ in cement-based materials. Recent work by Zichao et al. (2014) demonstrated interesting aspects of chloride diffusivity of concrete using probabilistic characteristics at meso-scale. Recently, Lina and Yang (2014) presented a simplified method to determine the chloride migration coefficient of concrete by the electric current in steady state. Example of service life prediction of a reinforced concrete bridge exposed to chloride induced deterioration was demonstrated by Papadakis (2013).

From these brief reviews it is reflected that, there have been numerous experimental and numerical studies on the diffusion of chloride ions in concrete specimens. Yet, there has been very less studies conducted on the chloride diffusivity in different types of concrete compositions. The main motivation of the present work is to systematically carrying out the chloride diffusion study for various concrete mixes. The other different parameters like chloride binding capacity, age of concrete etc. are also considered for the completeness purpose.

Numerical modelling has now been extensively embraced in the study of corrosion-affected RC structures. Several reasons may be cited for the increased use of modelling in the field of corrosion-affected RC structures but the main reasons are: (i) laboratory and field experiments (even with accelerated tests) are relatively expensive and time consuming and (ii) difficulty in replicating different test scenarios, i.e., isolating different variables in the test environment to replicate different real exposure conditions for RC structures. So, if there are some analytical and numerical tools, it would be very easy to predict the diffusion behaviour of chloride in various concrete samples (i.e. with various concrete mix, various ingredients properties etc.) and the chloride penetration profile in a concrete sample by following some simple steps. From this it can

jmrm abe analyzed for a concrete structure how much it is susceptible to corrosion. Hence one can have the idea about the durability of that structure.

Based on these scopes and the literature surveys the following objectives arrived at this study:

• Understanding the chloride diffusion procedure in cracked concrete considering various parameters like age of concrete, temperature, free chloride concentration etc.

• Analyzing the diffusion process in various types of concrete mixes with the help of the Virtual Rapid Chloride Permeability Test.

• Finding a way to predict the diffusion procedure in a concrete sample by integrating the Virtual Rapid Chloride Permeability Test with the FEM model.

2. Basic theory and mechanism

The following section gives an overview of the theory of diffusion and background about the mechanism.

According to Fick's second law for one dimensional case

$$\frac{\partial C_f}{\partial t} = D_{eff} \frac{\partial^2 C_f}{\partial x^2} \tag{1}$$

Where, D_{eff} is the effective diffusion coefficient, C_f is the free chloride concentration in concrete. Martín-Pérez *et al.* (2000), Yuan *et al.* (2009) introduced a new term ω_e , the evaporable water content (m³ evaporable water / m³ concrete) for diffusion in concrete. The solution for the equation becomes,

$$\frac{C_f(x,t)}{C_0} = 1 - erf\left(\frac{x}{\sqrt{4\omega_e D_{eff} t}}\right)$$
(2)

Here, erf() is the error function, which is a mathematical construct found in math tables or as a function in common computer spreadsheets. The influencing factors over the D_{eff} are given in Fig. 1 and discussed below.

(a) Chloride binding capacity

Diffusion Coefficient depends on chloride binding capacity of concrete (Martín-Pérez *et al.*, 2000). Thus, the influencing factor

$$f_{cl,1c}(\mathcal{C}_b) = \frac{1}{1 + \frac{\alpha}{\omega_e \left(1 + \beta C_f\right)^2}}$$
(3)

where, C_b is the bounded chloride concentration. Ishida *et al.* (2008) proposed the values of the concrete binding parameters α , β as 11.8 and 4.0 respectively for Ordinary Portland Cement.

(b) Influence of concrete age

Kwon et al. (2009) suggested another influencing factor for age of concrete

For
$$t < 30$$
 years, $f_{cl,2}(t) = \frac{1}{1-m} \left(\frac{t_{ref}}{t}\right)^m$
For $t > 30$ years, $f_{cl,2}(t) = \left[1 + \frac{t_r}{t} \left(\frac{m}{1-m}\right)\right] \left(\frac{t_{ref}}{t}\right)^m$ (4)



Fig. 1 Influencing factors over diffusion coefficient in concrete

where $t_r = 30$ years, $t_{ref} = 28$ days and 'm' is a time-reducing exponent describing how fast the diffusion coefficient reduces with time, depending on mix proportions.

