- *Technical Paper* -

MODELING OF MOISTURE LOSS AND SHRINKAGE BEHAVIORS OF BFS CONCRETE BASED ON ENHANCED PORE DISTRIBUTION MODEL

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ABSTRACT

A multi-scale model which is enhanced from microstructure aspect is applied to modeling behaviors of BFS concrete. Through investigation on pore size distribution, hydration degree-dependent specific surface area evolution is proposed for hydration product of BFS blended cement. Accordingly BFS blended cement matrix which has finer microstructure than OPC at later age can be simulated properly. Finally, verification shows that with the enhanced model, moisture loss and shrinkage behaviors of BFS concrete are predicted reasonably.

Keywords: blast furnace slag, specific surface area, pore distribution, moisture loss, shrinkage

1. INTRODUCTION

Blast furnace slag (BFS), which is a by-product obtained during steel manufacture, nowadays has already been widely used as a mineral admixture for cement in Japan. It was broadly agreed that concrete made with BFS has many advantages, including improved workability, low permeability and higher strength at later age. On the other hand, some disadvantages were also reported for BFS concrete, such as larger drying and autogenous shrinkage [1, 2], which tend to induce cracks thus decrease long time durability. Since those different behaviors from Ordinary Portland Cement (OPC), in order to promote efficient application of BFS and assess life-time performance of relevant structures effectively, it is of great necessity to model and predict properties of BFS concrete.

For life-time simulation of concrete structures, a computational system called DuCOM, which couples thermo-hygro-physical information of cementitious composites with multi-scale constitutive model, was developed by Maekawa et al [3]. With this analytical system, various properties during the whole life of concrete such as shrinkage, creep, carbonation, and chloride ion penetration can be predicted.

With regard to BFS blended cement concrete, DuCOM system has been improved by enhanced porosity development model, and compressive strength development of BFS concrete can be simulated and predicted properly [4]. However, other properties which are related to both moisture state and pore-structure, such as moisture loss and shrinkage under drying conditions are still not investigated. In this paper, the DuCOM system is enhanced with the purpose of modeling those properties. Analyses based on original model are conducted and the disagreement with experiment is pointed out. Pore size distribution of BFS blended cement matrix which is considered as the reason for the disagreement is discussed. Then enhanced specific surface area model for hydration product of BFS blended cement is proposed and therefore finer pore structure at later age compared with OPC can be obtained with the enhanced model, which is verified by water desorption isotherm. Finally, verification on moisture loss and shrinkage properties of BFS concrete is carried on based on the enhanced model.

2. MICROSTRUCTURE MODEL IN DUCOM

2.1 General Scheme

In DuCOM, micro-pore information including pore volume and distribution are computed through microstructure development model, which is the basis and foundation of the whole system. In this study, different properties of BFS concrete from OPC are considered essentially due to microstructure of harden paste and therefore enhanced work mainly focuses on modification of microstructure model, which will be described in detail in Section 3. First, the concept and whole scheme of microstructure development model and key parameters which controls pore volume and size distribution directly are introduced briefly.

Fig.1 shows the scheme of microstructure model, including porosity and pore size distribution. Micro pores in harden paste are categorized into three types in DuCOM: capillary pore, gel pore and interlayer pore, according to different size dimension. During hydration process, C-S-H gel grains precipitate outside cement particles and therefore fill in large voids in the paste, and remain of the voids are categorized as capillary

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pores. On the other hand, for gel grain generated outside or inside cement particles during hydration, it is assumed that inside there are much smaller voids than capillary pores, called gel pores. Besides, gel grain itself consists of numerous layers, and between those layers are extremely tiny spaces named interlayer pore which is only accessible for sole water molecule. Herein gel pores and interlayer pores are called internal pores together. Besides, the intrinsic porosity ϕ_{ch} is defined as the volume ratio of the gel and interlayer pores to the whole gel grain including those pores [3].

In DuCOM, size distribution functions of capillary and gel pores are calculated separately, and their superposition is used as assessment of pore fineness in the cement matrix. Since pore size distribution depends on not only porosity but also pore surface area, besides porosities of capillary (ϕ_c) and gel (ϕ_g), their surface area values per unit volume of matrix (S_c and S_g) are also computed in the model. Here there are another two intrinsic properties necessary in calculation: equivalent size of gel grain (ζ) and internal specific surface area of gel grain (s_g).

