Research Article

Evaluation Technique of Chloride Penetration Using Apparent Diffusion Coefficient and Neural Network Algorithm

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Diffusion coefficient from chloride migration test is currently used; however this cannot provide a conventional solution like total chloride contents since it depicts only ion migration velocity in electrical field. This paper proposes a simple analysis technique for chloride behavior using apparent diffusion coefficient from neural network algorithm with time-dependent diffusion phenomena. For this work, thirty mix proportions of high performance concrete are prepared and their diffusion coefficients are obtained after long term-NaCl submerged test. Considering time-dependent diffusion coefficient based on Fick's 2nd Law and NNA (neural network algorithm), analysis technique for chloride penetration is proposed. The applicability of the proposed technique is verified through the results from accelerated test, long term submerged test, and field investigation results.

1. Introduction

Chloride ions induced into concrete cause a severe corrosion in embedded steel and the durability degradation propagates to structural safety problem [1]. In the earlier researches on deterioration of chloride attack, studies based on field investigations and apparent diffusion have been performed [2–4]. Recently, micromodels based on mass conservation law and behaviors in early aged concrete like porosity, hydration, and saturation have been proposed [5–7]. Furthermore various phenomena like enlarged diffusion and permeation due to cracks and cold joint are considered for quantitative modeling on chloride penetration [8, 9].

Apparent diffusion coefficient based on Fick's 2nd law is conventionally utilized for evaluating chloride behavior, however migration test and the related techniques are frequently utilized for measuring a resistance to chloride penetration [10, 11] since apparent diffusion coefficient experimentally obtained needs considerably long period. Chloride diffusion coefficients from migration tests indicate ion velocity in electrical field so that they cannot be directly employed to Fick's

2nd law. For evaluation of chloride behavior using diffusion coefficient from migration test, complicated analysis frame is required [12, 13]. For evaluation of total chloride content, special relationship between free and bound chloride ion, so called isotherm, should be considered in the analysis frame [6, 14, 15]. Apparent diffusion coefficient can provide direct solution-chloride content based on Fick's 2nd Law to engineers, and this technique has been widely applied for its simple formulation and several familiar-powerful programs like Life 365 [3, 16]. Additionally several engineering advantages like easy employing time effect on diffusion behavior [16] and random variables for stochastic approach [8] are found through treating apparent diffusion coefficient.

NNA (neural network algorithm) is one of the optimization techniques and this has been widely utilized for determination of mix proportions and strength evaluation in concrete research field [17–20]. For analysis of chloride behavior and carbonation, NNA technique is recently adopted [21, 22] but the related analysis technique needs such complicated micromodels and major assumptions that it is not widely used for engineers.

TABLE 1: Chemical and physical properties of cement and mineral admixtures.

Types	Chemical composition (%)						Physical properties		
	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	CaO	MgO	SO ₃	Ig. loss	Specific gravity (g/cm ³)	Blaine (cm ² /g)
OPC	21.96	5.27	3.44	63.41	2.13	1.96	0.79	3.16	3,214
GGBFS	32.74	13.23	0.41	44.14	5.62	1.84	0.2	2.89	4,340
FA	55.66	27.76	7.04	2.70	1.14	0.49	4.3	2.19	3,621
SF	93.3	0.5	1.21	0.27	1.03	0.02	1.1	2.21	190,620

FIGURE 1: Flowchart for this study.

In this paper, apparent diffusion coefficients, which can provide a direct solution (chloride content), are obtained from chloride-submerged condition for 6 months. Major mix components are selected as neurons and training for learning is carried out for optimum apparent diffusion

coefficients. The simulated diffusion coefficients are verified with test results. A simple and deterministic analysis technique for chloride behavior is proposed considering time-dependent diffusion characteristics and the apparent diffusion coefficient from NNA. In this paper, diffusion

(a) Simple neural network architecture

(b) Activation function

FIGURE 2: Schematic diagram for simple NNA architecture [22, 24].