(c) Influence of temperature

Based on Arrhenius' law, both Martin-Perez et al. (2000) and Kong et al. (2002) suggested the influencing factor for temperature as

$$f_{cl,3}(T) = exp\left[\frac{E_a}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$
(5)

 E_a = Activation energy in kJ/mol, which depends on cement type and w/c ratio. For ordinary Portland cement (OPC) the value is 41.8 ± 4.0 kJ/mol with w/ c of 0.4, 44.6 ± 4.3 kJ/mol with w/ c of 0.5, 32.0 ± 2.4 kJ/mol with w/c of 0.6.

R =Universal gas constant = 8.314 J/K-mol

 T_0 and T are the reference and actual temperature in concrete ($T_0 = 296$ K).

(d) Influence of free chloride concentration

According to Xi and Bazant (2000) and Kong *et al.* (2002), the factor used to account for the influence of free chloride concentration on the chloride diffusivity is

$$f_{cl,4}(C_f) = 1 - k. (C_f)^n$$
 (6)

where, k and n are empirical parameters, k = 8.333 and n = 0.5.

2.1 The enhanced chloride diffusivity

Considering the dependence of chloride diffusivity on the four important influencing parameters as above mentioned, Fu *et al.* (2010) presented the enhanced general expression of chloride diffusivity as,

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$$D_e^* = D_c. f_{cl,1c}(C_b). f_{cl,2}(t). f_{cl,3}(T). f_{cl,4}(C_f)$$
(7)

Herein, the D_c is the diffusivity of the concrete at the age of 28 days in saturated state (m²/h) and

$$D_e^* = D_c. f_{cl,1c}(C_b). f_{cl,2}(t). f_{cl,3}(T). f_{cl,4}(C_f)$$
(8)

where, (w/c) is the water cement ratio.

2.2 Chloride diffusivity in concrete crack

Djerbi et al. (2008) presented the chloride diffusion coefficient through the crack that is

For,
$$30 \,\mu \,\mathrm{m} \le \mathrm{w} \le 80 \,\mu \,\mathrm{m}$$
 $D_{cr} = 2 \times 10^{-11} \,\mathrm{w} - 4 \times 10^{-10}$

For, w
$$\ge 80 \,\mu \,\mathrm{m}$$
 $D_{cr} = 14 \,\times \,10^{-10}$ (9)

Where, '*w*' is the crack width.

Later, Wang *et al.* (2011) performing some experiments showed that the value of chloride diffusion coefficient in a crack is much higher than the stated values in Eq. (9).

They also stated that this phenomenon may be attributed to the additional transport mechanism of chlorides for moving through crack spaces, e.g. generation of some convection current because of the temperature gradient or small hydraulic pressure gradient. According to them, when the crack width is more than a critical value (i.e., 60μ m), the diffusion coefficient D_{cr} value becomes 10,000 mm²/hr.

When the crack width is less than the critical value D_{cr} value ranged from 1500 mm²/hr to 4500mm²/hr. So, they suggested a value of 3000 mm²/hr is to be taken as the diffusion coefficient value in a crack of width less than 60 μ m.

3. Proposed novel approach

First some preselected concrete mixes are taken for analysis. Then their corresponding 28 days saturated diffusion coefficient is determined. After that incorporating various other influencing parameters the FE modelling is carried out to determine the penetration profile of chloride ions in the concrete samples. The steps of the analysis are shown Fig. 2. Detail discussion for better understanding is given below.

3.1 Step 1: Concrete mix selection

The diffusion property of concrete also depends upon the concrete mixing compositions. Thomas *et al.* (1999) carried out some experimental studies on effect of concrete composition on the diffusivity of chloride ions in concrete. It is observed from their study that if in an OPC concrete mix a certain quantity of OPC is replaced by fly ash or slag, it affects the chloride diffusion in a concrete block very much. So, the effects of their existence in a concrete mix should



Fig. 2 Steps for analysis

also be considered during an FEM study of chloride diffusion in concrete. The effects of such concrete compositions are analysed with the help of Virtual RCPT lab. Details about is discussed in the next section.

