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A Numerical Simulation Approach to Calculating Hygro-thermal Deformation of Concrete Based on Heat and Moisture Transfer in Porous Medium

D. P. Chen, C. X. Qian and C. L. Liu

287

A Model for Estimating the Aggregate Content for Self Compacting Riber Reinforced Concrete (SCFRC)

P. Ghoddousi, R. Ahmadi and M. Sharifi

297

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Theme: Concrete Technology

D e c .
2 0 1 0
V O L . 8
N O . 4

Influence of Sodium Oxide on Properties of Fresh and Hardened Paste of Alkali-Activated Blast-Furnace Slag

A. Allahverdi, B. Shaverdi and E. Najafi Kani

304

Load Bearing Strength of Fly Ash Modified with Cement and Waste Sludge

M. Shoeb Ahmad and S. Salahuddin Shah

315

Durability of Concrete Cylinder Specimens Strengthened With FRP Laminates under Penetration of Chloride Ions

A. Gharachorlou and A. A. Ramezaniapour

327

High-Temperature Mechanical Properties of Concrete

M. Bastami, F. Aslani, and Mo. Esmailnia Omran

337

Biodeterioration of Coastal Concrete Structures by Marine Green Algae

S. Jayakumar and R. Saravanane

352

Fast Set and High Early Strength Cement from Limestone, Natural Pozzolan, and Fluorite

E. Najafi Kani and A. Allahverdi

362

A Numerical Simulation Approach to Calculating Hygro-thermal Deformation of Concrete Based on Heat and Moisture Transfer in Porous Medium

D. P. Chen¹, C. X. Qian² and C. L. Liu^{3,*}

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Abstract: Concrete deformation due to temperature and moisture condition will always develop simultaneously and interactively. The environmentally (hygral and thermally) induced stress and deformation are essential to concrete durability. To simulate the deformation of concrete caused by the coupling effect of temperature and moisture, a numerical simulation approach is proposed comprising analytical process and finite element analysis is proposed based on the mechanism of heat and moisture transfer in porous medium. In analytical method, Laplace transformation and transfer function were used to simplify and solve the coupled partial differential equations of heat and moisture transfer. The hygro-thermal deformation of concrete is numerically simulated by finite element method (FEM) based on the obtained temperature and moisture stress transformed from the solved moisture distribution. This numerical simulation approach avoids the complex eigenvalues, coupling difficulty and low accuracy in other solving method, and also effectively calculates the moisture induced shrinkage which is almost impossible using familiar FEM software. Furthermore, a software named Combined Temperature and Moisture Simulation System for concrete (CTMSOft) was represented and developed by a mix programming of Visual Basic, Matlab and ANSYS. CTMSOft provided a simple and more intuitive interface between user and computer by providing a graphical user interface (GUI). The validity of the numerical simulation approach was verified by two cases analysis.

Keywords: hygro-thermal deformation, porous media, concrete, numerical simulation, mix programming

1. Introduction

Durability of concrete structures is strongly influenced by cracking caused by shrinkage of the concrete material, by external loading and by other environmentally (hygral and thermally) induced stresses. Along with the development of the industry of cement and concrete, crack and damage to durability of concrete induced by the volume change since concrete have been placed in the building site have attracted most attention in the research of durability, which, in fact, is a problem of the concrete deformation (volume stability). It must be mentioned that the crack induced by ill volume stability, no matter what

small they are, would remarkably reduce the permeability and make the deterioration easier to occur, and thus heavily deteriorate the durability [1-3].

Nevertheless, it would be more practical to study the volume stability of concrete using a coupled temperature and moisture model, provided this model concept would lead to accurate predictions of the deformations in the concrete structure under actual environmental conditions. Predicting the hygro-thermal deformation of concrete, and controlling it, is made difficult by the complexity of the material and the varying environment conditions. This could not be realistically reproduced in experiments and field tests. Fortunately, a numerical simulation approach provides a powerful tool for analyzing the deformation of the concrete structure under such conditions.