FIGURE 3: Strength development with admixtures and curing periods.

coefficients from various HPC (high performance concrete) mix proportions, NNA application for reasonable selection of diffusion coefficients, and simple technique for chloride penetration prediction are dealt with. In Figure 1, flow chart for the work is shown.

2. Outline of NNA

It is reported that NNA was started by McCulloch and Pitt [23]. A neuron as a unit with process of stimulus and reaction is modeled in the system. The training for learning a data set

FIGURE 4: Comparison of measured diffusion coefficient with OPC concrete.

TABLE 2: Physical properties of aggregates.

Types	Items			
	$G_{\max}$ (mm)	Specific gravity (g/cm ³)	Absorption (%)	F.M.
Fine aggregate	—	2.58	1.01	2.90
Coarse aggregate	25	2.64	0.82	6.87

is conducted with connection strength, transfer function, and biases. The errors between calculated and expected results are reduced with increasing epochs. The training for learning is completed when the error decreases to a target convergence level. In this paper, a back-propagation algorithm is adopted for the neural network. Figure 2 shows an outline of simple neural network architecture [22, 24].

In this network, each element of input is connected to each neuron input through the weight matrix. Neurons (N_j) and activated values (H_j) in the hidden layer are formulated

as (1) and (2). Activated value, O_k can be written as (3). Consider

$$N_j = \sum W_{ji} I_i, \quad (1)$$

$$H_j = f(N_j + B_j), \quad (2)$$

$$O_k = f\left(\sum W_{kj} H_j + B_k\right), \quad (3)$$

where I_j is input vector, W_{ji} is weight or connection strength, f is transfer function, and B_j is bias. In the back-propagation, error (E) is calculated through (4) considering target value (T_k). Consider

$$E = \frac{1}{2} \left(\sum_{k=1} O_k - T_k \right)^2. \quad (4)$$

TABLE 3: Mix proportions for HPC.

Names of mix	w/b	Items							Binder × % Admixture	
		W	C	Unit weight (kg/m ³)			S	G		
				Binder Materials						
				GGBS	FA	SF				
o100-37	0.37	168	454	—	—	—	767	952	1.0	0.017
o100-42	0.42	168	400	—	—	—	787	976	0.9	0.015
o100-47	0.47	168	357	—	—	—	838	960	0.85	0.017
g30o70-37	0.37	168	318	136	—	—	762	946	0.8	0.018
g30o70-42	0.42	168	280	120	—	—	783	972	0.75	0.013
g30o70-47	0.47	168	250	107	—	—	835	956	0.65	0.015
g50o50-37	0.37	168	227	227	—	—	760	943	0.75	0.017
g50o50-42	0.42	168	200	200	—	—	780	969	0.7	0.0135
g50o50-47	0.47	168	178	179	—	—	832	853	0.6	0.015
f10o90-37	0.37	168	409	—	45	—	760	943	0.75	0.018
f10o90-42	0.42	168	360	—	40	—	780	969	0.9	0.021
f10o90-47	0.47	168	321	—	36	—	832	952	0.75	0.017
f20o80-37	0.37	168	363	—	91	—	752	934	0.75	0.018
f20o80-42	0.42	168	320	—	80	—	774	961	0.85	0.025
f20o80-47	0.47	168	286	—	71	—	826	946	0.7	0.017
f30o70-37	0.37	168	318	—	136	—	745	952	0.75	0.2
f30o70-42	0.42	168	280	—	120	—	768	953	0.75	0.015
f30o70-47	0.47	168	250	—	107	—	820	939	0.65	0.019
f10s05-37	0.37	168	386	—	45	23	756	938	1.0	0.023
f10s05-42	0.42	168	340	—	40	20	777	965	0.9	0.021
f10s05-47	0.47	168	303	—	36	18	829	950	0.9	0.021
f20s05-37	0.37	168	340	—	91	23	749	929	0.9	0.023
f20s05-42	0.42	168	300	—	80	20	771	957	0.85	0.025
f20s05-47	0.47	168	268	—	71	18	810	927	0.9	0.025
g30s05-37	0.37	168	295	136	—	23	759	942	0.75	0.015
g30s05-42	0.42	168	260	120	—	20	765	949	0.75	0.015
g30s05-47	0.47	168	232	107	—	18	832	952	0.8	0.015
g35f15-37	0.37	168	227	159	68	—	751	932	0.65	0.014
g35f15-42	0.42	168	200	140	60	—	773	959	0.65	0.014
g35f15-47	0.47	168	178	125	54	—	804	921	0.7	0.014

w/b: water to binder ratio.