3.2 Step 2: virtual rapid chloride permeability test

Rapid chloride permeability test is a very old test for measuring the diffusion coefficients in a concrete sample. It was standardized as ASTM C1202 in 1991. While the shortcomings of the test are numerous and have been critically assessed by several authors, the current widespread usage of the test and the fact that is has been standardized suggest that it will continue to be one of the evaluators of concrete performance of choice for the foreseeable future. In this process a water-saturated concrete specimen (mainly cylindrical with dimensions provided as per ASTM C1202) is positioned in a cell containing fluid reservoirs on both sides. One reservoir is filled with a 3% NaCl solution and the other with a 0.3N NaOH solution. A potential of 60 V DC is applied across the cell. The negative terminal is connected to the electrode in the reservoir with the NaCl solution and the positive terminal is connected to the electrode in the NaOH solution. The negatively charged chloride ions will migrate towards the positive terminal. Then the current is measured for 6 hours. After the total current passed for 6 hours (Q_{6hrs}) is measured, applying Berke's empirical formula the diffusion coefficient in the concrete sample can be calculated

$$D_i = 0.0103 \times 10^{-8} \times (Q_{6hrs})^{0.84}$$
(10)

Where Q_{6hrs} is the total charge passed through the sample in 6 hrs in Coulombs and D_i is in cm²/sec.

Bentz (2007) provided a virtual test method that includes prediction of the conductivity of the

cementitious binder, pore solution and the total charge passed during an ASTM C1202 RCPT. The governing equations have been implemented in a set of forms-based HTML documents using the JavaScript script programming language and afterwards verified against numerous existing experimental results. There are many parameters that can be changed as per user's requirement in this test, eg. cement content, water-cement ratio, silica fume content, fly ash content, aggregate properties etc. The main advantage of this test is that it is very user-friendly. One can take various concrete mixes with various ingredients properties as per their requirement and can obtain the result for that particular scenario

3.3 Step 3: numerical modelling

By using Galerkin method we can do an FE formulation of the diffusion procedure. For the one dimensional Fick's second diffusion formula the desired function $C_f(x,t)$ can be represented by a finite series approximation as (Lapidus *et al.* 1982)

$$C_{f}(x,t) = \hat{C}_{f} = \sum_{i=1}^{n} N_{i}(x) C_{fi}(t)$$
(11)

Where, N_i = Interpolating function and C_{fi} = Undetermined coefficient. Now, by Galerkin formulation this equation can be expressed as (Lapidus *et al.*, 1982)

$$\iiint_{N_i} L\{\hat{C}_f\} = 0, \ \forall_i \tag{12}$$

The above function implies that there exist N equations requiring N basis functions that need to be solved for simultaneously. The finite elementization of Fick's Second Law can be expressed as

$$\int_{0}^{L} N_{i} \left\{ \frac{\partial^{2} \widetilde{N}}{\partial x^{2}} \widetilde{C_{f}} - \widetilde{N} \frac{\partial \widetilde{C_{f}}}{\partial t} \right\} dx = 0, \quad \forall_{i}$$
(13)

Now the above form is reduced to

$$A\dot{\widetilde{C}_f} + B\widetilde{\widetilde{C}_f} + f = 0$$
(14)

By integrating the concentration-flux relationship matrix (i.e., the [B] elemental matrix) can be represented as

$$[B] = -D \begin{bmatrix} \int_{L_e} \frac{\partial N_i}{\partial x} \frac{\partial N_i}{\partial x} dx & \int_{L_e} \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} dx \\ \int_{L_e} \frac{\partial N_j}{\partial x} \frac{\partial N_i}{\partial x} dx & \int_{L_e} \frac{\partial N_j}{\partial x} \frac{\partial N_j}{\partial x} dx \end{bmatrix}$$
(15)

Similarly the temporal term can be evaluated [A] elemental matrix for linear basis function as

$$[A] = \begin{bmatrix} \int_{L_e} N_i N_i \, dx & \int_{L_e} N_i N_j \, dx \\ \int_{L_e} N_j N_i \, dx & \int_{L_e} N_j N_j \, dx \end{bmatrix}$$
(16)

Then suitable number of nodes and elements are assumed and corresponding basis function is assumed. Then applying zero-Neuman boundary conditions i.e., zero-flux and putting the initial

	Diffusion in concrete	Diffusion in crack
Diffusion coefficient	D_{e}^{*} [from Eq. (7)]	D_{cr} [from Eq. (9)]
Boundary concentration	Exposed surface: C_s Crack surface: C_{cr} (x,t)	At the face open to the solution C_s
Diffusion equation(for 2D analysis)	$\frac{\partial C_f}{\partial t} = \frac{\partial}{\partial x} \left(D_{e,x}^* \frac{\partial C_f}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_e^* \frac{\partial C_f}{\partial y} \right)$	$\frac{\partial C_f}{\partial t} = \frac{\partial}{\partial x} \left(D_{cr} \frac{\partial C_f}{\partial x} \right)$

Table 1	Modelling	parameters
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Dirichlet boundary values i.e. concentration values the problem is solved.

