Multi-scale modeling to link observed behavior, characterization and analysis

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**ABSTRACT:** This paper provides an overview of the mathematical modeling for time-dependent behaviour of cementitious materials. Since the cementitious materials have complex and multi-scale structures, the modeling need to bridge a very wide range of the order from nano-scale for material science level to meter-scale for structural analysis. Furthermore the structure of the cementitious materials is formed through chemical reaction and changes with time as a function of the environmental condition. Thus analytical models for observed behaviour in the cementitious materials need to be sufficiently comprehensive and precise characterization for material structure and measurement of the environmental conditions are essential for building up the constitutive models.

### 1 INTRODUCTION

For durability design and/or prediction of life time of concrete structures, nowadays it is essential to apply some relevant mathematical models to simulate the time-dependent behaviour of concrete. Cementitious materials such as concrete have complex multi-component and multi-scale structures that first form through chemical reaction and then continue to change with time (e.g. Jennings et al. 2008). As a result, various aspects of the behaviour have been observed but sometimes the real mechanisms are not clarified. If the observed behaviour is just simplified as a material law, the potential of modern numerical methods for computerized structural design is not fully used.

It could be noticed that a lot of information on the cementitious materials exists dealing with the various aspects of formation and development of the micro-structure and strength. In the field of cement chemistry, chemical reaction process, hydration products and micro-pore systems were deeply studied. Material structure of the heterogeneous composite system, mechanism of crack initiation and propagation, and mass transportation through the internal network of the porous micro-structure and cracks were studied in the field of material engineering. For the analysis and design of buildings and infrastructures, however, those scientific knowledges are limited to be transferred but averaged material laws have been obtained by a large amount of experimental studies.

One way to come to more realistic and more reliable material laws is to link the observed time-dependent behaviour with details of the material structure and with real mechanisms (Wittmann, 1983). However, the observed behaviour of concrete cannot be linked directly each other and a hierarchic system of at least three different levels needs to be introduced. Table 1 shows an example proposed by Wittmann (1983). For combining all of these observed behaviour into a unified system, conceptual modelings are essential to integrate carefully all of the important findings on these different levels into a general computational framework based on mathematical modelling. Here the modelling of concrete should cover microstructure, hydration, temperature, moisture content, state of equilibrium, and mechanical and volumetric changes. The integration is to be sought in terms of a computational tool that can take into consideration the development of micro-structure and various changes of concrete exposed to any arbitrary environment. Furthermore, for predicting the life time of concrete structures, it needs to predict the structural performance of concrete together with the transport of various external agents into the concrete microstructure (Maekawa et al. 1999).

In this paper, some examples of such mathematical modelling and computational tools together with some experimental technologies to characterize the material structure are overviewed.
2 MATHEMATICAL MODELING FOR TIME-DEPENDENT BEHAVIOR OF CEMENTITIOUS MATERIALS BASED ON MICRO-MESOSCOPIC APPROACH

2.1 Microstructural modeling of concrete

As a starting point for predicting the time-dependent behavior of concrete or concrete structures, i.e. heat production and resultant thermal deformation, autogenous shrinkage, drying shrinkage and creep behavior, microstructural modeling of concrete is discussed. For the initial state of concrete, which is determined by the properties and performance of raw materials, mixture proportion, work operation, and hydration process, a couple of models have been proposed with which the evolution of the initial state of the concrete can be predicted as a function of the mixture composition and curing condition. The five most frequently discussed micro-structural models are the HYMOSTRUC (van Breugel 1991), CEMHYD3D (Bentz & Garboczi 1993), Navi’s model (Navi & Pignat 1999), DuCOM (Maekawa et al. 1999, Maekawa et al. 2003) and CCBM (Maruyama et al. 2007). Regarding, especially deformation phenomenon, HYMOSTRUC, CEMHYD3D, CCBM, and DuCOM are dealing with, and consequently, these models are overviewed here.

HYMOSTRUC predicts the degree of hydration from the data of water to cement ratio, mineral components of cement, particle size distribution, and curing condition (i.e. humidity and temperature). The particle size distribution is represented by Rosin-Rammler function and the particles are uniformly placed in the space in statistical way. Shape of cement particles is assumed to be spherical, and it keeps the geometry during hydration process. Inter-particle contact with each other occurs when the cement particles grow. The effect of inter-particle contact on the rate of hydration is modeled with the concept of ‘cell density’.

The rate of hydration is described as a function of basic rate of hydration and coefficients of diffusion process in hydrates with Arrhenius’ law for curing temperature effect. The basic rate of hydration is determined by the amount of C₃S and C₂S. The coefficients of diffusion process in hydrates take into account of density of hydrates, residual water and relative humidity in pore structure.

Using HYMOSTRUC, van Breugel & Lokhorst (2001) explained the creep behavior of early age concrete based on the concept proposed by Ghosh (1973). Assuming inherent creep of cement hydrates and strain conservation among cement hydrates, redistribution of stress between old hydrates and new hydration products was mathematically solved in his study.

Koenders & van Breugel (1997) developed a model for autogenous shrinkage based on the HYMOSTRUC. In this model, a simple pore size distribution curve was used, and this pore size distribution, residual water, and adsorption curve gave the thermodynamic equilibrium, and relative humidity in cement paste matrix. Thermodynamic equilibrium and a similar approach to Munich model (Wittmann 1982), which is based on the surface tension concept, can produce the deformation of cement paste in early age.

CEMHYD3D is using the method of Cell Automaton, and accumulation of reaction in local cells represents the total reaction of cement paste and gives the discrete (or voxel) 3-dimensional cement paste structure. The accumulation is determined by the local chemical reaction rule which is a function of density of substances in target cell and neighborhood cells. This unique model can take into account many chemical reactions at once. But discrete system in size and time, may produce some other problems, such as evaluation of time with changing curing temperature and reaction of fine particles like silica fume. In spite of these problems, combining with statistical approach, CEMHYD3D has been successfully applied to many engineering problems.

### Table 1 Three structural levels of concrete and corresponding characteristic features, mechanisms and models. (Wittmann 1983)

<table>
<thead>
<tr>
<th>Structural Levels</th>
<th>Characteristic features</th>
<th>Mechanisms</th>
<th>Type of Models</th>
</tr>
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<tbody>
<tr>
<td>Micro-level</td>
<td>Structure of Hardened Cement Paste, Xerogel</td>
<td>Particle Displacement, Capillary Tension, Disjoining Pressure, Surface Free Energy</td>
<td>Materials Science Models</td>
</tr>
<tr>
<td>Meso-level</td>
<td>Pores, Cracks, Inclusions</td>
<td>Crack Formation and Extension, Differential Stresses</td>
<td>Materials Engineering Models</td>
</tr>
<tr>
<td>Macro-level</td>
<td>Quasi-homogeneous Structural Elements</td>
<td>Apparent Mechanisms</td>
<td>Structural Engineering Models Material laws</td>
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Regarding shrinkage problem, combining CEMHYD3D and geometrical algorithm (Bentz et al. 1995) can take into account the thermodynamic equilibrium and relative humidity in the cement paste matrix. Using these parameters, and considering specific surface free energy and Bangham equation (Bangham & Fakhoury 1931) it can simulate the deformation of porous material (Bentz et al. 1998).