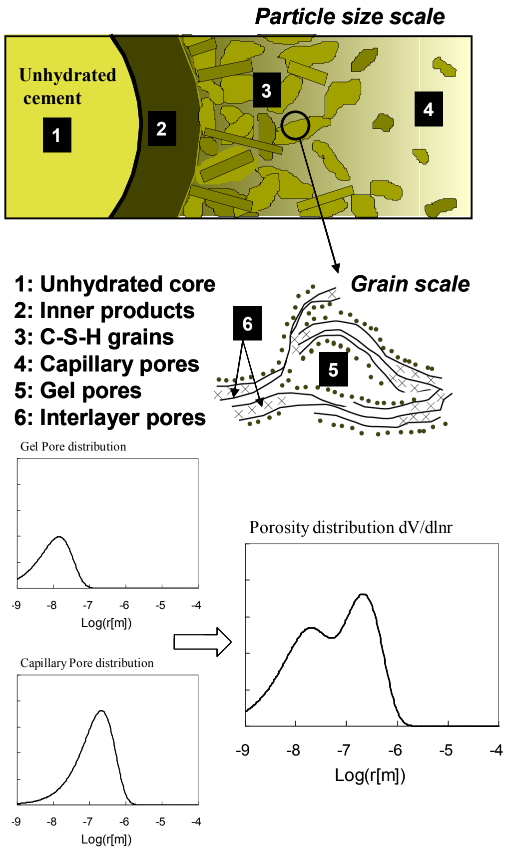

Fig.1 Microstructure model [3]

It has to be emphasized that ϕ_{ch}, ζ and s_g are keys for modifying microstructure of harden cement paste. Since ϕ_{ch} represents internal pore volume (sum of interlayer and gel pores) per volume of C-S-H gel grain. At the same hydration degree, the higher ϕ_{ch} the more internal pores insides gel grain. Therefore hydration product is more capable of expanding and filling in large voids, resulting less capillary pores and more gel pores. On the other hand, ζ and s_g dominate capillary and gel pore distribution. Since ζ represents size of gel grain and when smaller grains fill in voids in the paste, large surface area thus finer capillary pore distribution is expected. Besides, larger surface area and finer distribution for gel pores are available with higher value of s_g. In DuCOM ϕ_{ch}, ζ and s_g for gel product of OPC are assumed to be constant, and the values are 0.33, 30nm and 30m^2/g under normal temperature (20 ℃).

2.2 Modified Porosity for BFS Cement Matrix

The microstructure model introduced above has been modified by porosity modification based on water content measurement inside the pores and verification on compressive strength of BFS concrete gives good agreement [4]. Here the modified model is introduced briefly, and Fig.2 presents analysis and experiment result of internal water and compressive strength based on both original and modified model during the study. Cement pastes made of ordinary Portland cement (N), medium heat cement (M) and low heat cement (L) with w/c ratio 0.5 and 45% BFS replacement were cast respectively. After cured at 20°C until different ages, specimens were dried at 40°C for 24 hours and the weight loss was considered as capillary water. Then the specimens were exposed at 105°C to remove all the internal water inside gel grains. Finally, the specimens were heated up to 1000°C to remove chemically combined water. Besides, mortar specimens with size ϕ5×10cm were cast for compressive strength test.

Compressive strength is calculated based on capillary porosity model proposed by Otabe [5]. Generally speaking, the lower capillary porosity, the higher strength will be obtained. However, when the model is applied to concrete with BFS added in, compressive strength computed is always less than OPC as Fig.2 (b) shows. Since it is widely recognized BFS has higher strength than OPC at later age, it seems that there may be some discrepancy when calculating porosity of BFS concrete. Therefore, after examined by various experiment such as hydration degree, chemically combined water and physical water inside micro-pores, it was found that for BFS harden paste, analysis underestimated internal pore water (sum of gel and interlayer water) content insides gel grain at later age, which means gel porosity is underestimated and capillary porosity is overestimated. As mentioned in Section 2.1, intrinsic porosity ϕ_{ch} controls ratio of internal and capillary pore, therefore, intrinsic porosity of gel grain formed from slag hydration (ϕ_{ch}^{sg}) was proposed as follows:

$$\phi_{ch}^{sg} = 0.53 \cdot \alpha_{sg} + 0.28 \qquad (1)$$

Where, α_{sg} is the hydration degree of slag component.