Fu *et al.* (2010) presented the parametric guideline for modelling the diffusion procedure in a cracked concrete. They provided these guide lines for simulating the diffusion procedure in a 2D concrete model. The parameters are mentioned in Table 1.

As discussed earlier the diffusion of chloride into concrete can be modelled by using Finite Element Method. In this study the COMSOL MULTIPHYSICS software is used for this modelling purpose. Here conventional models for one type of physics can be extended into multiphysics models that solve coupled physics phenomena simultaneously.

The software runs the finite element analysis together with adaptive meshing and error control using a variety of numerical solvers, including a time-dependent solver for linear and non-linear problems. The mesh generation process can be performed through a set of control parameters. After solving, there are a number of tools for plotting and post-processing any model quantity and parameter.

4. Numerical simulation

As discussed in Section 3 and explained in Fig. 2, here systematic study is carried out for various concrete mixes.

4.1 Step 1: Selection of concrete mixes

Three mixing cases are selected in this study with different mixing ratios of different ingredients (e.g. cement, fly ash, slag). The slag and fly ash contents are selected as per the guidelines provided by Slag Cement Association and IS codes. In Table 2 the various mix proportions of the three different cases are given.

Four trial cases are considered for the concrete mixes:

Case 1 – Only OPC is taken without taking any slag or fly ash in the mixing.

Case 2 – According to Slag Cement Association slag cement can replace up to 80% of cement in a concrete mix. So, two mixes are considered where OPC is replaced by 50% and 80% of slag cement.

Case 3 – As per IS 456 : 2000, fly ash, conforming to IS 3812 Part-1, can be mixed with OPC for normal concreting. So, four mix proportions of fly ash (varying from 20% to 35%) are

		Mix Proportions									
	CASE 1	CA	SE 2		CAS	E 3			CA	SE 4	
Mix Designation	PC	P/S1	P/S2	P/F1	P/F2	P/F3	P/F4	P/SF1	P/SF2	P/SF3	P/SF4
Portland Cement	400	200	180	320	300	280	260	200	200	200	200
Fly Ash	-	0	0	80	100	120	140	80	100	120	140
Slag	-	200	320	0	0	0	0	120	100	80	60
Water Water	200	200	200	200	200	200	200	200	200	200	200
to Cementetious material ratio	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Coarse aggregate	1200	120 0	1200	1200	1200	1200	1200	1200	1200	1200	1200
Fine aggregate	600	600	600	600	600	600	600	600	600	600	600

Table 2 Different mix proportions

considered in the mix.

Case 4 – In this case both the slag and fly ash are mixed in the concrete to replace the OPC content by proportions as mentioned in the previous cases.

4.2 Step 2: Rapid chloride permeability test

In the Virtual RCPT, discussed earlier, the user can change the mixture proportions or test conditions and the total charge passed along with the effective w/c ratio, estimated degree of hydration of the binder, estimated final temperature, and concrete density will be calculated. Also, the estimated final temperature can be manually changed in the test conditions box and the results recalculated in an iterative fashion (at the user's discretion). But this virtual test was developed with data for water-to-cement ratios ranging from 0.3 to 0.5, silica fume additions of 0 % to 10 % by mass and aggregate volume fractions of 0.62 to 0.70. Thereafter the computation of the total charge passed during a rapid chloride permeability test is relatively straightforward. In Fig. 3 the Virtual RCPT result is shown for the P/SF concrete mix.

4.3 Step 3: FEM modelling

The FEM model analyzed here is similar to the model analyzed by Fu *et al.* (2010) and based on the experimental tests done by Wittmann *et al.* (2008). It consists of a two dimensional quadratic concrete section with a straight vertical crack starting at the midpoint of the bottom edge. Penetration of chloride ion is allowed through the bottom face only. The values of the different parameters are given as follows.