Bazant and Najjar [4] carried out a prior research on concrete deformation based on heat transfer and moisture diffusion in concrete. Fick's second law for drying shrinkage and Fourier's heat conduct equation for thermal shrinkage are the basic equations to calculate the

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concrete deformation numerically. Luikov has proposed the governing equations for coupling heat and mass transfer in porous materials, quite a few researchers have given different solution methods. Mikhailov and Ozisik [5] had the analytical solutions based on the classical integral transform method. Gaur and Bansal [6] used periodic approximate method to obtain closed-form solutions. Chang and Weng [7] applied a decoupling technique to coupled governing equations. Cheroto et al. [8] proposed a modified lumped system analysis approach to get approximate solutions. But the methods referred are either complicated or incorrect. The modified Luikov's equations and the transfer function are applicable to simulate the temperature and moisture distribution in concrete [7, 9].

The investigations of shrinkage or cracking of concrete induced by the coupling effect of heat and moisture were mostly carried out to analyze the concrete in fire or at high temperature [10-14]. The similar research at normal temperature was rare, and the mechanism of heat and moisture transfer in concrete was different in such condition. The research on hygro-thermal deformation with time-dependent boundary condition was even less. Besides that, the numerical simulation process faced a difficult dilemma in applying moisture effect as load on nodes when using finite element method.

Therefore, to resolve the above difficulties, we proposed a numerical simulation approach

comprising analytical solution of moisture-temperature distribution, theoretical calculation of moisture induced stress and finite element analysis of coupling hygro-thermal deformation. And computer-programming techniques were used to develop software for numerically calculating the heat and moisture transfer in porous materials like concrete and the deformation induced by their coupling effect based on the transfer mechanism. The program provided a simple and more intuitive interface between user and computer by providing GUI. This software quantitatively evaluated the heat and moisture distribution, the stress induced by variation of relative humidity, and the hygro-thermal deformation of concrete with different boundary conditions.

This paper presents the numerical simulation approach to calculating hygro-thermal deformation of concrete based on heat and moisture transfer in porous media and describes the corresponding software named Combined Temperature and Moisture Simulation System for concrete (CTMSOft). Two cases analysis were investigated according to the approach proposed and the CTMSOft developed.

2. Numerical Simulation Approach

The proposed numerical simulation approach comprising three steps as shown in Fig.1: (1) analytical solution of the moisture and

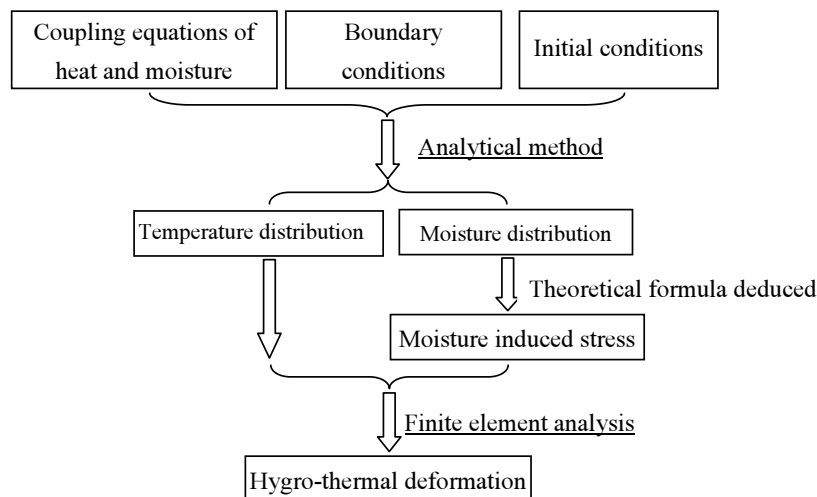


Fig.1. Schematic of the numerical simulation for hygro-thermal deformation of concrete

temperature distribution in concrete in the varying temperature and moisture circumstance; (2) theoretical calculation of moisture induced stress; (3) finite element analysis of coupling hygro-thermal deformation of concrete.

2.1. Analytical Solution of Moisture and Temperature Distribution

An analytical procedure based on the mechanism of heat and moisture transfer in porous medium as an original methodology for predicting and estimating the heat and moisture transfer in porous media, was defined as a stand-alone and comprehensive frame for a real simultaneous solution, which was connected to the heat and moisture transfer inside the materials, environmental temperature and moisture.

Material properties are considered to be uniform throughout whole material body. The heat and moisture transfer equations resulting from mass and energy conservation during the transfer process can be expressed as Eqs. (1) and (2).