Recently, CCBM was proposed by Maruyama et al. in Japan. This model is based on the fundamental kinetic model for Portland cement developed by Tomosawa (1974 & 1997). The kinetic model is expressed as a single equation composed of four rate determining coefficients which represent the rate of surface solution, formation and destruction of initial impermeable layer (for dormant period), and the following diffusion controlled process. This model also assumes that cement is spherical and it keeps its shape during hydration. Aiming for the universality, CCBM introduced the particle size distribution, reaction of each mineral compositions, coefficients for precipitation rate, and difference of density of cement gel which is affected by the temperature history. Model parameters were determined according to the cement reaction data obtained by X-ray/Rietvelt method (Hoshino et al. 2006, Matsushita et al. 2007). Phase composition problem was also modeled according to experimental data (Maruyama et al. 2007). Fig. 1 shows the comparison of degree of hydration between the experimental results and calculated results by CCBM. This model focused on the problem of early age cracking in RC members. Heat capacity and coupling of the heat and moisture transport were modeled precisely and succeeded in predicting the temperature history and distribution (Maruyama et al. 2006). Using capillary tension and disjoining pressure approach for autogenous shrinkage, self-induced stress in RC members coupled with thermal deformation and autogenous shrinkage was evaluated with FE analysis (Maruyama & Sato 2005).

Another Japanese micro-structural simulation model named DuCOM was also developed by Maekawa, Ishida, Kishi and others in the University of Tokyo (Maekawa et al. 1999, Maekawa et al. 2003). The analytical system can simulate hydration reaction, micro-pore structure formation, moisture transport/equilibrium and their system dynamics based on thermodynamics. DuCOM is comprised of mainly the multi-component hydration heat model, microstructure development model and moisture transport and equilibrium model. Each model is briefly explained below.

In the multi-component hydration heat model of DuCOM, the chemical compounds of Portland cement are aluminate (C$_3$A), alite (C$_3$S), belite (C$_2$S), ferrite (C$_4$AF), and gypsum. Other blending materials, such as blast furnace slag, fly ash or limestone powder, are incorporated into the model as individual components. The total heat generation rate per unit volume of such a blended cement is represented as the sum of the specific heat generation rate of the individual clinker component. The temperature-dependent heat generation ratio of each clinker component is based on the Arrhenius law. The heat generation rate can be idealized by two material property parameters, i.e. the reference heat rate and activation energy, when temperature is constant at 293K. In the heat generation, the following factors are taken into account as mutual interaction: retardation of the cement-slag reaction at an early stage caused by the presence of fly ash and organic admixtures, free water consumption due to hydration progress, heat generation rate change of slag and fly ash based on the amount of calcium hydroxide in the liquid phase, the interdependence between C$_3$S and C$_2$S and relative fineness of each mineral component. Finally, the temperature distribution and the degree of hydration of the concrete can be obtained by applying thermodynamic energy conservation to the space and time domain of interest. The hydration degree of hardened cement paste in this model is assumed to be the ratio of accumulated heat Q of hydrated products to final heat generation Q$_{o}$. According to the hydration model, the hydration reaction process for an arbitrary cement powder can be simulated rationally.

Next, the microstructure development model is summarized. The model can simulate the microstructure formation process of the hardening cement paste matrix for any mix proportion under arbitrary environmental conditions based on the information from the above multi-component hydration model. In the microstructure model, micro-pores in the concrete are classified into three types: capillary pores, gel pores, and interlayer pores. The capillary pores are located in the relatively large interparticle spaces between the powder particles; they act as free space for the precipitation of hydrate products. The gel pores are thermo-dynamically defined as the spaces where new C-S-H gel grains conditionally precipitates only when the temperature rises (Nakarai et al. 2007). The interlayer pores are located between the layer structures of the C-S-H gel grains; the layer thickness is defined as 2.8 Å corresponding to water molecular size. From the average degree of hydration and the weight of chemically combined water computed in the hydration model, the volume of gel products and porosity of capillary pores, gel pores and interlayer pores are calculated in the model. The entire micro-pore structure is idealized as the total porosity of the above-mentioned capillary pores, gel pores and interlayer pores. The pore distribution of each pore is represented by a simple Raleigh Ritz function, postulating that the pores are cylindrical in shape.
Moisture in the cementitious microstructure can be presented in both liquid and vapor phases in the moisture transport and equilibrium model. The vapor and liquid phase transports are formulated based on mass conservation laws. The pore moisture is classified as adsorbed water, condensed water in capillary pores and gel pores, and interlayer water in the interlayer pores in the model.

Firstly, the moisture equilibrium model is explained. Considering the surface equilibrium between the vapor and liquid phases in fine pores, the relationship between the radius $r_s$ of pore where the meniscus is formed and pore humidity can be obtained from Laplace equation and Kelvin’s equation, when the interface is a part of an ideal spherical surface. The amount of water in the microstructure at a given ambient relative humidity can be calculated because the porosity distribution of the microstructure is known from the above mentioned microstructure development model. Pores of radius less than $r_s$ would be completely filled, while the other pores would be empty. Thus, the model gives the saturation of pores by integrating the total pores volume from zero to $r_s$. The pores include physically adsorbed water in their solid walls. In the model, the adsorbed layer is idealized based on the modified BET theory (Hillerborg 1985). The degree of moisture saturation in concrete is then given as the total of saturation in micro-pores consisting of capillary pores, gel pores and interlayer pores, and the volume of adsorbed layer. The adsorption-desorption hysteresis is explained as the inkbottle effect in the model. It is assumed that moisture can be trapped in inkbottle-shape pores owing to the complex geometrical characteristics of the microstructure. During the wetting stage, as relative humidity increases, liquid water can gradually condense in the smaller pores. On the other hand, during the drying stage, evaporation of moisture occurs from larger pores. During virgin drying, the evaporation of trapped water in larger inkbottle-shaped pores can be inhibited due to connection to smaller pores. The result is an apparent adsorption-desorption hysteresis. In the model, the saturation in monotonic drying is idealized based on the inkbottle effect. Since the stability of the condensed water in inkbottle-shaped pores is strongly dependent on the ambient temperature according to experimental findings, the temperature sensitivity in saturation-humidity paths is implemented (Ishida et al. 2007). The hysteresis of interlayer water is also modeled based on the experiments that revealed the hysteresis has a temperature dependence, too (Ishida et al. 2007).

