# AN INTEGRATED MODEL FOR PERFORMANCE ASSESSMENT OF CEMENT-BASED MATERIALS

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## 1. INTRODUCTION

The deterioration of cementitious materials in concrete structures is causing concern over the world today. The long-term service life of infrastructures can be achieved through improved quality control of materials, methods, and design and construction practices. A detailed knowledge is essential on these aspects, and this knowledge need to be incorporated into models for understanding the phenomena and hence for predicting the actual service life of the structures. A multi-scale simulator, which was developed in Concrete Laboratory at the University of Tokyo Japan, can predict the state of the concrete from its birth to entire life (Maekawa et al. 2009). The simulator is able to predict the performance of concrete structures in aggressive environments. For very accurate prediction however, additional mechanisms and processes affecting the performance should also be incorporated into the multi-scale simulator. DUrability COncrete Model DuCOM (Maekawa et al. 2009) and geochemical transport code PHREEQC (Parkhust et al. 1999) will be used to achieve this purpose. The developed model will consider not only the hydration of cement particles and the transport of multi-species into cementitious materials but also the chemical interaction of multi-species with cement phases simultaneously.

### 2. THE COMPUTATIONAL PLATFORM

DuCOM and PHREEQC were coupled in a previous work to develop a multi-scale physicochemical and geochemical model (Elakneswaran et al. 2012). The governing equation which is to be solved by numerical analysis for transport of ions at pore scale can be expressed as follows (Maekawa et al. 2009):

$$\frac{\partial (\phi \cdot S \cdot C_{ion})}{\partial t} + div J_{ion} - Q_{ion} = 0 \quad (1)$$

Where  $\Phi$  is the porosity, S is the degree of saturation of porous media,  $C_{ion}$  is the concentration of an ion in pore solution,  $J_{ion}$  is the total flux of an ion, and  $Q_{ion}$  is the sink term.

In Eq. [1], the first term represents the rate of change in total amount of ion per unit time and volume, the second term gives the total flux due to both diffusion and advection, and the last term called the sink or source term which represents the rate of removed or precipitated ions by reactions. In the governing equation, Nernst-Plank equation is used to express diffusive flux of ions considering electrical potential gradient and activity coefficient in porous media. The sink term can be calculated as the rate of dissolved or precipitated ions due to geochemical reactions.

The framework of coupled physicochemical and geochemical model is shown in Figure 1. DuCOM consists of several sub-models, which work together and are interlinked. PHREEQC has incorporated into DuCOM as a model to perform speciation and geochemical calculation after hydration and microstructure computation as well as in each ionic model. Each sub-model in the framework satisfies the governing equation (Eq. [1]) for FEM calculation through continuous iterations.



Figure 1 Framework of coupled DuCOM and PHREEQC

**3. SIMULATION RESULTS AND DISCUSSIONS** Simulation results provide many details such as hydration of cement particles, microstructure formation, pore solution concentration, ionic profiles during the transport, mineralogical distributions, etc. as a function of time and depth. The coupled model was used to predict hydration of cement particles and the formation of porosity. The simulation result for hydrating Ordinary Portland Cement (OPC) with water to cement ratio (W/C) of 0.5 is shown in Figure 2. Beside some un-hydrated clinker, Calcium Silicate Hydrates (C-S-H), Ettringite (Aft), and monosulfate are the main phases in the hydrated OPC. It can further be seen that the formation of monosulfate correlates with the disappearance of ettringite. Ettringite is completely changed to monosulfate at later age (after one days of hydration). The amount of C-S-H and portlandite continues to slowly increase with time. However, the formation of monosulfate does not change with time. The simulated hydrated products are compared with experimental observations. The XRD Rietveld analysis in the hydrated OPC samples which cured until 91 days showed the same kind of phases as simulated one (Elakneswaran, 2009). The comparison of experimentally determined portlandite and monosulfate with the simulated results are shown in Figure 2. The simulated results agree well with experimental observation. In order to determine the total (gel and capillary) porosity in hydrated OPC, Mercury Intrusion Porosimetry (MIP) and nitrogen gas adsorption were used (Elakneswaran, 2009). Very good agreement is obtained between experimentally determined and simulated porosity after hydration of 91 days for OPC sample (Figure 2).

The performance of cementitious materials in seawater environment was evaluated the using coupled model. In the simulation, one side of the concrete was considered to be contact with seawater and the other side was free. A one-dimensional multi-ionic transport coupled with geochemical reactions was considered. The hydration products are dominated by C-S-H (with CaO to  $SiO_2$  ratio of 1.6), portlandite, ettringite, monosulfate, and gypsum. In addition to these hydrates, other phases expected to form under these environment have also been included. As for the multi-ionic transport, the main ions in pore solution and exposure solution such as  $Na^+$ ,  $K^+$ ,  $SO_4^{2-}$ ,  $Ca^{2+}$ ,  $OH^-$ ,  $Mg^{2+}$ ,  $Al^{3+}$ ,  $H_2SiO_4^{2-}$ , and  $HCO_3^{--}$  were considered. The simulation result of mineralogical evolution in terms of volume percentage for 20 years of seawater transport is shown in Figure 3. As indicated in the figure, the left-hand side of the figure corresponds to the exposure surface



Figure 2 Hydrates and porosity changes as function of hydration time for OPC with W/C of 0.5(Lines represent the simulated results while marks show the measured data (Elakneswaran, 2009) after 91 days of hydration)



Figure 3 Representation of the distribution of phases after 20 years of seawater ingress

which in contact with seawater solution. The figure indicates that the reorganization of cement hydrates due to seawater ingress and equilibrium between solids and solution.

#### 4. SUMMARY AND CONCLUSIONS

A robust and reliable model has been required to take into account the fundamental physicochemical and geochemical reactions resulting due to detrimental effects during the service-life of concrete structures. A multi-scale model developed by Concrete Laboratory at the University of Tokyo is extended in this study by coupling geochemical code PHREEQC with the model. The newly developed multi-scale modeling framework capable of addressing physiochemical and geochemical processes in cementitious materials such as hydration of cement particles, pore structure formation, multi-species transport, activity effect, ionic interaction with cement hydrates, etc. The modeling results have compared with experimental data reported in the literature. It can be inferred that the modeling results capable of capturing the actual occurring phenomena in the aggressive environments.

#### REFERENCES

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