G: gravel.

AE: air entrainer.

S: sand.

SP: superplasticizer.

For minimizing the error, connection strength (W_{ij}) is modified backward from neurons in output layer like

$$\begin{aligned} \Delta W_{kj} &= \eta \delta_k H_j, & \Delta B_k &= \eta \delta_k, & \delta_k &= (T_k - O_k) f'(N_k), \\ \Delta W_{ji} &= \eta \delta_j H_i, & \Delta B_j &= \eta \delta_j, & \delta_j &= (W_{kj} \delta_k) f'(N_j), \end{aligned} \quad (5)$$

where δ_j and δ_k are gradients of the total error, and η is the learning rate.

After the modification of connection strength, NNA repeats the process of calculation and modification until the error decreases within the target convergence.

For the data set, each input should have boundary limits from 0.0 to 1.0. Through data process like (6), each value satisfies the boundary limit. Consider

$$P_n = \frac{P_{\text{act}} - P_{\text{min}}}{P_{\text{max}} - P_{\text{min}}}, \quad (6)$$

where P_n is input value for training, P_{act} is actual input data, and P_{max} and P_{min} are maximum and minimum values of input data. After calculation, the output value with a range of 0.0~1.0 is obtained and it should be converted to actual value using (6).

TABLE 4: Results of apparent diffusion coefficient.

Mixture	Diffusion coefficient (m^2/sec)
o100-37	$4.1E-12$
o100-42	$5.2E-12$
o100-47	$7.3E-12$
g30o70-37	$2.1E-12$
g30o70-42	$3.0E-12$
g30o70-47	$3.2E-12$
g50o50-37	$1.4E-12$
g50o50-42	$1.6E-12$
g50o50-47	$1.7E-12$
f10o90-37	$3.5E-12$
f10o90-42	$5.2E-12$
f10o90-47	$6.2E-12$
f20o80-37	$3.2E-12$
f20o80-42	$4.0E-12$
f20o80-47	$5.9E-12$
f30o70-37	$3.9E-12$
f30o70-42	$4.3E-12$
f30o70-47	$5.9E-12$
f10s05-37	$2.2E-12$
f10s05-42	$2.8E-12$
f10s05-47	$3.3E-12$
f20s05-37	$2.5E-12$
f20s05-42	$3.6E-12$
f20s05-47	$3.8E-12$
g30s05-37	$1.4E-12$
g30s05-42	$1.9E-12$
g30s05-47	$1.8E-12$
g35f15-37	$1.8E-12$
g35f15-42	$1.9E-12$
g35f15-47	$2.3E-12$

3. Test Program for Apparent Diffusion Coefficient

3.1. Outline of Test Program. In this section, tests for learning and training of NNA are explained. Thirty mix proportions for HPC are prepared. Target slump and air content are 150 ± 15 mm and $4.5 \pm 1.0\%$, respectively. Three w/b (water to binder) ratios are set as 0.37, 0.42, and 0.47. After 28 days of water curing, the specimens were kept in 3.5% of NaCl solution for 6 months. For 1-dimensinal intrusion of chloride ion, sides and bottoms were coated with epoxy except top surface. After 6 months of submerging in NaCl solution, chloride profiles were measured based on AASHTO T 260. Through regression of chloride profile, surface chloride contents and apparent diffusion coefficients are obtained. For binding materials, OPC (ordinary portland cement) was used. GGBFS (ground granulated blast furnace slag), FA (fly ash), and SF (silica fume) were added for mineral admixtures. In Table 1, chemical compositions and physical properties of cement and the used mineral admixtures are listed.