Next, the moisture transport model is described. Moisture transport in a porous body is driven by the pore pressure gradient and the temperature gradient. Ishida et al. (2007) proposed a formulation of vapor flux that can be applied to arbitrary temperature conditions. The model takes into account of factors reducing the apparent diffusivity of vapor, such as the complexity of the pore network. The vapor flux is driven by the gradient of absolute vapor density $\rho_v$ of the system, instead of by relative humidity.

### 2.2 Mesoscopic modeling for time-dependent behaviour of concrete

Recently, a project has been in progress, which couples the microscopic thermo-physical information obtained from DuCOM with macroscopic structural information such as stress, strain, deformation, cracking and others computed by a 3D FEM structural system named COM3.
One of the targets of this project is the development of a multi-scale constitutive model that can simulate the time-dependent deformation of concrete such as shrinkage and creep based on the hydration reaction, pore structure and moisture state in the pores (Maekawa et al. 2003, Zhu et al. 2004, Asamoto et al. 2006). Outline of the multi-scale constitutive model is described below.

In the model, concrete is idealized as a two-phase composite with aggregate and hardening cement paste. The aggregates are modeled as elastic particles with a stiffness determined by their density, while the hardening of cement paste is expressed by the progressive formation of finite fictitious clusters as the hydration proceeds based on solidification theory (Bazant & Prasannan 1989). The number of clusters is dependent on the degree of hydration as obtained from DuCOM. The stress in the hardening paste is given as the summation of stresses applied to all clusters. Both volumetric terms and deviation of stress and strain are computed, taking into account of interactions between aggregate particles and the cement paste matrix.

According to the model, the mechanical behavior of a fictitious cluster is associated with the thermodynamic state of moisture in micro-pores such as capillary pores, gel pores and interlayer pores. Recently, moisture migration in gel pores was divided into moisture transport through the internal pores of C-S-H gel grains and water in motion within the inter-particle spaces of hydrate micro-products (Asamoto et al. 2006). The motion of moisture in capillary and gel pores is idealized based on seepage theory, which describes moisture in the pores migrating gradually under sustained stress.

Since the rate of motion depends on pore size, it takes longer for moisture in smaller pores to reach the equilibrium. The moisture in interlayer pores diffuses and causes the volumetric change only at high temperature. Each component is composed of an elastic spring, a dashpot and a slider whose parameters are determined by temperature, moisture saturation, pore size distribution and other factors of the hardening cement paste.

The driving force behind volumetric change in the model is assumed to be related to capillary pressure and solid surface energy. These phenomena are computed, coupling with the thermodynamic state of moisture in the micro-pores. The capillary force is calculated based on the Laplace equation, the Kelvin equation and the degree of saturation of capillary and gel pores subjected to pore pressure. Shrinkage under a relatively high humidity condition is caused mainly by the capillary force in the model. On the other hand, in the case of a relatively low humidity condition, the increase in the solid surface energy of gel particles due to desorption of water is idealized as the main mechanism to drive the shrinkage. By coupling the above volumetric stress depending on moisture states in pores with the C-S-H skeleton stress, the equilibrium between skeleton stress and external loading can be satisfied. Thus, the time-dependent deformation can be computed according to the boundary conditions without conventional classification such as autogenous/drying and basic/drying creep. Currently, the model is able to reasonably simulate the time-dependent deformation of cementitious composites under arbitrary boundary conditions (Zhu et al. 2004, Asamoto et al. 2006). Fig.2 summarizes DuCOM and multi-scale constitutive model concept.
Some of model components, especially related with the phenomena in micro-pores, are dependent on various macroscopic assumptions arising from experiments. Regarding CCBM, model parameters of hydration process are determined according to the experimental data of X-ray/Rietvel analysis, DSC, and MIP with several assumptions for amorphous phase component. And the accuracy of the model is discussed with experimental data of ig. loss, calorimeter, and X-ray/internal standard method. In the case of DuCOM, the modeling of the temperature-dependent hydration process and microstructure formation of gel pores is based on indirect information obtained from the adiabatic temperature test and the thermogravimetric analysis. The hysteresis and the temperature sensitivity of moisture such as trapped water in inkbottle-shaped pores and interlayer water are simply idealized according to macroscopic experimental findings. The ultimate recoverable and irrecoverable time-dependent deformation in the model is also based on the various experimental data of shrinkage and creep. The hydration, microstructure, moisture states, and time-dependent deformation in fine pores have been extensively studied over several decades, but it has been difficult to directly observe the phenomena and verify the theories, particularly at nanometer scale. Thus, the modeling must be postulated from macroscopic information and remain empirical. According to the model, the computational prediction can give a good agreement with the phenomena that have been experienced, while the unusual extending conditions and phenomena in the far future are hardly predicted at convincing level. In order to predict the long-term durability of RC structures and to utilize a variety of cementitious materials for various structures, the intrinsic micro information from experimental analysis is necessary.

Recent remarkable development of the experimental technique is expected to reveal the above unclear microphysical phenomena. It may enable us to investigate the microstructure and moisture behavior at micrometer and nanometer scale. Directly observing the time-dependent behavior of cement hydrates in fine pores, each phenomenon can be clarified and the various theories assuming from macroscopic information can be verified. Since the molecule behavior is dominant at nanometer scale and should be modeled not only by classical thermodynamics but also by molecular dynamics, statistical theories and others, the experimental studies are useful for idealizing the phenomena at nanometer level. Identifying the dominant phenomenon and physics in each scale for the time-dependent behavior at macro-scale, the modeling of the time-dependency of cement hydrate at the multi-scale is possible and enables to predict the deterioration process of RC structures under arbitrary boundary conditions. Thus, as shown in Fig.3, the linkage between the phenomenon, experimental analysis and modeling based on theories at each scale is quite important. In the next chapter, the state-of-the-art of experimental techniques to verify the theory at each scale will be described.