4.3.1 Parameters and properties

The following dimensions and parameters are considered for the modelling

4.3.2 Mesh parameters

Three noded triangular mesh is selected for the analysis of the model. Each node has two degrees of freedom. The parameters used for meshing this model are stated in Table 4. The meshed model is shown in Fig. 4.

The element growth rate signifies the ratio mesh element edge lengths of two succeeding layers of elements. That is, a maximum 20% increase in mesh element edge length with each succeeding layers of elements in the present model. The resolution of curvature determines the size of boundary elements compared to the curvature of the geometric boundary.

4.3.3 Boundary conditions

As mentioned earlier applying zero-Neuman boundary conditions i.e. zero-flux and the initial concentration in the domains as Dirichlet boundary values, the model is solved. The boundary conditions at different boundary are shown in Table 3.

Material	Mass (kg)	SiO ₂ content (%)	Specific Gravity	Fineness (m ² /kg)
Water	200	Not applicable	1.0	Not applicable
Cement	200	20.0	3.2	375
Silica Fume	0	99.0	2.2	Not applicable
Fly Ash	80	50.0	2.6	Not applicable
Slag	120	Not applicable	2.8	Not applicable
Limestone filler	0	Not applicable	2.7	Not applicable
Fine Aggregate	600	Not applicable	2.81	Not applicable
Coarse Aggregate	1200	Not applicable	2.7	Not applicable

Mixture Proportions

Hardened Concrete Air Content (%): 5.0 Estimated pore solution conductivity (S/m): 25.0 Help available



Applied Voltage (V): 60 Time (min): 360 Specimen length (mm): 60.8 Specimen diameter (mm): 95.25 Initial Temperature (°C): 30 Final Temperature (°C): 30

Curing/Saturation: Saturated Sealed ©

Compute Predicted Total Charge Passed (Coulombs): 3529 Predicted Initial Current (mA): 163.4

Predicted Initial Resistance	(Ohms)):	367.19	
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Estimated Effective Water to Cement Ratio: 0.526

Predicted Degree of Hydration at 28 d (%): 87.7 (user may change)

Fig. 3 Virtual RCPT for P/SF concrete mix



Fig. 4 Geometry and mesh of the model

Table 3 Parametric values

Modelling parameters	Values
Dimension of the block	$100 \text{ mm} \times 100 \text{ mm}$
Crack length	60 mm
Crack width	0.2 mm
Water-cement ratio(w/c)	0.5
'm' value in Eq.(4)	0.2
"T" in Eq.(5)	303 K

Table 4 Mesh properties

Mesh geometry	Triangular
Maximum element size (m)	0.002
Minimum element size (m)	$7.5 imes10^{-6}$
Maximum element growth rate	1.2
Resolution of curvature	0.25

Table 5 Boundary values

Boundary parameters	Values
Surface chloride concentration at the bottom face of the whole block (C_s)	7.06 kg/m ³ (198.87 mol/m ³)
Flux at each face	0
Concentration(C_f) value inside the concrete block and crack zone at $t = 0$	0

5. Results and discussion

The dimensions of the samples are as per the standards given in ASTM C1202. In all three cases samples are taken as saturated. The total charge passed for 6 hrs is obtained as per the calculations of the Virtual RCPT. A constant potential of 60V is provided for 6 hours. The temperature is considered 30° C.

The diffusion coefficient values obtained here are the 28 days saturated diffusion coefficient values, i.e., D_c in Eq. (7).

After the 28 days saturated diffusion coefficient is obtained the model was prepared in COMSOL MULTIPHYSICS. The convection and diffusion module is used for the simulation. The Eq. (7) is then incorporated in the model. So, all the influencing parameters mentioned earlier are considered in the simulation. After that, three noded triangular mesh is generated. Next, a time dependent analysis is carried out.

The analysis is run for various time durations and the result and penetration pattern is noted at different time durations.

Fig. 5 demonstrates the penetration depths at the crack tip and at a region far away from the crack. From the plot it is clear that the penetration values are not so different at the crack tip at the end of 700 hours.

Case 1

The diffusion of chloride ion is maximum in this case among all the cases. It is observed in the penetration profile as shown in Fig. 6.