FIGURE 5: Relationship between compressive strength and diffusion coefficient.

FIGURE 6: Decrease in errors with increasing epochs.

The physical properties of aggregates are listed in Table 2. Thirty mix properties which are used for learning and training of NNA are listed in Table 3.

3.2. Test Results

3.2.1. Compressive Strength with Ages. Compressive strength is measured at the age of 7, 28, 91, and 270 days. In Figure 3, the results of compressive strength with different ages are shown. The results show typical strength development, higher strength with lower w/b ratio. The smallest strength at the age 7 days is measured in f30o70 (30% replacement of FA) in Figure 3. Compared with the results in OPC, the strength ratio is only 69.9%, however, in the long term (270 days), concrete with mineral admixtures mostly shows higher strength than OPC concrete. It is reported that the ability of a mineral admixture to react with calcium hydroxide present in the hydrated Portland cement paste and to form additional calcium silicate hydrates can lead to significant reduction in

TABLE 5: Result of multiregression analysis.

$D = [a_1(w/b) + a_2(C_e) + a_3(\text{GGBFS}) + a_4(\text{FA}) + a_5(\text{SF}) + a_6(S) + a_7(G) + I] \times 10^{-15}$							
a_1	a_2	a_3	a_4	a_5	a_6	a_7	I
293.86	26.58	11.01	24.34	-42.41	12.78	11.80	-39491.61

TABLE 6: Mix proportions for verification (long-term submerged condition).

Type	w/b	Binder (kg/m ³)		Sand (kg/m ³)	Coarse aggregate (kg/m ³)
		C	FA		
OPC 100%	38.1	449	0	616	1,050
OPC 80% and FA 20%	38.1	359	90	616	1,050

porosity of both the matrix and the transition zone. Consequently, considerable improvement in ultimate strength and water-tightness can be achieved by incorporation of mineral admixtures [25]. Silica fume is very effective to strength development both in the short and in the long term. In the case of 270 days, the highest strength is measured in f10s05 (17.5% increase for OPC result, w/b 0.37), g30s05 (16.7% increase for OPC result, w/b 0.42), and g30s05 (31.0% increase for OPC result, w/b 0.47). In many researches, the effect of silica fume is found to be considerable both to strength and to durability [26, 27].

3.2.2. Apparent Diffusion Coefficient. In Table 4, the results of apparent diffusion coefficient are listed. The maximum and minimum results are measured in o100-47 ($7.3 \times 10^{-12} \text{ m}^2/\text{sec}$) and g30s05-37 ($1.4 \times 10^{-12} \text{ m}^2/\text{sec}$), respectively. The lower w/b ratio concrete has, the lower diffusion coefficients are measured. The mix proportions with mineral admixture have lower results than those with only OPC. Since the mix proportions with lower w/b ratio and large amount of binder have more hydrates amount and smaller porosity, penetration of chloride ion is impeded [7, 13, 15]. Concrete with FA can have large amount of hydrates due to pozzolan reaction and this leads low diffusion of chloride ion. In the case of GGBFS, low diffusion coefficients are measured due to the small porosity from latent hydraulic properties and chemical binding of chloride ion [5, 6, 28]. The comparisons of mineral admixture group with OPC series are shown in Figure 4.

In order to evaluate the relationship between strength and diffusion coefficient, linear regression analysis is performed and the results are shown in Figure 5 with test results.

The regression results are listed in (7a)~(7d). Consider

$$C_3 = -1.3477D + 37.064, \quad (7a)$$

$$C_{28} = -1.8815D + 46.954, \quad (7b)$$

$$C_{91} = -2.8811D + 61.963, \quad (7c)$$

$$C_{270} = -3.0938D + 68.342, \quad (7d)$$

where C_i denotes the compressive strength (MPa) at i days, D is measured diffusion coefficient ($\times 10^{12} \text{ m}^2/\text{sec}$). It is

observed the gradients of (7a), (7b), (7c), and (7d) increase with ages and this shows higher strength is related with lower diffusion coefficient with aging.

