Development of a calculation model for ionic transport using a migration test

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Introduction

Recently, the calculation model for ionic transport through concrete has been developed [1]. The multicomponent system of ion diffusion in the pore solution of concrete should be mainly considered for reality. Therefore, the calculation model concerning the multicomponent concentrated system has been developed. However, in this model the physical characteristics of such the porous material still cannot be certainly determined. The purpose of this research is to apply the existing mutual diffusion model with the physical characteristic parameter of the pore structure by using the results from steady state migration test. Moreover, ions-solid interacting phenomena are also implemented in this model. As a result, the concentration profile of each ion and the amount of ion through concrete can be calculated.

Calculation model of mutual diffusion coefficient and migration test results

The generalized form of the Fick's first law $J_i = -K\sum_{j=1}^{n_s} D_{ij}\frac{\partial C_j}{\partial x}$ suggested by Onsager relates the flux of i_{th} species (J_i) to the concentration gradient of j_{th} species by the mutual diffusion coefficient (D_{ij}). From the definition of the Onsager coefficient and the thermodynamic force equations, D_{ij} of i_{th} ion that influenced by j_{th} ion can be calculated from Eq. (1). The schematic diagram of mutual transport of ions in a multicomponent solution is shown in **Fig.1**.

$$D_{ij} = \delta_{ij} D_i^0 \left(1+\frac{\partial \ln \gamma_i}{\partial \ln C_i}\right) - \left\{ \frac{z_i D_i^0 C_i}{\sum_{k=1}^{n_s} z_k^2 D_k^0 C_k} z_j D_j^0 \left(1+\frac{\partial \ln \gamma_j}{\partial \ln C_j}\right) \right\} \quad (1)$$

where, δ_{ij} designate to the Kronecker delta function, D_i^0 is the diffusion coefficient in the infinite dilute solution and the derivative of activity coefficient (γ_i) which respected to concentration of each ion (C_i) can be determined by Debye-Hückel theory.

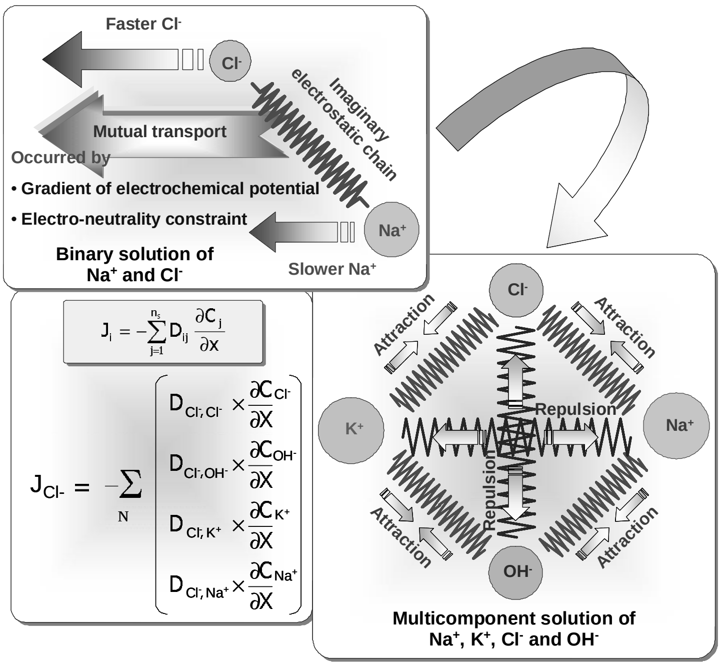

Fig.1 Mutual diffusion model for ions in a multicomponent concentrated solution system

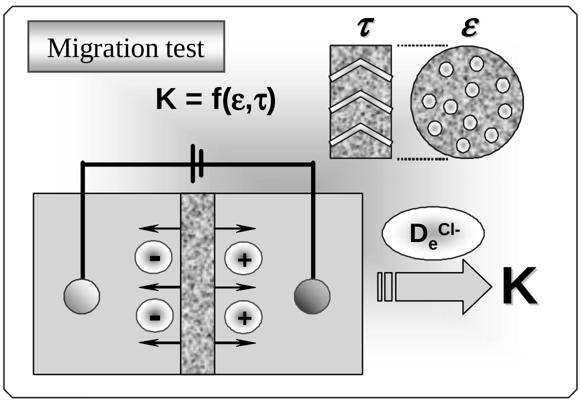

Fig.2 Physical characteristic parameter of pore structure determined by steady state migration test

Keywords: ionic transport, generalized Fick's law, multicomponent concentrated solution, migration test, ion-solid interaction
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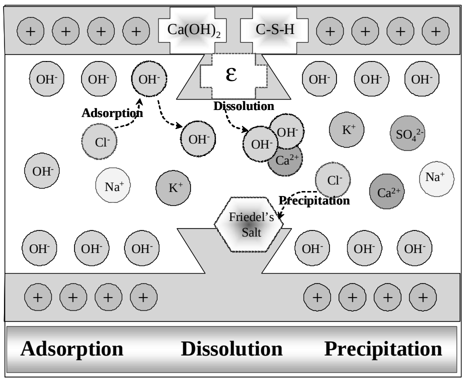

