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Evaluation of Fiber and Blast Furnace Slag Concrete Chloride Penetration through Computer Simulation

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Abstract

Durability of concrete is an important issue, and one of the most critical aspects affecting durability is chloride diffusivity. Factors such as water cement ratio, degree of hydration, volume of the aggregates and their particle size distribution have a significant effect on chloride diffusivity in concrete. The use of polypropylene fibers(particularly very fine and well dispersed micro fibers) or mineral additives has been shown to cause a reduction in concrete's permeability. The main objective of this study is to evaluate the manner in which the inclusion of fiber(in terms of volume and size) and blast furnace slag(BFS) (in terms of volume replacement of cement) influence the chloride diffusivity in concrete by applying 3D computer modeling for the composite structure and performing a simulation of the chloride penetration. The modeled parameters, i.e. chloride diffusivity in concrete, are compared to the experimental data obtained in a parallel chloride migration test experiment with the same concrete mixtures. A good agreement of the same order is found between multi scale microstructure model, and through this chloride diffusivity in concrete was predicted with results similar to those experimentally measured.

Keywords : blast furnace slag, chloride penetration, computer model, concrete chloride diffusivity, polypropylene fibers

1. Introduction

The durability of concrete is an important issue, and must be considered in the initial stage of design by taking the performance specifications into account. These specifications are still under development and approval. However, the acceptance of durability based design codes would to a great extent assure a better service life and performance estimation of concrete structures. One of the aspects of durability is the concrete resistance towards chloride ion penetration. Factors such as water-cement ratio, degree of hydration, volume of the aggregates and particle size distribution of cement, blast furnace slag and aggregates have a significant effect on chloride diffusivity in concrete. The use of polypropylene fibers (especially very fine and well dispersed micro fibers) is shown to produce a significant reduction in permeability through a modification of crack topography. At the same time, the use of only macro polypropylene fibers produces higher permeability, mostly because of poor dispersion.

Recently, the use of blast furnace slag(BFS) as a replacement of some of the cement in concrete has been considered in order to restrain chloride ion penetration and improve chloride ion penetration resistance[1]. The microstructure of BFS concretes is less permeable than that of ordinary concrete, and thus slower penetration of chloride ions and water from the outside may be expected[2].

The main objective of this study is to evaluate

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the manner in which fiber inclusion (in terms of volume, length and diameter) influences the chloride diffusivity in concrete by applying 3D computer modeling for the composite structure and simulation of the chloride penetration. In the same way, the influence of BFS replacement ratio on the chloride diffusivity in concrete is evaluated.

The simulation procedure includes a cellular-automation based 3D model for cement paste hydration and microstructure development (CEMHYD3D)[3] with modifications made to the code, and some new code has been added in order to reflect the differences between ordinary Portland cement hydration and cement with mineral additives hydration. Another part of the multi-scale simulation is a 3D hard core/soft shell(HCSS) model for concrete[4]. The public-domain source code of HCSS has been modified in order to incorporate fibers considering not only their volume, as has already been studied in Staneva et al.[5], but also the fiber size.

2. Multi scale Modeling, Techniques and Experimental Setup

The multi-scale modeling approach has been proposed and applied by Bentz[6] to predict the chloride ion diffusivity of plain concrete. Here, this model has been extended to both plain and fiber reinforced concretes.

2.1. Modeling Steps

The approach includes the generation of a multi-scale microstructure computer model of both plain and polypropylene fiber concretes, and the simulation and evaluation of chloride diffusivity of these systems by applying the random walker algorithm. The multi-scale microstructure model at micro scale describes the cement paste surrounding a single aggregate, the hydration development and percolation in cement paste, and in the Interfacial Transition Zone (ITZ), as proposed by Benz and Garboczi[7]. The model at a millimeter scale describes the aggregate particles in the considered volume, as well as the fibers when they are employed. The multi-scale model is illustrated in Figure 1. The models at these two scales are interconnected together with the technique to compute the relative diffusivity of a three-dimensional microstructure, and finally to compute the diffusivity of a concrete[8].