3.2.3. NNA Application to Diffusion Coefficient. NNA technique is applied to simulation of diffusion coefficient and the results are compared with those from multiregression analysis. Seven mix components like w/b ratio, unit content of cement, GGBFS, FA, SF, sand, and coarse aggregate are considered as input neurons. Output neuron is fixed as apparent diffusion coefficient. MATLAB program is used for this regression analysis. Back propagation algorithm is adopted and Tan-Sigmoid function is used for transfer function among various functions like linear transfer and log-sigmoid [24]. Training number is set as 2,000 and the error to target convergence is set as 10^{-12} for learning process. The number of neuron is only 7 so that the simulation is usually completed within 2,000 trials. The decrease in error with increasing epoch is shown in Figure 6.

In Table 5, the result from multiregression analysis is listed. From the analysis, the average of relative error is 19.8%, which is reasonable; however 70.6% of relative error is calculated in the case of g50s05-47.

In Figure 7, the results from multiregression in Table 5 are compared with those from NNA and experiment. The results from NNA show more reasonable prediction with average relative error of 4.1%, which is very close to test results compared with 19.8% of average relative error from multiregression analysis. The comparisons of relative error from each technique are shown in Figure 8.

The chloride profiles based on the diffusion coefficient from NNA are compared with test results which were kept in submerged condition for 6 months in Figure 9. Concrete with lower w/b ratio and larger mineral admixture shows the more reduced chloride penetration. The proposed technique shows reasonable prediction for chloride penetration.

4. Analysis Technique of Chloride Penetration with Time-Dependent Diffusion

4.1. Time-Dependent Diffusion of Chloride Ion. It is reported that chloride diffusion coefficient based on Fick's 2nd law decreases with time [3, 8]. The governing equation for

TABLE 7: Analysis conditions for verification (submerged condition).

Type	m	D from NNA (m^2/sec)	D_{28} ($10^{-12} \text{ m}^2/\text{sec}$)	Surface chloride content (% of concrete wt.)
OPC 100%	0.2	2.509	2.912	0.709
OPC 80% and FA 20%	0.36	1.801	2.252	0.709

FIGURE 7: Comparison with results from test, multiregression, and NNA.

chloride penetration is listed in (8) and time-dependent diffusion coefficient is listed in (9) [3, 8, 16]. Consider

$$C(x, t) = C_s \left[1 - \operatorname{erf} \left(\frac{x}{2\sqrt{D(t) \cdot t}} \right) \right], \quad (8)$$

$$D(t) = D_0 \left(\frac{t_0}{t} \right)^m, \quad (9)$$

where, t_0 and D_0 are reference time (28 days) and diffusion coefficient at reference time, $D(t)$ is time-dependent diffusion coefficient. m is time exponent which is changed with type and amount of mineral admixtures [3, 16], which is defined as

$$m = 0.2 + 0.4 \left(\frac{\text{FA}}{50} + \frac{\text{SG}}{70} \right), \quad (10)$$

where FA and SG denote the replacement ratio of fly ash and slag. For solving (8) with (9), numerical analysis like finite

differential method should be employed, however if time term is fixed, averaged diffusion coefficient can be derived as (11a) and (11b) [29]. Consider

$$D(t) = \frac{1}{t} \int_0^t D_0 \left(\frac{t_0}{\tau} \right)^m d\tau = D_0 \frac{t_0^m}{t} \left[\frac{\tau^{1-m}}{1-m} \right]_0^t = \frac{D_0}{1-m} \left(\frac{t_0}{t} \right)^m, \quad (t < t_c), \quad (11a)$$

$$D(t) = D_0 \left[1 + \frac{t_c}{t} \left(\frac{m}{1-m} \right) \right] \left(\frac{t_0}{t_c} \right)^m, \quad (t \geq t_c), \quad (11b)$$

where t_c is the time after which diffusion coefficient keeps almost constant and it is usually assumed as 30 years.