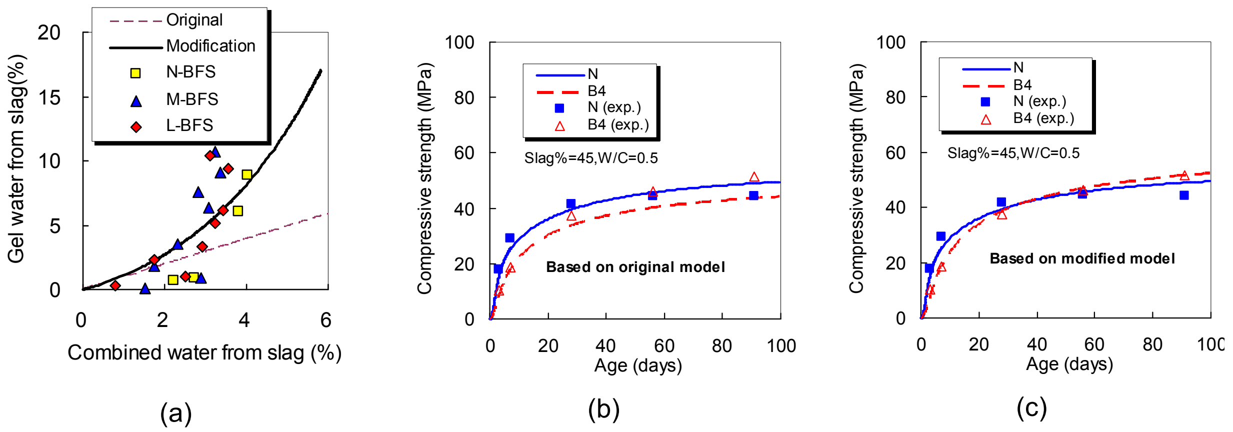

Fig.2 Water content and compressive strength [4]

Here the intrinsic porosity for BFS gel grain is not a constant but hydration degree-dependent variable. Meanwhile, internal porosity of gel grain formed from Portland cement component hydration (ϕ_{ch}^{pc}) is kept the same value as in Section 2.1. Average intrinsic porosity is calculated by weight fractions of Portland cement and slag. Therefore, for BFS blended cement, with hydration degree goes on gel grain tends to gain more internal porosity. Accordingly the total volume of hydration product becomes much higher and fills in voids more sufficiently, so less capillary porosity and higher compressive strength can be expected.

With modified intrinsic porosity for BFS blended cement, internal water content was calculated again and compared with experiment data (Fig.2 (a)). It is obviously showed that the enhanced model shows nonlinear increment and much higher internal water content at later age, which is also agreeably consistent with experiment. Finally, verification by compressive strength experiment in Fig.2 (c) shows validity of the modification. At early age compressive strength of BFS is less than OPC. With hydration degree goes on, BFS tends to contains finer pores (internal pores) and less capillary pores, therefore higher strength at later age is computed.

3. ENHANCED PORE DISTRIBUTION MODEL

3.1 Discrepancy for Moisture Loss and Shrinkage Simulation

Based on microstructure model in DuCOM and the modification on intrinsic porosity introduced above, porosity of BFS harden matrix can be simulated and compressive strength of BFS concrete is predicted reasonably. However, some properties such as moisture loss and shrinkage depend on not only porosity but also pore fineness, i.e. pore size distribution. Therefore, in this study, first of all applicability of current model on those properties of BFS concrete is investigated.