Case 2

In this case of OPC is replaced with slag by certain proportions. When slag quantity is 50%, not much difference is observed in penetration profiles. But, when, slag replaces 80% of OPC, diffusion coefficient decreases as well as diffusion depth as shown in Fig. 7 and 8.

In this case OPC is replaced with fly ash. It is observed that addition of fly ash reduces the chloride diffusivity manifolds than normal OPC concrete (Fig. 6). The penetration profiles are shown in Figs. 9-12. Reduction in diffusion is even more in this case than addition of slag cement. The reason for this high resistance to chloride diffusion can be explained if the constituting elements in OPC, slag cement and fly ash are studied. Slag Cement Association has provided the quantities of oxides present in these cases (Table 7). From the table, one can observe

	PC	P/S1	P/S2	P/F1	P/F2	P/F3	P/F4	P/SF1	P/SF2	P/SF3	P/SF4
Total charge passed (Q _{6hrs}) in coulomb	17446	17839	4385	3483	2250	1406	846	3529	2275	2233	851
Diffusion coefficient (10 ⁻¹² m ² /s)	37.66	38.37	11.81	9.73	6.74	4.54	2.96	9.84	6.80	6.70	2.98

Table 6 Results obtained from Virtual RCPT



Fig. 5 :Plot of penetration depth for different cases







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Fig. 8 Penetration profile for P/S2



Fig. 9 Penetration profile for P/F1



Fig. 10 Penetration profile for P/F2





Fig. 12 Penetration profile for P/F4 and P/SF4



Fig. 13 Penetration profile for P/SF1



Fig. 15 Penetration profile for P/SF3

Table 7 Typical chemical oxides for various cementitious materials

	Portland cement	Slag cement	Fly ash C	Fly ash F
CaO	65	45	25	3
SiO_2	20	33	37	58
Al_2O_3	4	10	16	20
Fe_2O_3	3	1	7	10
MgO	3	6	7	1

that lime (CaO) content is much less in case of fly ash. Besides the silica (SiO_2) and alumina (Al_2O_3) content is much higher in fly ash than Ordinary Portland Cement. Fly Ash is also pozzolanic in nature. So, during hydration it also reduces the pores in concrete. These properties in fly ash make it less prone to chloride diffusion and chloride attacks. But the quantity of fly ash

should not be increased to a very high level. Namagga *et al.* (2009) showed that there is an optimum quantity (35%) of fly ash. If more quantity of fly ash is mixed it will decrease the rate of strength gain in concrete. Thus the ultimate strength gain may take even 56 days or more. Hence the mix proportion of fly ash is limited to 35%. Besides, addition of fly ash increases the setting time of concrete. Moreover, fly ash decreases the air entrainment and pores in concrete. Concrete is susceptible to damage from freeze/thaw cycles if its air content is very low.

Case 4:

Keeping these disadvantages of fly ash addition in mind finally both slag and fly ash are mixed with the OPC. Here, 50% OPC content is kept constant for the trials. The fly ash content is varied from 20% to 35% and rest amount of slag is added. The diffusivity and penetration is little more than the Case 3 but it is also very low compared to Case 1 and Case 2. The penetration profile is shown in Fig. 12, 13, 14 & 15.

6. Concluding remarks

The paper presented novel integrated approach of Virtual RCPT with FEM for various concrete mixes. From the study it is observed that if in a concrete mix of OPC, some quantity of OPC is replaced with fly ash, it gives better resistance against chloride diffusion and thus makes it less prone to chloride attack. It has been corroborated in many previous experimental researches. Naik *et al.* (1996) tested some concrete samples with fly ash content upto 55% of cementitious materials and observed significant decrease in the chloride penetration, than the OPC. Thomas *et al.* (1998) carried out experiments with some concrete blocks, containing different quantities of slag and fly ash. The blocks were exposed to sea water for 8 years. They also observed the increased resistance to chloride ingress in concrete is to be increased in order to make a structure less corrosive. This study can be extended for a cross section of a real life RCC structure case and thus explore the corrosion in a reinforced concrete structure. Further, it may be possible to build an FE model which can describe the whole procedure starting from diffusion of chloride into a concrete section to the corrosion damage in the same. Such a model can really give a fair idea of the serviceability of a concrete member in a saline environment.