![Phenomena](image)

**Characterization of structure**
- Neutron Radiography (1mm~10nm)
- Digital & 3D laser microscope (1mm~1μm)
- Internal pore humidity sensor
- Mercury intrusion porosimetry (1μm~10nm)
- Gas adsorption isotherm (1μm~10nm)
- SEM (10μm~10nm)
- SAS (1μm~1nm)
- NMR (10nm~1nm)

**Modeling**
- Pore pressure, Kelvin equation
- BET theory
- Munich model
- Spring and dashpot for visco-elasticity
- Dashpot and slider for visco-plasticity

Fig.3 Schematic illustration of the linkage of phenomena, characterization of structures and modeling
3 EXPERIMENTAL TECHNOLOGY AND METHODOLOGY TO MEASURE MICROSCOPIC INFORMATION OF CEMENTITIOUS MATERIAL

3.1 Propagation and distribution of micro-crack and moisture transport in micro-crack (1mm~1μm level)

3.1.1 Time-dependent behavior in micro-crack

The behavior of microcracks in cementitious materials has been extensively studied because the microcracks can affect the diffusivities of chloride ion, CO₂ and other harmful agents in concrete and they lead to the reduction of the durability. Gran (1995) reported an impregnation technique based on fluorescent ethanol that can be slowly replaced with the pore water. This technique is called as Fluorescent Liquid Replacement(FLR) technique and does not need traditional preparation procedures such as drying and evacuation that may induce microcracks. The FLR technique gives impregnation depths that are several orders of magnitude larger than the measurable impregnation obtained with traditional procedure using epoxy. According to him, the FLR technique can be used to observe the crack development due to loading, freezing/thawing, corrosion etc., even in the case of low W/C concrete and does not need traditional preparation procedures. Ammouche et al. (2000 & 2001) proposed an image analysis technique for the quantitative assessment of microcracks in cement-based materials. The highlighted microcracks and other microdefects of the polished samples were observed by using an optical microscope. The various micro information such as porosity, air bubble and microcracks was extracted from the observed image conducting a pretreatment of the color image and an automatic thresholding on the gray level histogram. The characteristics of the crack network were quantified using classical stereological methods. The technique enabled to determine the specific crack length, the degree of orientation and other crack pattern characteristics and seemed to lead to the basis of the micromechanical discussion.

Recently, the development of laser microscopes and digital microscopes has been progressive. The advantage of these technologies is to observe the phenomenon in micro-pores with high resolution and color under arbitrary conditions such as wetting conditions, while SEM, X-ray diffraction and others need some preprocessing of samples, for example, vacuum drying and evaporation coating. In the case of laser microscopes, 3D laser scanning technology has been advanced and enables us to examine the surface roughness of specimens at high resolution of nm level (http://www.keyence.co.jp/microscope/laser/index.jsp?). The observable 2D range of 3D laser microscopes and latest digital microscopes is about from 1 μm to 1 mm. Although these technologies are not applicable for studying phenomena at nanometer scale, it is expected that the propagation of micro-crack under sustained stress and the meniscus formation in micro-meter pores are observable because they are able to continuously measure such behavior. An example of observation on the surface of hardened cement paste by using the above mentioned 3D laser microscopes is shown in Fig.4.
3.1.2 Moisture transport around crack and between aggregate and cement paste matrix

Recently, Neutron Radiography (NR) technique was adopted for the observation of moisture transport behavior around crack. Kanematsu et al. (2007) observed moisture behavior in different crack width ranging from 0.05 to 0.3mm in the specimen whose size was 100 x 100 x 20mm. Relative water content in the concrete was also the one of parameters. According to the experiment, it was confirmed that the speed of penetration of moisture in the crack is affected by the relative water content in the concrete. The typical figure of NR is shown in Fig.5.

For mitigation of autogenous shrinkage, recently saturated porous aggregate was applied to the concrete of low water to binder ratio. For the performance-based design of these kinds of material and evaluation of concrete performance, effect of water in porous aggregate on the reduction of shrinkage of concrete should be evaluated. Regarding this aspect, Lura (2003) used ink for the observation of the effective distance from the aggregate surface, and this experiment revealed that the range within 1mm from the cement paste matrix to the aggregate surface was colored, and, at least, 1mm distance from the aggregate was supplied water from the aggregate. Bentz et al. (2006) used the X-ray tomography technique for getting the information of water distribution around saturated light weight aggregate. From this experiment, water was supplied to the position of 2mm away from the aggregate surface. Maruyama et al. (2007) also carried out a similar experiment using NR, which is shown in Fig.6. In this experiment, porous aggregate was limitated by hardened cement paste with W/C=0.55, and W/C of cement paste matrix was 0.30. Subtraction of water strength obtained by NR test, that the range of supplied water in hardening cement paste was 4mm from the surface of imitated aggregate was detected. Fig.6 shows the distribution of water strength of NR around cement paste matrix - aggregate interface.
3.2 Microstructure and moisture state in micro-
pores (1μm~10nm level)

3.2.1 Pore distribution and volume

The mercury intrusion porosimetry has been widely used to study the microstructure of hardened cement paste. It measures the volume of mercury which infiltrates into sample pores according to injection pressure. By converting the injection pressure of the test results into the cylindrical pore radius, and assuming the mercury intrusion volume as volume of the pores which corresponds to the cylindrical shaped pores, the relationship between the pore radius and volume can be obtained. This relationship is said to be the cumulative pore capacity curve and is the most basic relationship which describes the distribution characteristics of pores in the microstructure. The specific surface area of sample pores is also evaluated from the mercury intrusion porosimetry results. Based on the modeling which assumes the geometry as the cylindrical shape, specific surface area is evaluated as a total sum of pore surface of cylindrical shape.

A gas adsorption test is also an accepted methodology to examine the pore structure. It measures the specified volume of gas adsorption to adsorbent which it balances in relative humidity under an isothermal environment, that is, the test measures the adsorption isotherm. In the gas adsorption test, as well as the mercury intrusion porosimetry, the volume of gas adsorption corresponds to sample pore volume. There are various gases that can be used in the gas adsorption tests. From a viewpoint of microstructure evaluation, nitrogen is often used because it is an inert gas. Kelvin equation is generally used to analyze the pore size distribution from the adsorption isotherm. Applying the Kelvin equation to the results of the adsorption isotherm relationship, the accumulated pore capacity curve similar to the mercury intrusion porosimetry is gained. The adsorption volume is obtained with the volumetric method, while the mercury intrusion volume in the mercury intrusion porosimetry directly corresponds to the volume of pores.

The BET theory is used for evaluating the specific surface area based on the adsorption isotherm. The theory is expanded from the Langmuir theory and multilayer adsorption state is considered, assuming the adsorption site on the adsorbent. The adsorption isotherm expressed with the BET theory nearly corresponds to the II type adsorption isotherm. The range of relative humidity in which the BET theory is accepted is about from h=0.05 to 0.35 in the case of hardened cement paste. The monolayer adsorption volume and interaction constant are determined from the results of the BET plot within this range. In Fig.7, the solid line in the graph is the fitting results of the relative humidity range of h=0.05 to 0.35 in a straight line. The monolayer adsorption volume, specific surface area and interaction constant are calculated based on the fitting results and are marked in each graph.

Davis (1984) showed the correlation of the BET specific surface area using nitrogen adsorption isotherm and the mercury intrusion porosimetry by targeting a variety of samples. Davis pointed out that the mercury intrusion porosimetry gives a larger specific surface area than the BET methods does. However, the results in both methods are not so different and they can be directly compared for practical purposes. Fig.8 shows the comparison of the specific surface of hardened cement paste measured with these two different methods. In these results, the mercury intrusion methods tend to give larger specific surface area than the BET method does.