It is reported that moisture loss of BFS concrete at later age under drying condition is less than OPC due to low permeability, while drying and autogenous shrinkage are usually larger. Fig.3 shows computational result of moisture loss and shrinkage of BFS and OPC concrete and comparison with experiment. The authors conducted the moisture loss experiment mentioned here. OPC and BFS mortar specimens were seal-cured for 1d, 3d, 7d and 28d respectively and then exposed at 60% RH to measure water loss. In the autogenous shrinkage experiment [7], mortar specimens with size ϕ5×10cm were cast and sealed. A 70mm long thin strain sgauge was embedded before casting to measure the shrinkage deformation. The specimens were stored under at constant 20°C. Apparently for BFS case cured for 28d analysis overestimates moisture loss, showing more water loss than OPC, which is opposite to the experiment. On the other hand, drying and autogenous shrinkage are underestimated, and gives inconsistent trend when compared with OPC. Therefore, it can be concluded that with current model, moisture loss and shrinkage could not be predicted correctly.

Since moisture loss and shrinkage is significant influenced by microstructure of cement matrix especially pore fineness, it is necessary to examine pore size distribution evolution. It has been widely reported that pore distribution of harden cement paste with BFS replacement is quite different through both morphology observation by electron microscope and pore analysis experiment such as Mercury Intrusion Porosimetry (MIP). Generally speaking, at very early age BFS blended paste has coarse pore structure, while with hydration progress gradually it tends to be finer than OPC. Pore distribution curve obtained by MIP method indicated that for matured matrix usually peak of the curve moves towards finer direction if replaced by BFS. However, Fig.4 presents an example of pore size distribution calculated by current model. For early age such as 1d, indeed BFS matrix has a coarser pore distribution. However, for long term age of 90d, peak of distribution curve stays at the similar position with OPC, which implies that in analysis pore size are estimated similar. In other words, calculation based on current model does not reflect the main difference on pore fineness between BFS and OPC, which maybe also the reason for discrepancy on shrinkage and water

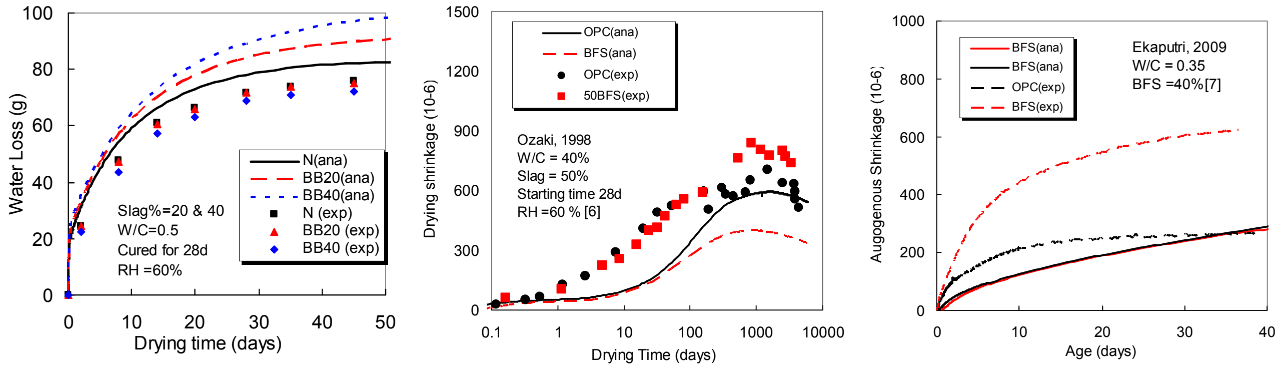

Fig.3 Moisture loss and shrinkage based on original model

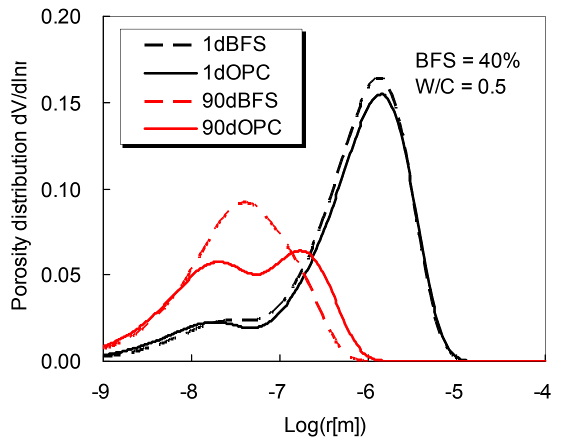

Fig.4 Pore distribution based on original model

loss. Therefore with regard to multi-scale model applicable to BFS concrete, the crucial issue is to develop pore distribution model which is consistent with the true pore fineness.