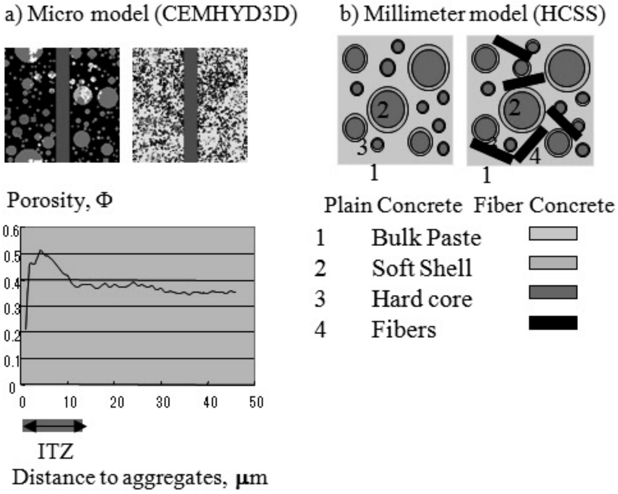


Figure 1. Multi scale microstruture concrete model

The simulation procedure includes a cellular-automation based 3D model for cement paste hydration and microstructure development (CEMHYD3D)[3] and a 3D hard core/soft shell (HCSS) model for concrete[4]. The public-domain source code of HCSS has been modified in order to incorporate fibers considering not only their volume as already studied in Staneva et al.[5] research, but also the fiber size as well. Additionally, modifications are made and some new codes are added to the code of the cement hydration program in order to reflect the differences between ordinary cement and BFS hydration processes.

The modeling approach consists of several steps. Aggregate particles are placed in the computational volume of modeled concrete, as the placement is random from largest to smallest particles, and the particle distribution follows the supplied sieve analysis classification. Fiber particles are placed according to the designed volume of fibers for each fiber type considered, and assuming a cylindrical shape.

Initial execution of the HCSS model is performed, with thickness of ITZ, t_{ITZ} to be equivalent to the median cement particle diameter known from cement particle size distribution. Cement particles are placed according to desired w/c ratio, and the thickness of a single aggregate particle (d_{agg}) is determined as the output of the initial run of HCSS (namely the ratio of ITZ volume, V_{ITZ} to the volume of bulk (cement) paste, V_b)[6]. Then, CEMHYD3D is executed and simulation of cement paste microstructure hydration is performed until the given degree of hydration. The porosity in the bulk (cement) paste as a function of distance from the aggregate surface is achieved, and the calculation of local relative diffusivity in the bulk (cement) paste and in ITZ region according to the suggested by Garboczi & Bentz[9] relationship (1) is performed.

$$\frac{D_b}{D_0} = 0.001 + 0.07\Phi^2 + 1.8\,H[\Phi - 0.18](\Phi - 0.18)^2 \cdots (1)$$

$$\Phi\text{-Porosity, H-Heaviside function} \quad \begin{cases} 1, \text{ for } \Phi > 0.18 \\ 0, \text{ otherwise} \end{cases}$$

Based on the results of the ratio of average ITZ diffusivity, D_{ITZ} to the average bulk (cement) paste diffusivity, D_b, the random walker algorithm[10] in HCSS model is executed and the effective diffusivity of concrete system relative to the average bulk (cement) paste diffusivity (D_c/ D_b) is achieved. Finally, a calculation of the absolute chloride ion diffusivity for the concrete, D_c is performed according to the relationship(2).

$$D_c = (D_c/D_b)(D_b/D_0)D_0 \ \ldots (2)$$

2.2. Variables of the Model

Previous research[7] on the identification of significant factors influencing concrete diffusivity has shown that the factors with the highest effect are the w/c ratio, degree of hydration and volume fraction of aggregates. Factors like aggregates' PSD, t_{ITZ}, and air content also have an influence on the diffusivity, but to a lesser extent. In this study, the w/c ratio and volume fraction of aggregates were kept constant, as that was the case in the experimental mixtures as well. Degree of hydration was selected as an equivalent to the age of 90 days. Fiber volume and fiber size were considered as major factors. Several different polypropylene fiber types were employed in the computational model and in the experiment as well. Details of mixture proportions, cement type, and fiber type and volume in the case of monofilament fibers only and for the same diameter of 0.1 mm are presented in Table 1.

Fibers of different types (monofilament, mesh) and of different diameter were applied previously[5] and the results of the multi-scale microstructure model that was built are discussed together with these of the present simulation run. The information about these fibers and mixtures is available in earlier literature[5].

The fiber diameters and volumes explored in the computation and experiment are 45, 60 and 100 μm, and 0.05, 0.1 and 0.3 % respectively. In a addition, an influence of the use of blast furnace slag (BFS) as a replacement of a portion of cement is considered by computing the diffusivity coefficients for 30%BFS, 0%BFS and 70%BFS replacement cases based on the established computer image-based models, and then these are compare to the PC case.