References

- Martín-Pérez, B., Zibara, H., Hooton, R.D. and Thomas, M.D.A. (2000), "A study of the effect of chloridebinding on service life predictions", *Cement Concrete Res.*, **30**, 1215-1223.
- Bentz, D.P., Garboczi, E.J., Martys, N.S., Snyder, K.A., Guthrie, W.S., Kyritsis, K. and Neithalath, N. (2009), "Virtual Testing of Concrete Transport Properties", *Presented at ACI Fall 2009 Session on "Material Science Modelling as a Solution to Concrete Problems"*, New Orleans.

COMSOL MULTIPHYSICS 4.2a user manual (2011).

- Conciatori David, Sadouki Hamid, Brühwiler Eugen (2008), "Capillary suction and diffusion model for chloride ingress into concrete", *Cement Concrete Res.*, **38**(12), 1401-1408.
- Djerbi, A., Bonnet, S., Khelidj, A., Baroghel-bouny, V. (2008), "Influence of traversing crack on chloride diffusion into concrete", *Cement Concrete Res.*, **38**, 877-883.
- Fu, C., Jin, X. and Jin, N. (2010), *Modelling of Chloride Ions Diffusion in Cracked Concrete*, Earth and Space: Engineering, Science, Construction and Operations in Challenging Environments, ASCE, 3579-

3589.

- Ishida, T., Prince, O.L. and Anh, H.T.L. (2009), "Modelling of chloride diffusivity coupled with non-linear binding capacity in sound and cracked concrete", *Cement Concrete Res.*, 39, 913-923.
- Ismail, M., Toumia, A., Françoisa, R. and Gagné, R. (2004), "Effect of crack opening on the local diffusion ofchloride in inert materials", *Cement Concrete Res.*, 34(4), 711-716.
- Lina, K.T. and Yang, C.C. (2014), "A simplified method to determine the Chloride migration coefficient of concrete by the electric current in steady state", *Comput. Concr.*, **13**(1), 117-133.
- Dao, L.N., Dao, V.N., Kim, S.H. and Ann, K.Y. (2010), "Modelling steel corrosion in concrete structures", Int. J. Electrochem. Sci., 5, 302-313.
- Naik, T., Singh, S. and Hossain, M. (1996), "Permeability of high-strength concrete containing low Cement factor", J. Energy Eng., 122(1), 21-39.
- Namagga, C. and Atadero, R.A. (2009), World of Coal Ash (WOCA) Conference Lexington, KY, USA.
- Sillanpää, M. (2010), "The effect of cracking on chloride diffusion in concrete, Master's thesis submitted in partial fulfillment of the requirements for the degree of master of science in technology", Department of Structural Engineering and Building Technology, Aalto University.
- Stanish, K.D., Hooton, R.D. and Thomas, M.D.A. (2000), "Testing the chloride penetration resistance of concrete: A literature review", Department of Civil Engineering, University of Toronto.
- Suwito, C.X.C. and Xi, Y. (2006), International Journal of Numerical analysis and Modeling, 3(4), 481-503.
- Thomas, M.D.A. and Bamforth, P.B. (1999), "Modelling chloride diffusion in concrete effect of fly ash and slag", *Cement Concrete Res.*, **29**, 487-495.
- Wang, L. and Ueda, T. (2011), "Mesoscale modelling of the chloride diffusion in cracks and cracked concrete", J. Adv. Concrete Tech., 9(3), 241-249.
- Vagelis, G.P. (2013), "Service life prediction of a reinforced concrete bridge exposed to chloride induced deterioration", Adv. Concrete Construct., 1(3), 201-213.
- Yunping, X. and Zdeněk, P.B. (1999), "Modelling chloride penetration in saturated concrete", *J. Mater. Civil Eng.*, **11**, 58-65.
- Yang, C.C. and Weng, S.H. (2013), "A multi-phase model for predicting the effective chloride migration coefficient of ITZ in cement-based materials", *Adv. Concrete Construct.*, **1**(3), 239-252.
- Zeng, Y. (2007), "Modeling of chloride diffusion in hetero-structured concretes by finiteelement method", *Cement Concrete Compos.*, **29**, 559-565.
- Zichao, P., Xin, R. and Airong, C. (2014), "Chloride diffusivity of concrete: probabilistic characteristics at meso-scale", Comput. Concr., 13(2), 187-207.

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