A possible approach to modify pore distribution assessment is increasing surface area of pores, i.e. S_c and S_g introduced in Section 2.1, which depends on two intrinsic parameters of gel grain; equivalent size of gel grain (ζ) and internal specific surface area (s_g). By decreasing ζ larger S_c value will be obtained while increasing s_g can induce larger S_g value, consequently pore distribution curve in Fig.4 will move towards left direction and finer pore-structure will be achieved. On the other side, considering coarse structure at early age, it is appropriate to assume similar value with original model for ζ and s_g at low hydration degree.

Combining the considerations above, enhanced pore distribution model is proposed by modifying intrinsic properties of pore grains formed from slag hydration as follows:

$$s_g^{sg} = 49 \cdot \alpha_{sg} + 0.5$$
$$\zeta^{sg} = -15 \cdot \alpha_{sg} + 10 \qquad (2)$$

Where, the unit of ζ^{sg} and $s_g{}^{sg}$ are 10^{-9}m and 10^3m^2/kg respectively. In DuCOM maximum hydration degree of slag is assumed to be 0.6, therefore ζ^{sg} remains positive number all the time.

As Eq.2 shows, for gel product generated from slag hydration in the cementitious powder, ζ^{sg} and $s_g{}^{sg}$ are dependent variables versus hydration degree of slag. Other the other hand, for gel product generated from Portland cement in the powder, ζ^{pc} and $s_g{}^{pc}$ are assumed the same values as original model in Section 2.1 thus constant during hydration. Average values of ζ and s_g for the total powder are obtained by weight fractions of Portland cement and slag.

Hence, average values of ϕ_{ch}, ζ and s_g are also dependent variables versus hydration degree. Accroding to Eq.2, in the new model individual gel grain becomes smaller, leading to denser capillary pore distribution. For gel pores inside gel grain, since surface area increase due to s_g, pore structure also becomes finer. Therefore, with the enhanced model much finer microstructure can be achieved for BFS harden paste, which qualitatively agrees with experiment such as morphology observation and pore measurement by MIP method. The size distribution in Fig.4 for 90d case is calculated again based on the enhance model and showed in Fig.5. For matured paste the peak of BFS size distribution curve obviously moves toward finer direction and finer pore structure is obtained compared with OPC paste.

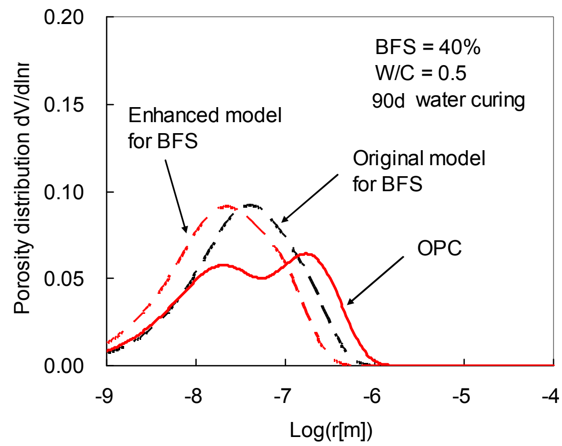

Fig.5 Pore distribution after enhancement

Here the scheme of microstructure formation for BFS harden paste is summarized in Fig. 6. The basic concept is the same with original model in Section 2.1. However, during the process that gel grains precipitate and fill in the void in the paste, grain dimension does not keep uniform. At the beginning, relatively large grains precipitate and with hydration degree goes on gradually smaller and smaller grains fill in the remained pores, resulting in finer capillary pores. On the other hand, when individual grain is inspected inside, it contains higher gel pore volume and finer pore distribution.