Fig.3 Schematic diagram for ion-solid interaction in pore structure system

In this research, the developed model of mutual diffusion coefficient (D_{ij}) [1] was applied with the physical characteristic parameter (K) which characterizes to the porosity and tortuosity of a cement-based material. This parameter was estimated base on the effective diffusion coefficient of chloride ion from steady state migration test which conducted on 8 mm thickness mortar specimen as shown schematically in **Fig.2**. The dissolution of $Ca(OH)_2$ which causes the increased porosity and the precipitation of Cl^- which produces the Friedel's salt are also included in this model. Moreover, the effect of positively charged of solid structure was also implemented for the calculation. It is known that the solid structure of pore in a cement-based material was positively charged. At initial stage, OH^- is attracted by this charge, however it is replaced in the existence of Cl^- as shown schematically in **Fig.3**.

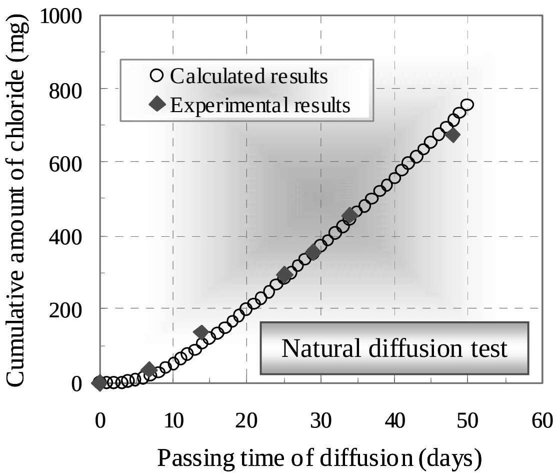

Fig.4 Comparison between calculated and experimental result of cumulative amount of Cl^-

Validation of the proposed calculation model

The natural diffusion test of 8 mm thickness mortar specimen was used to validate the proposed calculation model. The electrolytic solution in the up-stream compartment of the diffusion cell is 0.5 mol/l NaCl solution while that in the down-stream compartment is 0.3 mol/l NaOH solution. The pore solution component for calculation is assumed to compose of 6 ions; Ca^{2+}, Na^+, K^+, SO_4^{2-}, OH^- and Cl^- which the concentrations are 0.02, 0.2, 0.3, 0.03, 0.48 and 0 mol/l, respectively. The amount of Cl^- which diffuses to the NaOH side was investigated up to 50 days of diffusion. The result shown in **Fig.4** indicates that the cumulative amounts of Cl^- from the proposed calculation model exhibit good agreement with those from the experimental results. Moreover, by using this calculation model the concentration profile of some ions can also be calculated according to the passing time as shown in **Fig.5** (a) to (c).

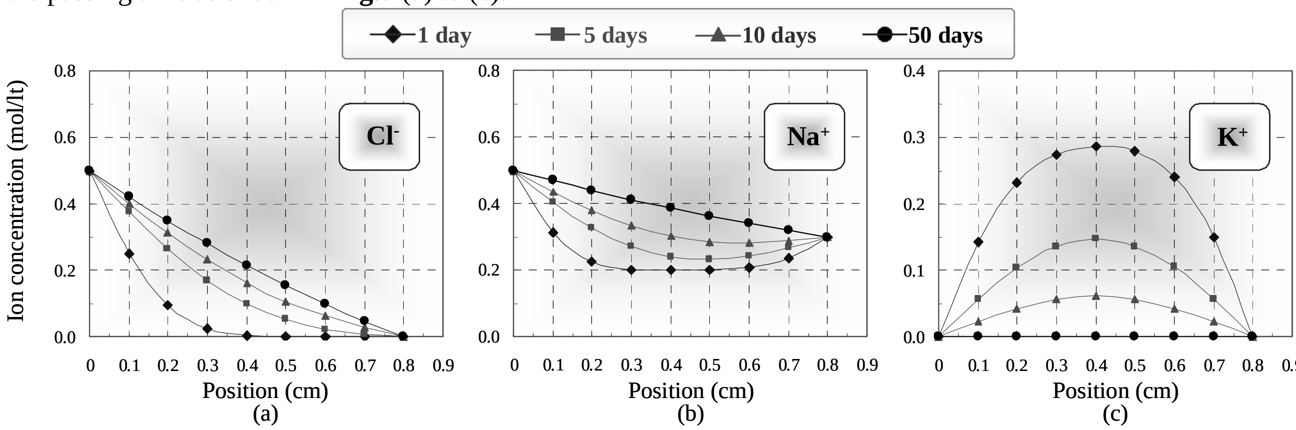

Fig.5 Calculated concentration profile of ions

Conclusion

The result from steady state migration test can be used to evaluate the physical characteristic parameter of concrete. Therefore, the migration test in addition to the mutual diffusion model resulted in more reliable ionic transport calculation for concrete.

Reference

1. Ritthichauy, W., Sugiyama, T. and Tsuji, Y., 2002. "Calculation of Diffusion Coefficient of Ion in Multicomponent Solution for Ion Movement in Concrete". Proceedings of JCI, Tsukuba. 19-21 July 2002. Tokyo: Japan Concrete Institute, 669-674.