The ordinary Portland cement used in all of the computer runs has Blaine fineness of 350 m^2/kg and has the following composition on a volume basis: C_3S – 0.702, C_2S – 0.132, C_3A – 0.083, C_4AF – 0.084. BFS with a fineness modulus of 6120 ㎠/g (specific density: 2.89 g/㎤) is used in experimental runs, and the one considered in the simulation part has the same physical parameters.

The cement paste (micro scale) model has a resolution of 1 μm/pixel. The concrete system (millimeter scale) model is a cube of 100 units per side and a real size of 30 mm. The simulation results received are compared with the experimental results obtained in an experimental setup explained below.

Table 1. Fiber type and size (mixtures proportions are: w/c=0.5; C=350 kg/㎥, S=927 kg/㎥, G=878 kg/㎥ and S/A=51% for all mixtures)

Mix& Fiber	Application	Fiber Size		
		L, mm	d,mm	Aspect ratio, Af
PC				
PP3,6, 10,12	Computation	3;6;10;12	0.1	30;60; 100;120
PP6,12	Experiment	6;12	0.1	60;120

2.3. Chloride Migration Experimental Procedure

The experimental setup and procedures are explained in the research of Antoni[11], but the test setup is presented simply in Figure 2. A major concern for selecting a chloride migration test based on Standard of NordTest Build 492[12] is that it must be a rapid test that produces consistent results, which can be used directly for service life prediction. Chloride diffusion coefficients of plain and polypropylene fiber reinforced concretes (mixtures in Table 1) were measured for both non-loading and under-loading conditions, but here only the former are of interest.

The fresh concrete was cast into 100x100x200 mm rectangular prisms, unmolded 24 hours later, and cured in water for 28 days. After the water curing, the prismatic specimens were cut into 50 mm thick specimens with 100x100 mm cross-section. All specimens were kept at room for an additional 60 days before the migration test.

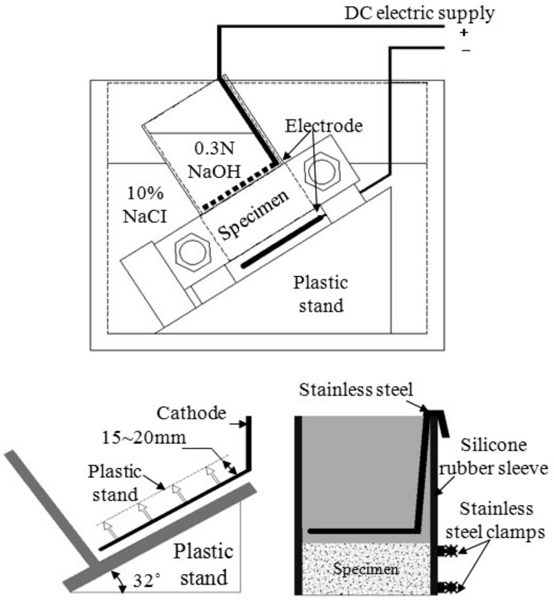


Figure 2. Migration test setup (NT BUILD 492)

3. Results and Discussion

3.1. Simulation Results of Multi scale Model and Migration Experiment

The multi-scale model was executed as explained in the previous section, and the predicted values of absolute chloride ion diffusivity for the concrete, D_c at 90 days and their graphical representation in relation with the fiber length and fiber volume are shown in Figure 3. The experimental results of chloride ion diffusivity for concrete $D_{c,exp}$ after the migration test are also presented in Figure 3.

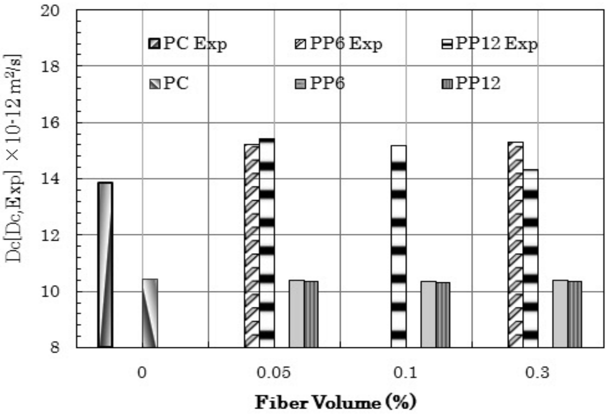


Figure 3. Effect of fiber volume on the absolute chloride ion diffusivity of concrete: Multi scale model's simulation and experimental results.