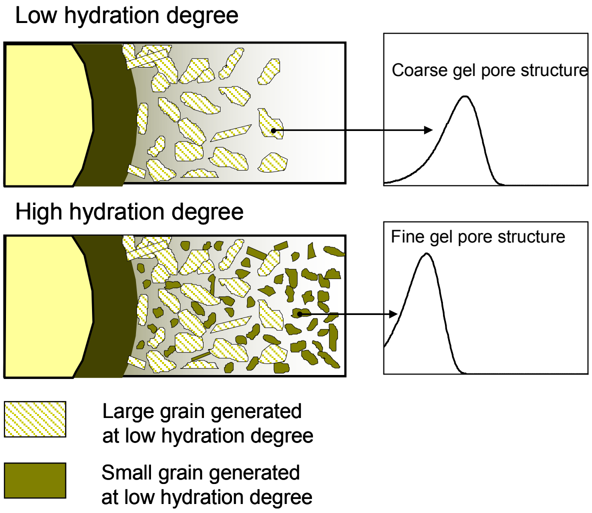

Fig.6 Scheme of new micro-pore model

3.2 Verification by Water Desorption Experiment

Since the basis of thermo-hygro-physical system in DuCOM is micro-scale information in the paste, it would be persuasive if the enhanced pore distribution model could be verified by experiment which is related to pore-structure directly. Morphology image obtained by electron microscope supports the enhanced model but can not be calculated quantitatively. Although MIP method provides proof for denser pore-structure of BFS concrete, it is not believed to provide the “true” porosity because pore structure may be altered during mercury intrusion, and therefore pore size distribution curve is not reliable for quantitative comparison. On the other hand, since water content contained inside the paste is strongly influenced by pore structure, experiment dealing with water content measurement is applicable for verification of enhanced model. In this section, pore size distribution is verified by water desorption isotherm from Maruyama’s experiment [8].

Water adsorption and desorption experiment can reflect pore fineness since capacity of keeping water at various relative humidity (RH) depends on fineness of pores. The finer the pores the more water remained inside. In DuCOM, the whole water isotherm of OPC concrete can be simulated. Herein the enhanced model is applied for BFS case.

In Maruyama’s experiment, OPC and BFS cement paste with w/c ratio 0.55 and 0.44 respectively were cured by $Ca(OH)_2$ solution for 150d and then water desorption experiment was carried out until RH lower than 0.3, at which most of gel and capillary water was considered evaporated. The same environment condition is applied in the analysis, and comparison is showed in Fig.7. It is obvious that analytical results based on the enhanced model agree with experiment and reflects the difference between BFS and OPC. BFS matrix keeps more water than OPC at the same RH, which is agreeably simulated by the enhanced model.

Therefore, based on the verification by water content experiments it can be concluded that the enhanced pore size distribution model can simulate microstructure development of harden cement paste with blended BFS reasonably.

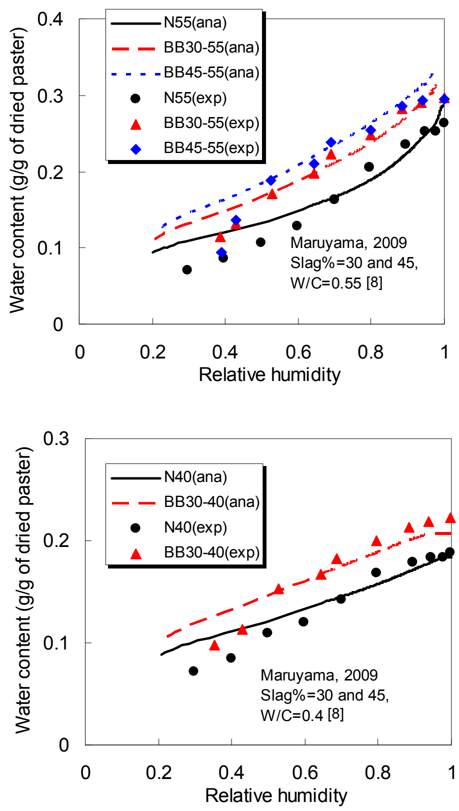

Fig.7 Water desorption analysis

4. VERIFICATION BY STRENGTH, DRYING AND AUTOGENOUS SHRINKAGE

In order to examine applicability of the enhanced model on prediction of performance of BFS concrete, verification by properties such as moisture loss, drying and autogenous shrinkage are carried out and the comparisons are shown in Fig.8 ~ Fig.9. With the enhanced model, these properties of BFS concrete are simulated reasonably. Especially the different trends from OPC can be traced. As Fig.8 shows, if exposed under drying condition after just short term curing, the matrix with BFS added in loses more water due to coarse pore-structure. With longer curing time, for example 28 days, BFS mortar tends to restrain much