![Fig.7 BET plot of hardened cement paste; N2 adsorption (Chiba Institute of Technology, Utsumi Lab.)](image-url)
Samples to be used in the mercury intrusion porosimetry and gas adsorption tests need to be dried before the tests. Gallé (2001) studied porosity obtained in the mercury intrusion porosimetry results at the maximum injection pressure of 413 MPa by targeting the dried sample using each drying method. It was found that samples executed in an oven-drying at 105 ℃ have the highest porosity in the mercury intrusion porosimetry. Juenger et al. (2001) deliberated the differences of the BET specific surface area and the pore volume based on the drying conditions targeting the nitrogen adsorption test. According to their experimental results, the oven drying at 105 ℃ has the lowest BET specific surface area compared to that of D-dry and a combination of methanol elution and D-dry in the nitrogen adsorption. The measured porosity is dependent on not only test method but also pre-drying conditions.

Odler (2003) deliberated on the difference of the BET specific surface area depending on each type of adsorbate. Fig. 9 shows the summarized results of the BET specific surface of H₂O adsorption and N₂ adsorption described in references (Odler 2003, Mikhail & Abo-El-Enel 1972, Mikhail & Selim 1966). From these results, it is found that water vapor adsorption evaluates the higher specific surface area than that of the nitrogen adsorption. Feldman and Sereda (1968) explained the difference in the specific surface area between water vapor adsorption and nitrogen adsorption in terms of the filling of interlayer pores only by water. Daimon et al. (1977) pointed out that the only water could absorb into intercrystallite pore of C-S-H gel and interlayer pores, while nitrogen cannot enter such small pores. Recently, Jennings and his co-workers (Thomas et al. 1999, Jennings 2000, Tennis & Jennings 2000) suggested that the calcium silicate hydrate (C-S-H) in cement paste is classified into two types: a high density C-S-H (HD C-S-H) and a low density C-S-H (LD C-S-H). HD C-S-H is made of densely packed particles into which nitrogen cannot penetrate. Particles of LD C-S-H are not packed as tightly as those of HD C-S-H, and nitrogen can penetrate partially into this structure. On the other hand, water can infiltrate into both types of C-S-H and as a result, the difference in the specific surface area by vapor adsorption from nitrogen adsorption arises. There is, however, no unified explanation about the variation of surface area due to adsorbents.

Due to the characteristic and theory of each test method, the range of pore size of the analysis target is specified. In the case of mercury intrusion porosimetry, the pore radius in which mercury can be infiltrated shall be specified depending on the injection pressure. Currently, equipment which can pressurize up to 400 MPa is widely used, and the minimum pore radius which the mercury can infiltrate during pressurization is about \( r = 1.8 \times 10^{-9} \) [m] according to Washburn equation. That is, based on the maximum injection pressure of the equipment to be used, the minimum limit value of the theoretically evaluable pore radius in mercury intrusion porosimetry is specified.

On the other hand, the evaluable minimum pore diameter in the gas adsorption test is the minimum value of pore diameter whose molecule diameter to be used can be detected from the gas adsorption tests. Generally, since adsorption potential of micro pores with less than \( 2.0 \times 10^{-9} \) [m] is extremely large, it is thought that Kelvin equation is not
approved in such fine pores. Dubinin equation (Dubinin 1960) is also used for evaluating micro pore size. In gas adsorption test, the maximum value of pore diameter is theoretically infinitely large. At the area close to saturated vapor pressure, however, the experimental error is perceptively sensitive to temperature control and pressure control, and practically, pore radius range which can be evaluated with Kelvin equation is assumed to be about from 1 to 100 nm (see Fig.10).

3.2.2 Internal humidity

Grasley et al. (2007 & 2006) developed a new internal relative humidity measurement system and proposed a model to predict drying stress gradient in concrete. The system involved embedding of a small, and digital, RH and temperature sensor in a small plastic tube with Gore-Tex caps into fresh concrete. The sensors were a capacitive type RH sensor and used a thermistor to measure temperature. In the system, the internal humidity could be measured at the accuracy of ±1.8% (when RH is less than 80%) and the temperature sensor had an accuracy of ±0.3°C (at 20°C). Using the system, the potential free shrinkage strain based on Kelvin-Laplace equation was calculated and the drying stress induced by internal and external restraint at any point across the cross-section was determined. The model revealed that the tensile stress in the surface layer routinely exceeded the tensile strength of concrete in drying concrete, even in the case of free shrinkage.

Ceramic humidity sensor is also used to measure internal pore humidity in concrete. When water vapor within a porous ceramic material diffuses and is adsorbed on its crystal surface, moisture dissociates into hydroxyl and proton on the surface, reducing the electric resistance of the ceramic. The humidity-sensing mechanism of a humidity sensor utilizes this phenomenon, ionic conduction by water adsorption. Among the wide variety of ceramic humidity sensors available with various materials, sensors made with NASICON ceramic materials have the potential to be used as humidity sensors for concrete, as they show a high ionic conductivity while having relatively high durability and long-term stability (Yagi & Saiki 1991, Ozawa et al. 2007). Fig.11 shows the configuration of a sensor element, which consists of an alumina substrate on which a ceramic moisture-sensitive film is deposited between two electrodes. With its body being small and thin (5 x 13 x 0.8 mm) as shown in Fig.12, this type of sensor embedded in concrete allows measurement of humidity in concrete without significantly disturbing the humidity profile of concrete.

The measurement range and accuracy of this sensor are 20 to 90% RH and ±3 to 5%, respectively, within the effective temperature range of 0 to 50°C. When embedding this sensor in concrete, it is necessary to calibrate its sensing characteristics beforehand by conducting controlled humidity testing, as various ions contained in the moisture in concrete can affect the ion conduction. Fig.13 and Fig.14 show typical sensing characteristics of this sensor in air and in concrete.

### Fig.10 Measurement range of mercury porosimetry and gas adsorption

<table>
<thead>
<tr>
<th>r [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1x10⁻¹⁰</td>
</tr>
<tr>
<td>micropore</td>
</tr>
<tr>
<td>○: H₂O Molecular radius</td>
</tr>
<tr>
<td>□: N₂ Molecular radius</td>
</tr>
</tbody>
</table>

Mercury porosimetry (p_{max}=400MPa, Washburn eq.)

Gas adsorption (Dubinin eq.)

Gas adsorption (Kelvin eq.)
respectively, obtained from controlled humidity testing for 400 days. Fig.13 reveals that the measurement error tends to increase as the humidity decreases in air. In concrete, however, the measurement error tends to increase both in the high and low humidity ranges as shown in Fig.14. When using this sensor, the measured data should be corrected accordingly based on the recognized sensing characteristics.