4.2. Chloride Penetration Analysis Using NNA and Time-Dependent Diffusion Coefficient. The diffusion coefficients from NNA are the results based on the test data which is

FIGURE 8: Comparison of relative errors from NNA and linear regression analysis with averaged relative errors.

obtained from 6 months submerged condition, so that they are converted to diffusion coefficient at the reference time (28 days). In Figure 10, analysis technique for chloride behavior using NNA is depicted.

4.3. Comparison with Previous Test Results. In this section, the results from the proposed technique are compared with the previous test results of chloride profiles. In the previous test [28], two types of concrete (FA and OPC) were kept in 3.5% NaCl solution for 46 weeks. Table 6 shows the mix proportions [28].

Conditions for analysis are listed in Table 7 and the analysis results are shown in Figure 11. From Figure 11, it is found that the obtained diffusion coefficient seems to be small but the results from the analysis reasonably agree with the previous chloride profiles.

Another verification is performed using the results from field investigation. In the previous research [28], the chloride profiles were obtained from RC columns after 1 and 10 years in submerged condition. Unfortunately, mix proportions could not be obtained but it was found that it was made up with OPC concrete and w/c (water to cement ratio) was 0.55. Conventional mix proportions are assumed as Table 8 based on the domestic typical mix proportions [30] and analysis conditions are listed in Table 9.

TABLE 8: Mix proportions for verification (field investigation).

Type	w/c	Cement (kg/m ³)	Sand (kg/m ³)	Coarse aggregate (kg/m ³)
OPC 100%	55.0	352	653	1,173

TABLE 9: Analysis condition for verification (field investigation).

Type	m	D from NNA (m ² /sec)	D_{28} (m ² /sec)	Surface chloride content (% of concrete wt.)
OPC 100%	0.2	3.647	4.233	0.709

In Figure 12, chloride profiles from field investigation are compared with the results from this study. With elapsed time, chloride profile moves to inside of concrete and the proposed technique is evaluated to reasonably predict the chloride penetration.

This study extends the applicability of NNA which is limitedly utilized for concrete strength and mix proportions to the research on durability. Through learning and training of diffusion coefficient, target value (diffusion coefficient) can be simulated in a given mix proportions. However this technique has still limitation since NNA technique closely

FIGURE 9: Continued.

FIGURE 9: Comparison of chloride profile between NNA and test results.

depends on data set for training. The data in this paper has limited material properties like w/b ($0.37 \sim 0.47$) and diffusion coefficient ($1.4 \sim 7.3 \times 10^{-12} \text{ m/sec}^2$) so that it is necessary to extend the range for enhancing application. Various mix proportions with mineral admixtures and variability of surface chloride content will be considered for future study.

5. Conclusions

The conclusions evaluation technique of chloride penetration using apparent diffusion coefficient and neural network algorithm are as follows.

- (1) Thirty mix proportions for HPC containing GGBFS, FA, and SF are prepared and apparent diffusion coefficients are obtained after 6-month submerged condition of NaCl 3.5%. Seven mix components (w/b, unit content of cement, GGBFS, FA, SF, and fine/coarse aggregate) are selected as neurons and NNA is applied to simulation of diffusion coefficient. The simulated data shows only 4.1% of relative error, which is very accurate compared with the results from multiregression analysis showing 19.8%.
- (2) Utilizing diffusion coefficient from NNA and time-dependent diffusion, chloride profiles are evaluated.

FIGURE 10: Prediction of chloride penetration using NNA and time-dependent diffusion.

FIGURE 11: Chloride profile between results from test and this study.

From the comparison with results of long term submerging test and field investigation, the proposed technique is evaluated to reasonably predict the induced chloride profile.

- (3) The proposed technique is closely dependent on quantitative data set for training and learning. With

FIGURE 12: Chloride profile between results from field investigation and this study.

more extended mix proportions and the related diffusion coefficients, this technique can be modified and more applicable to evaluation of chloride penetration.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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