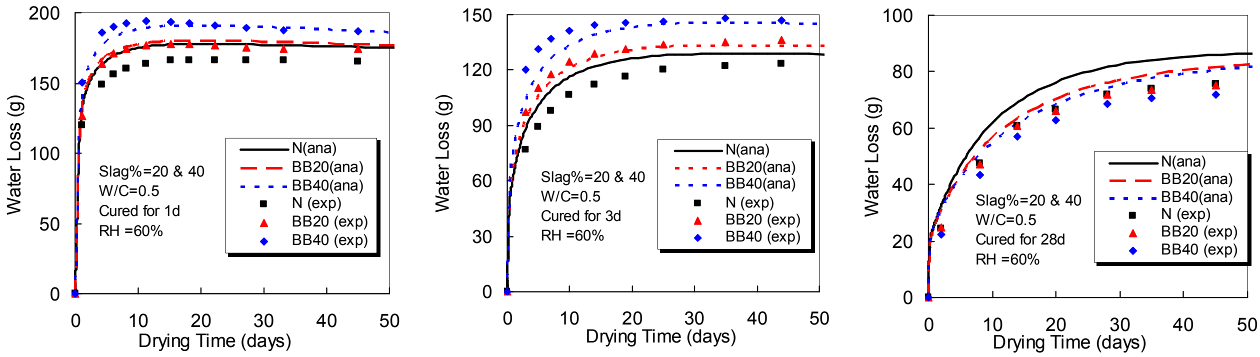

Fig.8 Water loss analysis

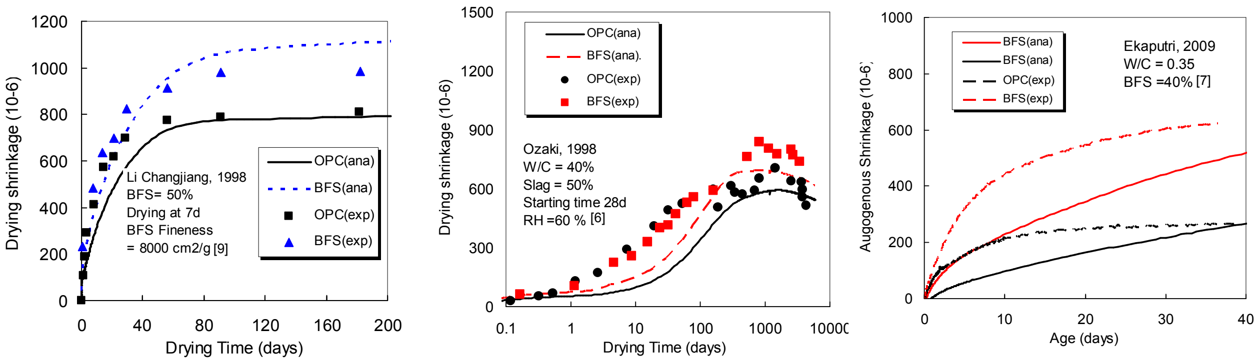

Fig.9 Drying and autogenous shrinkage analysis

water because of finer microstructure than OPC. For drying shrinkage, analysis agrees with experiment, indicating that BFS has larger shrinkage than OPC due to finer pore distribution. Besides, computation on autogenous shrinkage of low water to cement ratio also indicates consistency of the enhanced model with experiment. With low water to cement ratio, BFS concrete behaviors higher autogenous shrinkage.

5. CONCLUSION

(1) Original microstructure model with modified intrinsic porosity is not applicable to moisture loss and shrinkage prediction for BFS concrete, due to underestimation of pore size fineness in the calculation.

(2) With enhanced pore distribution model, finer pore-structure of BFS blended cement matrix at later age can be simulated agreeably, which is verified by water desorption experiment.

(3) Verification by properties of BFS concrete such as moisture loss and shrinkage confirms applicability of enhanced model on prediction of performance of BFS concrete.

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