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} + \rho r h_{iv} \frac{\partial M}{\partial t} + Q \quad (1)$$

$$\frac{\partial M}{\partial t} = D_{mk} \frac{\partial^2 M}{\partial x^2} + D_{mk} \delta \frac{\partial^2 T}{\partial x^2} + W \quad (2)$$

where ρ is the density of the material, c_p is the specific heat of constituent, T is the temperature, λ is the thermal conductivity, r is the phase change factor, M is the moisture content, h_{iv} is the heat of phase change, D_{mk} is the moisture diffusion coefficient considering the effect of Knudsen diffusion, x is location variable, t is time variable, δ is the thermal gradient coefficient, Q is the temperature sink and W is moisture sink in concrete.

In analytical method, Laplace transformation and transfer function were used to simplify the coupled partial differential equations of heat and moisture transfer in Laplace domain into a single fourth-order ordinary differential equation (ODE), which could be easily solved by conventional methods. Then the moisture and the temperature distribution in time domain yielded by inverse Laplace transformation [7, 9, 15].

2.2. Moisture Induced Stress

The deformations induced by temperature changes might be calculated by direct application of temperature loads to the nodes in the FE analysis. To the contrary, with the current FEM approach it is not possible to directly apply moisture loads to the nodes and must be transformed to moisture induced stress first.

Fortunately, Kelvin-Laplace equation and Mackenzie formula as described as Eqs.(3) and (4) make the transform of moisture distribution to stress be possible [9, 16, 17]. Eq. (3) describes the relationship between the negative pore fluid pressure and the internal relative humidity in the pore structure. Eq. (4) expresses the relationship between the hydrostatic pressure and the associated strain. And the relative humidity and its variation in concrete can be calculated according to the moisture content, which reckons on the experimental water loss and drying weight.

$$p = \frac{-\ln(RH)}{v_m} RT \quad (3)$$

Where p is the pore fluid pressure, RH is the relative humidity in concrete, v_m is the molar volume of water, R is the universal gas constant, T is the Kelvin temperature.

$$\varepsilon = \frac{\Delta p}{3} \left(\frac{1}{K} - \frac{1}{K_0} \right) \quad (4)$$

Where ε is the linear strain, Δp is the average of hydrostatic pressure caused by the variation of temperature or moisture, K and K_0 are bulk modulus of porous solid and bulk modulus of solid skeleton of the material respectively.

For a partially saturated porous medium like concrete, the average of hydrostatic pressure Δp can be substituted by pore fluid pressure p . Thus p can be expressed as

$$\Delta p = p_f - p_i = \frac{-\ln(RH_f)}{v_m} RT_f - \frac{-\ln(RH_i)}{v_m} RT_i \quad (5)$$

Where i and f indicate the initial and final state respectively.

Concrete is a composite material in which aggregate is volume stable and restrains the shrinkage of the cement paste. So the effect of

aggregate and its dosage must be considered when analyze the influence of Δp (or p) on the volume change of concrete [16, 18]. Once the mix ratio of concrete determined, the volume of aggregates is permanent even in the service life of concrete. So Eq. (4) could be modified again [16], therefore, to account for the volume fraction of aggregate

$$\varepsilon = \frac{\Delta p}{3} \left(\frac{1}{K} - \frac{1}{K_0} \right) \left(1 - \frac{V_a}{V_c} \right) \quad (6)$$

Where V_p / V_c is the volume fraction of the aggregate in the concrete

The bulk modulus for a porous medium as concrete is governed by the porosity and the elastic moduli of concrete[7], namely c , K_0 and G_0 . So, according to the theory of composite materials, the relationship between them can be described as:

$$\frac{K}{K_0} = 1 - \frac{c(3K_0 + 4G_0)}{4G_0} \quad (7)$$

Where G_0 is the shear modulus of porous skeleton, c is the porosity of concrete.

The stress on each node can be imagined as the arithmetic product of strain and elastic modulus. Consequently, the stress induced by moisture changes, namely σ_h , can be calculated by Eq. (7) [19].

$$\sigma_h = \frac{cR(3K_0 + 4G_0)}{12G_0 v_m} (T_i \ln(RH_i) - T_f \ln(RH_f)) \left(1 - \frac{V_a}{V_c} \right) \quad (8)$$

2.3. FEM for Simulating Hygro-Thermal Deformation

Once the temperature and moisture loads have been applied to the element's nodes, the shrinkage deformation of concrete can be numerically simulated by means of FEM method.