3.1.1 Effect of fiber volume on the absolute chloride ion diffusivity of concrete

The effect of fiber volume is examined, and a general trend of maintained (shorter fibers 3mm, 6mm) or slightly decreased (longer fibers) chloride ion diffusivity Dc was observed with the increase of the fiber volume up to 0.3%. This could be due to an inability of the shorter fibers (3mm, 6mm) in the applied volume range to disconnect the percolated pathways. The comparison of the diffusivity of plain concrete and fiber concrete shows very small differences, as the polypropylene fiber concrete diffusivity has lower values.

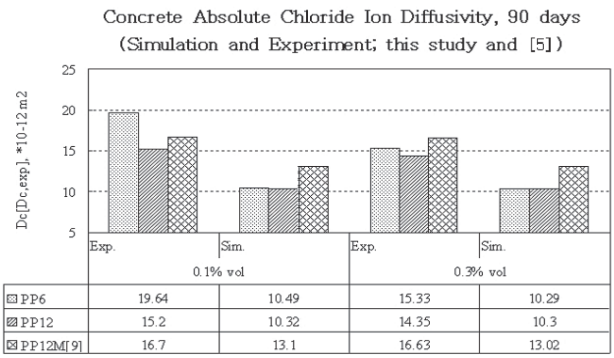
The experimental results in Figure 3 are similar to the computed behavior in the case of PP12exp concrete, namely, a decrease of the chloride diffusivity with the increase of fiber volume in the entire interval 0.05%~0.3%. Due to a preparation error of the PP6exp case at 0.1% fiber inclusion, the results obtained are not reliable and are excluded from this analysis. The other 2 cases of 0.05% and 0.3% fiber volume produce almost constant chloride ion diffusivity. The PP12exp case produces slightly higher chloride diffusivity compare to the case of plain concrete as well as the PP6exp case. The interval range of experimentally measured diffusivity is higher due to the effect of various factors (i.e. mixing, casting, preparing of test specimens etc.), which were not entirely considered and reflected in the simulation process. The simulation values and experimentally measured values are found to be of the same order and show a similar trend in the fiber volume – chloride ion diffusivity relationship; namely, a slight decrease in the chloride ion diffusivity when the fiber volume increases.

3.1.2 Effect of fiber length on the absolute chloride ion diffusivity of concrete

The multi-scale model results plotted in Figure 4 fall into a quite narrow interval, and no pronounced trend is found in terms of the effect of fiber length on chloride ion diffusivity. However, it is observed that with the increase of fiber length the chloride ion diffusivity decreases slightly, but that also depends on the fiber type as well. Concretes with a mesh type, 12 mm fiber studied in the research of Staneva et al.[5] show higher values of diffusivity coefficient. The experimental results (Figure 4) show that the shorter fiber PP6exp case produces higher diffusivity compared to longer one (PP12exp), with the increase of fiber volume over 0.1%. Previously, it was reported[13] that longer fibers are slightly superior to the shorter ones in terms of creating a percolated network. This is also seen in the simulation results for PP6 and PP10 cases. However, the experimental results for PP12exp and simulation results for PP12 show that it is possible in the considered length interval of 3~12 mm, and even in 12mm fiber at certain fiber volumes (0.1%; 0.3%) to create a less percolated pathway, and thus keep the chloride ion diffusivity at lower levels.

3.2. Simulation Results of Multi scale Model for Different Fiber Diameters

The multi-scale model is used also to compute the chloride diffusivity in concrete according to the data of Staneva et al.[5] The results in these cases are presented in Table 2. It can be seen that fiber diameter in the considered interval of 45μ m to 100 μ m does not uniformly influence the chloride diffusivity. The 60μ m diameter produces a maximum value of the diffusivity for all considered fiber lengths, except in the case of 10mm, where it is a minimum. Considering the above results together with the results reported by Staneva et al.[5] The following relationship is achieved and presented in Figure 5.



	Exp.	Sim.	Exp.	Sim.
	0.1% vol		0.3% vol	
▨ PP6	19.64	10.49	15.33	10.29
▨ PP12	15.2	10.32	14.35	10.3
▨ PP12M[9]	16.7	13.1	16.63	13.02

Figure 4. Effect of fiber length on the absolute chloride ion diffusivity of concrete: Multi scale model's simulation and experimental results

Table 2. Computational results for absolute chloride ion diffusivity of concrete, Dc (*10^{-12} ㎡/s) and V_f=0.05%.

