学　位　論　文　内　容　の　要　旨

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学　位　論　文　題　名

Multi-stage model for predicting the mechanical and durability characteristics of cement-based material

(マルチステージモデルによるセメント系材料の力学特性及び耐久性予測)

Cement based materials such as mortar and concrete are the most widely used building materials in the global construction industry. Owing to the diverse components such as hydration products, aggregates and cement-aggregate interfacial zone, they highly reveal a complicated microstructure. Different varieties of hydration products such as calcium silicate hydrate (C-S-H), calcium hydroxide, ettringite, hydrotalcite, and AFm phases are formed depending on the binder composition. The main hydration product, the C-S-H, has a complex pore structure with high specific area. It is also well-known that C-S-H in hydrated matrix exists in two different forms namely low-density C-S-H (LD C-S-H) and high-density C-S-H (HD C-S-H). Moreover, the occurrence of cement-aggregate interface (interfacial transition zone) is related to the wall-effect initiated by the aggregate surface that disturbs the normal packing of cement particles. Due to its higher porosity, the interfacial transition zone (ITZ) in cementitious composite is considered as a weaker phase compared to aggregate and hydrated matrix in concrete and mortar. The aforementioned microstructure of the cementitious materials are the utmost significant factors that govern the progress of mechanical and ionic transport properties.

Predicting the mechanical and transport properties of hydrated matrix are no doubt the most complicated processes. In most of the previously proposed models, the prediction relies on number of assumptions and simplifications which limit the application range and further developments of the models. Needless to say, to realistically simulate the responses of binder, the model should integrate all the constituents of hydration. Therefore, the purpose of this research work was to develop a model for reliably predicting the mechanical and transport properties from the detailed microstructure. A new model named HyMeC (Hydration and Mechanical properties of Cement-based material) was developed to predict the mechanical properties of cement-based material and this model was coupled with COMSOL Multiphysics (HyMeC-COMSOL) to perform the calculation of transport of ions and gas.

In the first part of this research work, a two-stage model is proposed to predict the mechanical properties of the cement paste from the micro-structure. Firstly, relative humidity, thermodynamic, cement hydration and model for volumetric prediction are integrated to accurately predict the volume fraction of hydration products. Subsequently, a multi-scale model is developed in three hierarchical levels, that initiates from C–S–H matrix considering the formation of two types of C–S–H (low- and high-density C–S–H) to cement paste for the computation of the mechanical properties of cement paste. As the volume fraction of C–S–H and capillary porosity are the most significant components which determines the mechanical properties of cement paste, prime consideration herein is given to C–S–H space ratio.

The proposed model is well verified at the predictions of relative humidity, chemical shrinkage and capillary porosity, compressive strength, Young's modulus and Poisson's ratio with independent sets of experimental results.

In the next part, the mechanical properties such as Young's modulus and Poisson's ratio of mortar and concrete are evaluated using a multi-scale model developed in five hierarchical levels: from nano-scale cement hydrates to the scale of concrete. In the proposed model, the microstructure of mortar/ concrete is considered as a three-phase material: fine/ coarse aggregates, ITZ of aggregates and bulk paste/ mortar. The primary input is the microstructure of cement paste and ITZ, which are predicted as the function of curing time using coupled cement hydration-thermodynamic model. The ITZ volume fraction is analytically computed based on aggregate particle size distribution. Multi-level homogenization methods (based on three-phase sphere model for two-phase composite material) are finally implemented to predict the effective properties of mortar and concrete. Here, the equivalent matrix consisted of fine/ coarse aggregate, bulk paste/ mortar and ITZ are obtained with the first and second levels homogenization procedures for mortar/ concrete. To validate the predictability of the models for mortar and concrete, predicted values are compared with independent experimental data sets. The influences of ITZ on properties of mortar and concrete are also discussed based on the outcomes.

The combined diffusion of both carbon dioxide and chlorides, and its effect on mechanical properties in the hydrated cement paste is carried out in the latter part of the research work. A COMSOL-IPHREEQC interface based on MATLAB language is developed to simulate a multi-dimensional and multi-species ionic transport for cement-based materials. The COMSOL Multiphysics is used to perform the ionic transport calculations, and IPHREEQC carries out the chemical reactions using thermodynamic database. Based on the thermodynamic insight, the phase-equilibrium model and the surface complexation model are used to express the physical and chemical interactions. More importantly, the proposed transport model (COMSOL-IPHREEQC) is coupled with cement hydration model to continue the hydration reaction while doing the transport reaction. The transport of carbon dioxide and chloride are influenced by saturation degree, concentration of exposure solution (chloride ion and CO2 gas in the atmosphere), and porosity of the cement matrix. The proposed model is verified with different set of experimental results as well as with previously developed model in order to confirm the predictability of this proposed model. Moreover, the effect of the ionic transport on mechanical properties of cement paste is discussed using the multi-scale model proposed in the first part of this research work.