3. CTMSoft Developing

3.1. CTMSoft Structure

According to the numerical simulation method

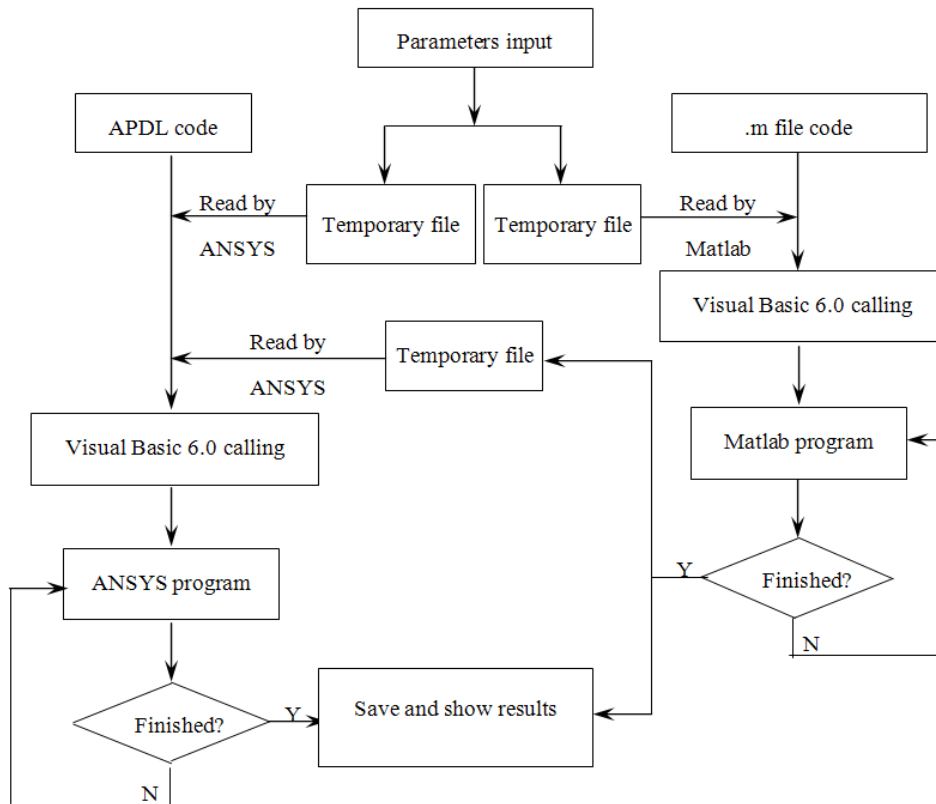


Fig.2. The holistic structure of CTMSoft

for concrete deformation based on heat and moisture transfer in porous medium (see Fig.1), the software development strategy of calling Matlab and ANSYS based on Visual Basic was proposed and the CTMSoft was developed by mix programming [20]. The holistic structure of CTMSoft concerning the different parts and their approaches is shown in Fig.2.

The CTMSoft was developed as an advanced Windows application by using the powerful features of Visual Basic (VB) programming to offer the user a graphical interface including the menu bar, commands buttons and figure viewer, etc. The GUI provided a simpler and more intuitive interface for data inputting, program running and results displaying. The core of performing the numerical simulation, which was written in and complied with Matlab or APDL of ANSYS, executed the virtual calculation process when triggered by click the related menu or command buttons. The displaying and saving of figures of numerical results were performed at the main user interface.

Although the program seemed clear and simple, a number of help features were included to allow the user to implement and understand it more easily. This comprehensive help function was documented to provide the user with a

variety of information, including an introduction to the CTMSoft and details of its methodology, how to get started using the program and many useful techniques to facilitate effective using, and so on.

3.2. Main Interface of CTMSoft

In the numerical simulation process using CTMSoft, the inputting, saving and transferring of basic parameters, the definition and selection of element type, size, initial and boundary conditions, the calling of Matlab and ANSYS, and the saving and displaying of numerical simulation results were all involved. The GUI provided a simpler and more intuitive interface for data inputting, program running and results displaying [21]. If the basic thermal and moisture parameters were considered as variables, or we considered the varying of environmental moisture and temperature, more relating data should be dealt with. At the main interface of CTMSoft, the positions for arranging the command menu, the shortcut buttons, the element definition and meshing, the basic conditions definition, the graphically displaying numerical results are defined and divided as shown in Fig.3.