Fiber Length, mm / Fiber Diameter, μm	3	6	10	12
45	10.30	10.47	10.49	10.39
60	10.37	10.48	10.37	10.40
100	10.37	10.34	10.43	10.35

In the wider interval of fiber diameter considered above, the chloride diffusivity in concrete has an ascending relationship with the fiber diameter factor. Diffusivity increases with the increase of fiber diameter and this is in agreement with the analysis and conclusions derived in Staneva and Horiguchi' s research[5], namely that the size of the fibers applied has an influence on concrete diffusivity.

3.3. Simulation Results of BFS Replacement

Finally, the simulation results of BFS replacement of cement and its influence on the diffusivity coefficient are as follows. The computed D_c,*$10^{-12}$$m^2$/s in 30% BFS case is 10.25, 6.79 in 50% BFS case and in 70% BFS case is 10.04. Higher replacement of cement with BFS produces a slightly lower diffusivity coefficient, and the relationship is a nonlinear one.

Replacement of up to 30% produces a diffusivity coefficient of 10.43, which is nearly the same as in plain concrete, but a replacement higher than that leads to some improvement of the transport properties. The experimental results confirm that with the increase in the replacement amount of BFS as a part of cement, the chloride diffusivity coefficient decreases. This suggests that the concrete permeability could be controlled by changing the BFS substitution ratio.

4. Conclusions

Based on the simulation, the multi-scale models established, the experimental results of the migration test and the comparison of the computed results with experimental results, it could be summarized that the computer 3D model is a good tool to predict and evaluate the transport behaviour of fiber reinforced concrete. The simulation values and experimentally measured values are found to be of the same order and to show a very slight influence of fiber volume and fiber length on the concrete chloride ion diffusivity. The simulation results are 25~35% less than the experimentally measured results. The applied fiber volumes influence the diffusivity to a very small extent, as the higher volume results in a lower or equal chloride ion diffusivity, which means that in the considered range the values of 0.1% and 0.3% could be more beneficial. This is also confirmed by the experimental results. The computer 3D model confirms the potential benefit of applying very fine micro fibers as well as blast furnace slag in order to improve concrete transport behavior. The approach described in this study can be applied in the process of predicting the transport behaviour of fiber reinforced concrete, as well as concrete with mineral additives, and used in the durability and service life design of the concrete.

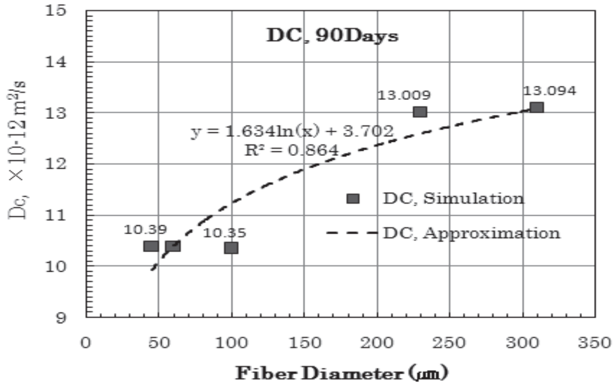


Figure 5. Effect of fiber length on the absolute chloride ion diffusivity of concrete: Multi scale model's simulation and experimental results.

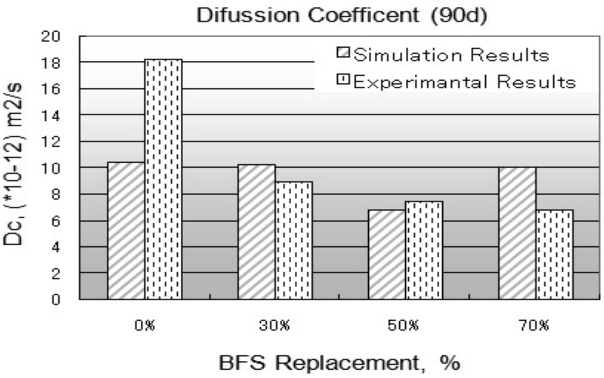


Figure 6. Effect of BFS replacement on the absolute chloride ion diffusivity of concrete: Multi scale model's simulation and experimental results.

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