Fig.15 shows typical humidity measurements at depths of 5, 10, and 50 mm from the surface of a concrete specimen with a cross-sectional size of 10 by 10 mm.

3.3 Measurable information in nano-pores

The microphysical information in nano-pores is considerable to evaluate the durability of concrete structures because it is known that the moisture in fine pores greatly affects long-term creep, shrinkage under low humidity and others. It has been, however, very difficult to measure or observe the structure and the moisture behavior in nano-pores because the preprocess, for example, vacuum drying and evaporation coating for experimental technologies such as SEM, X-ray diffraction and others can cause the destruction of the nano-pores structure and dispersion of moisture in nano-pores. Recently, the study focusing on the microstructure and the moisture behavior in pores of nanomaterial scale has been progressive using latest experimental technologies.

Nuclear Magnetic Resonance (NMR) is one of interesting technologies to be able to investigate the
time-dependent behavior in fine unsaturated and saturated pores. Valckenborg et al. (2001) examined the drying process and the pore water distribution of saturated mortar by means of NMR. It was found that the moisture cannot be extracted from gel pores (<10nm) until the water in capillary pores (10-1000nm) is drained as shown in Fig.16. Hazrati et al. (2002) measured water content profiles using proton nuclear magnetic resonance imaging (NMRI) technique during the capillary absorption of water in unsaturated mortar samples. The water diffusivity coefficient obtained in the experiment is strongly dependent on the water content and can be approximated by the sum of two exponential functions. Heijden et al. (2007) built a dedicated NMR setup in order to study the moisture transport in heated concrete. One-dimensional moisture profiles in fire-clay brick, calcium-silicate brick and concrete during heating were measured and compared with their model. Aono et al. (2007) investigated the change of microstructure of hardened cement paste due to drying and drying-wetting cycle using MIP, Archimedian method and Si29-NMR. It was found that the pore distribution is coarser due to drying because the condensation polymerization of silicate anion is progressive during drying.

Small-angle scattering techniques (SAS) using neutrons (SANS) or X-rays (SAXS) are also powerful method to study the microstructure of hardening cement paste. The angular profile of the small-angle scattered intensity from the sample is effectively a Fourier transform of the microstructure and can in principle be analyzed to determine the size distribution, volume fraction, and shape of the scattering features (Jennings et al. 2008). The advantage of the technique is also to examine the microstructure in saturated state. Thomas et al. (1998) reported the variation on the surface area of OPC with aging by SANS (Allen & Thomas 2007). They found that the surface area increases slightly with long-term curing and is greater in the case of higher water-to-cement ratio. In addition, it was suggested that the dense and inner product of C-S-H cannot be observed by SANS or SAXS and they interpreted the experimental findings as evidence for two-different morphologies of C-S-H. Allen et al. (2007) investigated the mean formula and mass density of the nanoscale C-S-H gel particles in hydrating cement by combining SANS and SAXS data and by exploiting the hydrogen/deuterium neutron isotope effect both in water and methanol. They have established a C-S-H formula \((\text{CaO})_{1.70} (\text{SiO}_2)(\text{H}_2\text{O})_{1.80}\) with a mass of density 2.604Mgm\(^{-3}\) and a water mass fraction of 0.174.

Studies by NMR and SAS techniques on microstructure and moisture behavior in micro-pores have been in progress recently. The nanoscale information may lead to further modeling of time-dependent behavior of cementitious materials under arbitrary conditions.
3.4 Summary of current technologies and future prospects

As described above, recent development of experimental techniques to study microphysical information has been remarkable and progressive. It is expected that the development enables us to reveal the classical assumption about time-dependent behavior of cementitious materials and to enhance the numerical models. Some of techniques, however, show different results even in the same measuring target. Since these differences appear to be caused by the characteristic and limitation of each test method, it is indispensable to understand the technique correctly and to analyze the varying test results comprehensively.

In order to verify various theories about micromechanics of cementitious materials, study on the microstructure related with moisture behavior in micro-pores is essential because hydration process, microstructure formation, transportation of ion, shrinkage and creep are strongly affected by moisture state in pores. Currently, NMR or SAS seems to be one of the effective techniques to examine such time-dependent behavior under various conditions. For further investigation for microphysical information, the application of various experimental techniques should be taken into account. Thus, the collaborative studies with researchers in other scientific fields such as chemical engineering, biotechnical engineering, nano-technology and others are necessary.

4 MATHEMATICAL MODELING FOR TIME-DEPENDENT BEHAVIOR OF CONCRETE COMPOSITES BASED ON MESO-MACROSCOPIC APPROACH

4.1 Effect of aggregates and interaction with cement paste phase (1μm ~ 1-10mm level)

Aggregates are used to reduce the shrinkage of concrete by restraining the shrinkage of the matrix paste. The roles of the type and amount of aggregate to reduce shrinkage were addressed by Pickett (1956), Roper (1959), and Hansen & Nielsen (1965) as shown in Fig.18. They also indicated that some types of aggregates often exhibit a large degree of shrinkage. Consequently, the selection of the type of aggregate can have a significant effect on the long-term behavior of a concrete structure. The water absorption of aggregates is directly related to the shrinkage strain of concrete in the same types of rocks. However, this correlation decreases when different types of rocks are used (Snowdon & Edwards 1962). It is well known that artificial lightweight aggregate does not exhibit so much large shrinkage strain in spite of its large water absorption ratio. Fujiwara (1984) found that internal specific surface areas (SSAs) of coarse aggregates measured by the BET method using nitrogen were in close agreement with the shrinkage strains, as shown in Fig.19. Larger SSA will be associated with a greater surface energy or disjoining pressure (Powers 1965), resulting in a higher shrinkage (or expansion) strain. On the other hands, a previous research showed that the measured SSAs vary with the adsorbates used (Brunauer et al. 1938). Hence, BET surface area of the shrinking aggregate using water vapor will be reasonable information. Fig.20 shows that the SSAs using water vapor have a good agreement with concrete shrinkage strains with various kinds of aggregates (Imamoto & Arai 2007). Furthermore, the evaluation of the shrinkage behavior from the viewpoint of the SSA will provide a perspective for new mixture design methodologies for concrete.
Recently, it was reported that a prestressed reinforced concrete (PRC) bridge in Japan had suffered severe cracking of RC member surfaces even though only three years had passed after the construction. A number of cracks were found on the surface of the RC members and vertical cracks were observed in the web even though it was horizontally prestressed. According to the emergency committee set up by JSCE, one of the reasons for this serious damage might have been excessive shrinkage of the concrete (JSCE Concrete Committee 2005). Since such serious concrete shrinkage was thought to be associated with aggregate properties, the committee studied the influence of aggregate properties on concrete shrinkage. Shrinkage experiments of three types of concretes with different types of aggregates were conducted. The aggregates for mix A were from the same source as used for the bridge concrete, while the aggregates for mix B were standard ones extracted from a different site. The sand in mix C was standard but the gravel was the same as that in mix A. The test results are shown in Fig.21. The concrete with the same type of aggregates as that of the PRC bridge exhibits extremely large shrinkage, about twice larger than that of concrete containing standard aggregates. Although little attention has been paid to the characteristics of aggregates themselves in the design process considering concrete mix proportion, structure size and boundary conditions, the above mentioned findings suggested that the effect of each property on mechanical behavior of concrete should be studied and taken into account in the design.