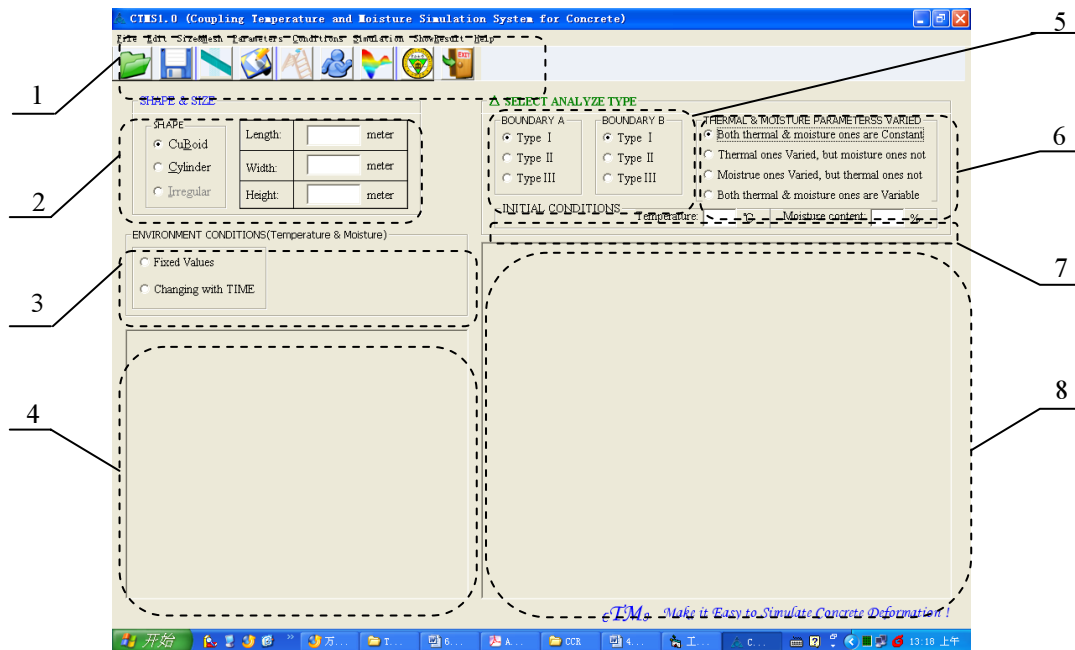


Fig.3. Main User Interface of CTMSoft

1-Menu and command buttons; 2-Type and size determination and inputting; 3-Temperature and moisture definition; 4-Showing meshing result; 5-Boundary conditions definition; 6-Defining thermal and moisture parameters; 7-Defining initial conditions; 8-Displaying numerical results graphically

4. Case Analysis

In order to validate the applicability of the present simulation approach in predicting the coupled heat and moisture transfer in concrete and the induced thermal-drying shrinkage of concrete, we applied the numerical simulation approach to two cases studies: (1) experiment of concrete deformation under isothermal condition; (2) test of coupling hygro-thermal deformation which carried out by Hundt which lasted for two years [22].

4.1. Isothermal Deformation of Concrete Experiment

In the experiment, a prismatic concrete specimen sized of 100mm×100mm×400mm was used and the concrete was cured for 28 days before test. The specimen has been isolated with

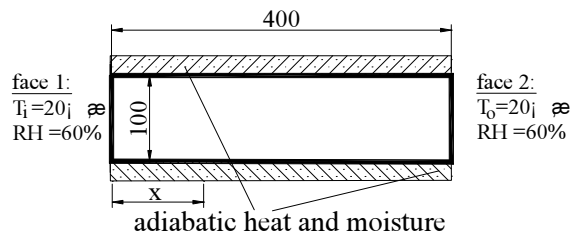


Fig.4. Schematic of layout and boundary conditions of drying shrinkage test

regards to thermal as well as moisture flux along the surfaces situated alongside to simulate plain 1D-conditions (Fig.4). In experiment, the specimen was placed in the laboratory where the temperature and moisture were constant at 20 and 60 RH respectively. Water loss and length change of concrete specimen were measured frequently.

The necessary initial and physical parameters in the calculation are determined according to experimental conditions, which are listed in Table 1. The testing data and the numerical results by present calculation procedure were shown in the Figures 5-6.

Fig.5 shows the average relative humidity in the three kinds of concrete numerically and experimentally. The calculation results by analytical and FEM method fit the experimental data very well.

