論文の内容の要旨

論文題目　Development of an Expansive Agent Model for Concrete in a Multi-scale Thermodynamic Platform based on Hydration and Microstructure Formation

(水和反応と空隙構造形成に立脚したマルチスケール型膨張コンクリートモデルの開発)

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Concrete structures, which are exposed to external climatic condition, tend to under-go shrinkage. Especially concrete structures with high surface-to-volume ratio experience the highest effect of shrinkage stress. Then, once the tensile strain caused by the shrinkage stress exceed the cracking strain, crack will occur. Consequently, deleterious ions such as chlorides and sulfates could migrate into concrete and cause immense degradation, structurally and aesthetically. This phenomenon is inevitable and has remained a major challenge in the field of civil engineering.

Up until recent times, engineers have been tackling this issue from designing, constructing and material aspects. For example, in the case of designing, structural elements with different shapes have been used. In the case of constructing, sequential constructing has been considered for bridge deck to mitigate the effect of moment distribution on the top surface. From material viewpoints, they have successfully mitigated the effect of shrinkage using shrinkage reducing admixtures, light-weight aggregates and expansive cements or expansive additive. Expansive additive has the capability to offset the shrinkage strain from reaching the cracking strain by enlarging the volume via the existence of expansive hydrates, that could be ettringites (Aft or trisulfoaluminate phase) or portlandites (calcium hydroxide) or magnesium oxide. Two major applications of expansive additives are:

1. To compensate the shrinkage of concrete due to thermal contraction; huge autogenous shrinkage; drying shrinkage.
2. To induce chemical pre-stress on pre-cast concrete elements.

Although a wide range of applications could be done with expansive concrete, there is still a lack of quantitative research to estimate the amount of expansion produced by the complex hydration of expansive additives for engineering applications. Usually, it depends on the conducted trial tests on different mix proportion and experience of engineers who have dealt with expansive concrete to estimate and judge whether the mix design and amount of expansive additive would be applicable for the concrete structures or not. Hence, estimating the amount of expansive additive to be used without creating harmful cracks in concrete structures could be a difficult task.

On the other hand, the Concrete Laboratory of the University of Tokyo has been developing a multi-scale thermodynamic analytical platform, coded as DuCOM-COM3, with the goal of being the *lifespan simulator* of concrete structures. This computational platform consists of, first, the material counterpart, that incorporates the hydration of cement particles, micro pore structure development, transports of multi-species and, second, non-linear structural analysis which deals with macroscopic response of structures. DuCOM covers the thermodynamic multi-chemo-physical modelling part whereby numerous thermodynamic models, such as multicomponent hydration, micropore structure formation and moisture equilibrium/transport. Its counterpart, COM3, is a nonlinear structural 3D finite-element analysis that implements constitutive laws of uncracked/cracked and hardening/aging/matured concrete. Time-dependent proper-ties of concrete such as elastic modulus, temperature, pore pressure, creep, moisture status, total porosity of interlayer, gel and capillary pores are calculated consequently after inputting the basic boundary conditions for a structure such as mix proportion, geometry and environmental conditions based on the micromodels of materials in-side the DuCOM system. The calculation sequence starts from multi-component heat of hydration model whereby the degree of hydration is determined through the amount of heat release by each phase in the system based on modified Arrhenius' equations. Then, the degree of hydration and mass of phases information retrieved from heat of hydration model would in turn be utilized to determine the volumetric balance and moisture status in the microstructure. Then, based on the solidification theory, time-dependent deformations such as creep and shrinkage would be superimposed to represent all the stresses existing in the cement paste matrix. Finally, models of concrete mechanics will deal with macroscopic structural responses based on the space-averaged constitutive laws on the fixed four-way cracked concrete model. Verification of the analytical models to real structures have been performed throughout the years. Due to the unstable nature of expansive additive, its practice in civil engineering field is quite limited as intended advantage of shrinkage compensating could not be attained if improper usage was conducted. Thus, the authors set out to extend a multi-scale thermodynamic analytical platform, coded as DuCOMCOM3, by incorporating an expansive additive model based on crystallization pressure theory.

The first part of the study involves the experiments to investigate the behavior of expansive additive from its hydration to its volumetric expansion. In addition to that, these experimental results were also used for developing and verification of the model. Preliminarily, hydration study of both CSA and free-lime type expansive study with 100% replacement ratio of ordinary Portland cement was done through XRD-Rietveld and TGA method. Such replacement ratio was decided in order to limit the parameters under investigation and to develop the reference heat rate for hydraiton model. After that, the hydration degree of each reactant phase, mass of both reactant and resultant phases inside the system was determined. Furthermore, isothermal calorimetry of different replacement ratio was also conducted and its results were specifically used to verify the heat model developed based on the multi-component heat of hydration model concept. Then, expansion behavior of cement paste bars and concrete with system of ordinary Portland cement and expansive additives at different replacement ratios was studied. As the very first step towards making the expansive additive model, this study aimed at tackling the effect of expansive additive at shrinkage compensating level, which is approximately 6 precents of addition into ordinary Portland cement mix.

The second part of the study is the development of the expansive additive model from its hydration to its volumetric expansion. Based on the combined XRD-Rietveld and TGA method to determine the degree of hydration of the phases in expansive additive, the reference heat rate for respective phases were determined and implemented as an extension on the multi-component heat of hydration model. Based on the hydration degree, the microstructure of cement matrix is formed whereby fractional volume of expansive hydrates, calcium hydroxide and ettringites, could be determined. However, not all the volume of the expansive hydrates are accounted for expansion. In fact, only the volume of expansive hydrates after adjacent particle contacts have been made would contribute in expansion. Then, as an initial step, the macroscopic expansive stress was expressed as linear isotropic pressure based upon upscaling through poromechanics from the local crystallization pressure of the expansive additive hydrates' crystals. Superimposing with the existing solidification model, which determines the creep and shrinkage of both cement paste and aggregates, this system of calculation could capture the behavior of both expansion and shrinkage of cement matrix based on the initial chemical composition of the binder. However, there was a limitation in this isotropic model as it could not capture the behavior of expansive cement pastes or concretes under restraints properly. Therefore, an investigation into using the ASR poromechanical model based on 2-phase Biot theorem was done.

The third part of the study is the implementation of ASR poromechanical model to simulate the effect of both restrained and unrestrained condition of expansive additive concrete. Due to the similar nature of expansion between ASR and expansive additive, as the scale of reaction and mechanism of expansion is closely related, it could be reasonably feasible to apply the ASR poromechanical model for expansive additives. By adapting the ASR poromechanical model to reflect the anisotropic behavior due to precipitation space when system is restrained, the model could capture the restrained effect in a more appropriate manner in uniaxial condition.