Asamoto et al. (2008) investigated quantitatively the influence of various aggregate properties on concrete shrinkage behavior using the multi-scale constitutive model described in Section 2.2. One of the aggregate properties could be possibly responsible for the large shrinkage of the bridge concrete. For example, the targeted aggregate had relatively softer elastic modulus in comparison with normal aggregate, (JSCE concrete committee 2005). According to the numerical simulation, however, such large shrinkage due to the soft stiffness of aggregate takes place only in the case of extremely low Young’s modulus (1.0GPa) as shown in Fig.22. Since aggregate shrinkage appeared to be dominant effect on concrete shrinkage as mentioned above, an aggregate shrinkage model was proposed based on an earlier pioneering research (Fujiwara 1984) and implemented in the multi-scale constitutive model in order to analytically examine the influence of aggregate shrinkage on concrete shrinkage. This demonstrated that the significant increase in concrete shrinkage could be calculated when aggregate shrinkage related to aggregate moisture states was taken into account as shown in Fig.23. According to the numerical simulation, it was also suggested that aggregate shrinkage was likely to cause the remarkable variation in concrete shrinkage.
4.2 Thermal stress and crack risk assessment of massive concrete (1cm ~ 1-10m level)

Technology for estimating the temperature cracking of massive concrete structures due to the hydration heat of cement has been dramatically developed in Japan over the past two decades, beginning with the publication of the 1986 edition of the Standard Specifications for Design and Construction of Concrete Structures by the Japan Society of Civil Engineers (JSCE 1986). These specifications introduced a quantitative index to the risk of thermal cracking, i.e. “thermal cracking index”. In current standard specification (JSCE 2002), the index including effect of drying shrinkage and autogeneous shrinkage, represented by the following expression is used.

\[
I_{cr}(t) = \frac{f(t)}{\sigma_{t}(t)} \geq \gamma_{cr}
\]

(1)

where, \(f(t)\): tensile strength of concrete and \(\sigma_{t}(t)\): maximum thermal stress in tension. The thermal cracking index should satisfy the safety factor \(\gamma_{cr}\) for the required functions and durability of the concrete structures as shown in Eq.(2).

Fig.22 Computed results of shrinkage with aggregates of varying Young’s modulus

Fig.23 Computed results considering aggregate shrinkage (maximum aggregate shrinkage is assumed to be 1400 μ)

Fig.24 represents the relationship between probability of cracking \(P_{f}\) and safety factor \(\gamma_{cr}\). For the ordinary reinforced concrete structures, the reference values of safety factors are provided according to the level of cracking risk as described below.

1) -1.75 and higher: when cracking is prevented.
2) -1.45 and higher: number of cracks is controlled as much as possible.
3) -1.00 and higher: when the crack width is controlled while allowing cracking.

In the Fig.24, the probability is larger than 50% when the safety value is 1.0, because the cracking index is evaluated from the tensile strength of the test cylinder that can be different form that of the real concrete structure. To calculate the cracking index, a specific procedure for determining the probability of cracking is also provided in the specifications. As a simple method of analyzing thermal stress, CP method is recommended in the specification, which was proposed by Japan Concrete Institute in 1985 (JCI 1985). CP method is a practically useful method allowing incorporation of the concrete placing process.

Fig.25 shows the relative proportion of analytical methods for thermal stress in Japan. The CP method
is used as the most practically method in Japan, because the thermal stress can be calculated easily and two-dimensionally for wall structures. In the case of FEM, three dimensional analysis is better for simulating such type of structures as well.

Fig.26 shows the comparative ratio of thermal crack control methods in Japan. As shown in Fig.26, selection of low-heat type cement and reduction of cement content are often adapted for preventing thermal cracking. The crack-inducing joint is also often applied to wall structures. The effective method according to the structure type is examined based on thermal crack index determined by JSCE specifications.

Next, a recent analytical system named JCMAC3 in Japan is described. The program can deal with not only thermal strain but also other initial strain at an early age comprehensively and three-dimensionally. Thermal strain, autogeneous shrinkage and drying shrinkage can be taken into account as initial strain at an early age (Fig.27). The initial strain is computed based on the recent research progress in Japan.

A discrete FEM solving three-dimensional heat conduction equation gives temperature distribution at each time-step and thermal strain is obtained. Drying shrinkage is computed by moisture transport analysis in the system. The moisture transport is idealized in Eq.(3) (Kagohashi et al. 2000). Vapor permeability and vapor capacity are dependent on relative humidity and lead to non-linear analysis.

![Fig.24 Relationship between Probability of cracking and safety factor](image1)

![Fig.25 Relative proportion of analytical methods for thermal stress in Japan (Tanabe 2004)](image2)

![Fig.26 Comparative ratio of thermal crack control methods in Japan (Tanabe 2004)](image3)

![Fig.27 Outline of JCMAC3](image4)
where, \( J \): moisture flux(g/h), \( \lambda_p \): vapor permeability(g/h-m-mmHg), \( dp/dn \): gradient of vapor, \( (dq/dn) \): vapor capacity(g/h-m\textsuperscript{3}-mmHg), \( q \): vapor density(g/m\textsuperscript{3}), \( n \): direction cosine, \( (\partial q/\partial t) \): varying vapor transfer density due to hydration reaction(g/h-m\textsuperscript{3}), \( P \): vapor pressure at the surface(mmHg), \( P_0 \): surrounding vapor pressure, \( \alpha \): evaporation ratio(g/m\textsuperscript{2}-mmHg) .Autogeneous shrinkage is determined from Eq.(4) (JSCE 2002) and distributed uniformly in each element.

\[
\varepsilon'_a(t) = \gamma \varepsilon'_{arc} \left[ 1 - \exp \left( -a(t-t_s)^b \right) \right] \tag{4}
\]

\( \varepsilon'_{arc} \): autogeneous shrinkage strain of concrete from start of setting \( t_s \) to age \( t \times 10^{-6} \), \( \varepsilon'_{arc} \): final value of shrinkage strain\( t \times 10^{-6} \), \( \gamma \): coefficient representing the influence of cement type, \( a \) and \( b \): coefficients representing the characteristics of autogeneous shrinkage progress.