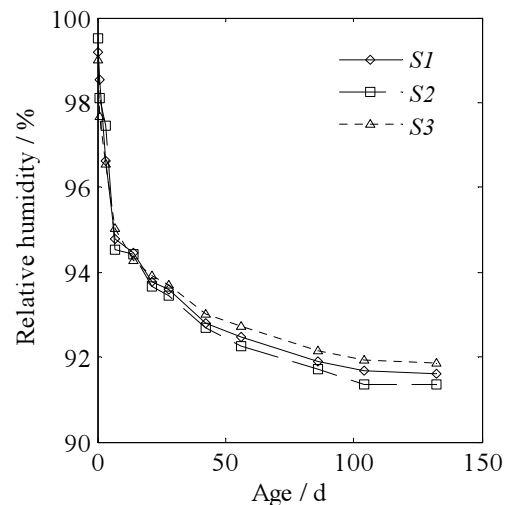


Fig. 5. Moisture content calculated from experimental data

Parameters	S1	S2	S3
Bulk modulus, GPa	24.12	23.56	23.89
Shear modulus, GPa	18.13	17.67	17.92
Porosity, %	9.6	10.2	9.8
Specific heat, J·g ⁻¹ ·K ⁻¹	0.85	0.87	0.84
Thermal conductivity, W·m ⁻¹ ·K ⁻¹	3.01	2.99	3.05
Aggregate volume fraction, %	65	67	69

Table 1. Parameters of concrete for simulation

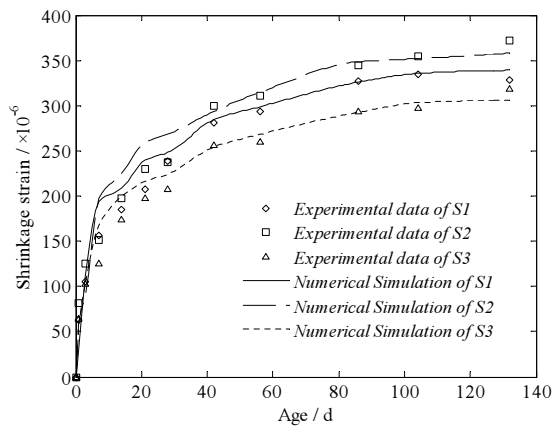


Fig. 6. Comparison of numerical and experimental shrinkage strain of concrete

Fig.6 shows a good agreement between the numerical and experimental shrinkage strain of the three kinds of concrete. Comparing Fig.5 to Fig.6, we can be sure that the lower relative humidity makes the shrinkage strain higher.

4.2. Hundt's Test

Hundt investigated different transport phenomena in six concrete specimens during a time period of three years, and the experiment results is suited to as a benchmark to verify the validity of numerical models. In the experiment, a prismatic concrete specimen sized of 2.4m×0.4m×0.4m was used and the concrete was cured for 28 days before test. The specimen has been isolated with regards to thermal as well as moisture flux along the surfaces situated alongside to simulate plain 1D-conditions (Fig.7). It was subjected to a temperature of 80 °C at one side and to a rapid decrease of external relative humidity (45%) at the other side.

At an internal relative humidity below approximately 45%, capillary menisci are not stable and the Kelvin-Laplace Equation is not

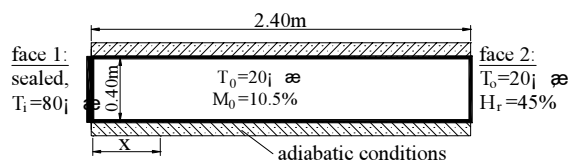


Fig.7. Schematic of layout and boundary conditions of Hundt's test on a concrete specimen

reasonable for expressing the moisture induced stress. While in Hundt's test, even though air relative humidity is 45%, the relative humidity inside the concrete rarely drops down below 50% [23]. Therefore, it is seemingly that the simulation procedure is applicable in this case.

According to the experiment conditions (see Fig.7), the boundary conditions in this case expressed as Eqs.(8)-(11). The initial conditions and some basic parameters are $l = 2.40$, $T_0 = 20^\circ\text{C}$, $M_0 = 10.5$, $T_i = 80^\circ\text{C}$, $T_e = 20^\circ\text{C}$, $M_e = 3.5\%$ (calculated from $\text{RH} = 45\%$). In the simulation analysis, the concrete specimen was discretized by 8-nodes block elements and a constant time step of 12 h was used.

$$\lambda \left. \frac{\partial T(x,t)}{\partial x} \right|_{x=0} = \alpha_i [T(0,t) - T_i] \quad (9)$$

$$\lambda \left. \frac{\partial T(x,t)}{\partial x} \right|_{x=l} = \alpha_o [T(l,t) - T_o] + (1-p)h_v \zeta_o [M(l,t) - M_o] \quad (10)$$

$$D_m \left. \frac{\partial M(x,t)}{\partial x} \right|_{x=0} + D_m \delta \left. \frac{\partial T(x,t)}{\partial x} \right|_{x=0} = 0 \quad (11)$$

$$D_m \left. \frac{\partial M(x,t)}{\partial x} \right|_{x=l} + D_m \delta \left. \frac{\partial T(x,t)}{\partial x} \right|_{x=l} = \zeta_o [M(l,t) - M_o] \quad (12)$$

The numerical results were compared with the experimental data of Hundt's test between the moisture content (volume ratio), the temperature and the length changing of the specimen (Figs.8-10). It must be noted that the simulated moisture

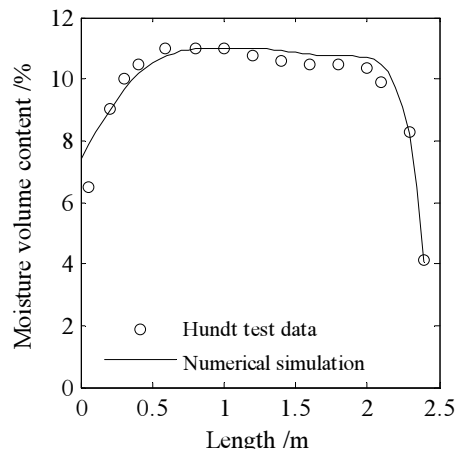


Fig.8. Comparison of numerically and experimentally moisture distribution (550d)

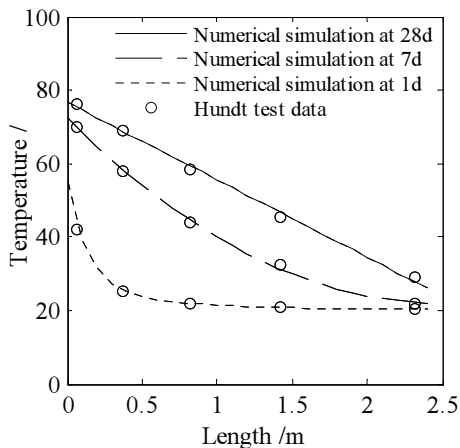


Fig.9. Comparison of numerically and experimentally temperature distribution

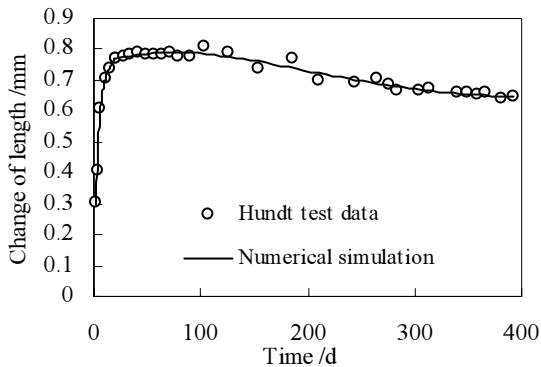


Fig.10. Comparison of numerically and experimentally of length changing of the specimen within the first 400 days

distribution is mass content of moisture directly from the analytic solution of heat and moisture transfer equations according to the boundary conditions. In order to compare the numerical results to the Hundt's test data, the numerical results of mass content were changed into volume content before comparing with experiment results of Hundt's test.

Obviously, Figs. 8-10 show a relatively good correlation between numerical and experimental data. The simulation procedure proposed in this paper is reliable and suitable for thermal-drying shrinkage simulation of concrete.

5. Conclusions

The simulation approach proposed in this paper is based on the coupling of heat and moisture transfer effects in the porous concrete. It

encompasses an analytical solution of temperature and moisture distributions in concrete, a numerical simulation of the stress fields induced by moisture and heat distributions, and the mathematical computation of hygro-thermal deformations in concrete specimen. The validity of analysis method was verified by two cases comparing test data with relevant analytical results. The results reveal the rationality and efficiency of the numerical simulation approach proposed and the CTMSoft developed.

The heat and moisture transfer inside porous materials like concrete is a complex phenomenon. More theoretical investigations are needed to be carried out for more insight into the variation of the heat and moisture transfer for different types of concrete and in various environment conditions.

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