JCMAC3 can comprehensively simulate initial strain at an early age including thermal strain, autogeneous shrinkage and drying shrinkage and lead to stress analysis at an early age. The addition of elements and change of heat transfer interface properties due to casting are possible. In JCMAC3, creep strain is calculated based on rate type theory (Ando et al. 1996), while the influence of creep is taken into account by using effective elastic modulus determined from the increment of effective strain at each step in the case of CP method. In JCMAC3, creep strain is determined by the strain at previous step.

Dirichlet series creep function is used for the computation as shown in Eq.(5).

\[
\phi(t, \tau) = \sum_{i=1}^{N} \frac{1}{C_i(\tau)} \left[ 1 - \exp \left( \frac{t - \tau}{\mu_i} \right) \right] \tag{5}
\]

where, \( C(\tau) \): function of time, \( \mu_i \): delaying time. Fig.28 represents the physical meaning. \( N \) Kelvin type creep models are connected in series and each dashpot works behind \( \mu_i \). Then, total visco-elastic strain is regarded as summation of creep strain in each dashpot. The increment of creep strain in three dimension \( \Delta \{\varepsilon^{cr}\} \) is idealized using stress increment \( \Delta \{\sigma^{cr}\} \).

\[
\Delta \{\varepsilon^{cr}\} = [L_1] \Delta \{\sigma^{cr}\} + \{L_2\} \tag{6}
\]

\[
\{L_2\} = \sum_{i=1}^{N} \left( 1 - \exp(-\Delta y_i) \right) \{q(i, t)\} \tag{8}
\]

\[
\{q(i, t)\} = \{q(i, t_s)\} \exp(-\Delta y_i) + \frac{\lambda_i}{C_i(t_{r+1/2})} \Delta \{\sigma\} \tag{9}
\]

\[
\Delta y_i = (t_{r+1} - t_r) / \tau_i \quad , \quad \frac{1}{E''} = \sum_{i=1}^{N} \frac{1 - \lambda_i}{C_i(t_{r+1/2})} \quad , \quad \lambda_i = \frac{1 - \exp(-\Delta y_i)}{\Delta y_i} \tag{10}
\]
where, \( \nu_{cr} \) is creep Poisson ratio. At step \( t = t_r + 1 \), \( \{L_2\} \) can be obtained from \( \{q(t_r)\} \) because \( [L_1] \) in Eq.(6) is known. Based on \( \{q(t_r)\} \) at previous step, the relationship between stress and strain considering visco-elastic effect can be computed. Dashpot parameters, \( C_i(t_r+1/2) \) and \( \mu_i \) can be determined by curve-fitting the creep function with Eq.(6).

In JCMAC3, computer memory can be effectively used by adapting the incremental creep model, so the analysis of massive structure having many elements is possible. In addition, there are several mathematical solvers that can solve simultaneous linear equations very fast. JCAMC3 is expected to be a useful tool for simulation of cracking in concrete, since it implements recent research results and has very practical aspect.

5 MATHEMATICAL MODELING FOR TIME-DEPENDENT BEHAVIOR OF CRACKED STRUCTURAL CONCRETE

5.1 Thermal crack control (1mm ~ 1cm level)

In the section 4.2, the evaluation for the crack risk of massive concrete with the thermal cracking index was described. In this section, the thermal crack control design and its analytical method after cracked are introduced from a practical point of view. The relationship between the thermal cracking index and the maximum crack width is given in JSCE guidelines for concrete (JSCE 2002), according to the reinforcement ratio, as shown in Fig.29. This relationship was proposed based upon the experimental results. The relationship enables us to determine the appropriate reinforcement ratio to control the maximum crack width based on the crack index.

On the other hand, Japan Concrete Institute proposed the following three kinds of analytical methods that extend the CP method.

1) Extended CP method (For calculating temperature, stress, and crack width).
2) Surface crack CP method (For tracing the crack propagation on the concrete surface).
3) Hybrid CP/FEM method (Focusing on the part where detailed information required).

According to the methods, it is possible to calculate crack propagation and crack width history. JCI implemented the above methods in the program named ‘JCMAC2’ that was released in the market for concrete engineers. The three analytical methods are summarized below.

5.1.1 Extended CP method (JCI 1992)

To directly calculate the crack width, the Extended CP method was developed by advancing the CP method. In the method, restraining body and restrained body are focused on and only the crack which penetrates over the restrained body is dealt with. It is postulated that the crack occurs when the thermal stress exceeds the tensile strength of concrete.

The procedure of Extended CP method is shown in Fig.30. The calculation is carried out in two steps. In the first step, the stress distribution in the restrained body is calculated ignoring the deformation of the restraining body. Here, Bernoulli-Euler theory is used. In other words, the stress transfer between the reinforcement and the concrete in the restrained body is calculated by the CP method, ignoring the deformation of the restraining body. The total stress balance in the whole section including the restraining body is taken into account in the second step. Bernoulli-Euler theory is also applied to the section of the entire system. The stress is computed by using CP method again. Then, the redistribution of the stress to balance the total stress in the whole system of the restrained and restraining bodies is calculated. As a result, the discontinuous plane is formed between the restrained body and the restraining body.

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![Fig.29 Relationship between cracking index and maximum crack width](image-url)
5.1.2 Surface crack CP method (JCI 2003)

Extended CP method is based on the assumption that once the crack occurs, it penetrates over the cross section. Thus, it cannot simulate the gradual crack propagation such as surface cracking. The surface crack CP method (JCI 2003) was developed in 2003, in order to calculate the crack depth from the surface of concrete in each age. This method was also developed based on the CP method. Whereas Extended CP method assumes that the height (or depth) of stress release zone is always constant, the height of the zone of surface crack CP method can increase according to the crack propagation. To determine the height, the calculation can be repeated as changing the stress release zone until the thermal stress is less than the tensile strength in the whole zone.

5.1.3 Hybrid CP/FEM method (JCI 2003)

The hybrid CP/FEM method combining the CP method and finite element method (FEM) was developed and commercialized with a program to analyze the temperature rise due to hydration reaction developed by Suzuki et al. (1990). In this hybrid CP/FEM method, the detailed structural responses such as stress and strain distribution in each element, cracking pattern and others can be simulated by nonlinear 3D FEM analysis, while the simple information can be obtained by the CP method based on the Bernoulli-Euler theory as shown in Fig. 31. The crack width can be computed considering not only internal penetration of crack but also the propagation at the surface and three-dimensional effect of steel confinement.

Fig.30 Flow of Extended CP Method

Fig.31 Concept of Hybrid CP/FEM Method
5.2 Time-dependent structural damage under sustained and repeated loads (1cm ~ 1m level)

The meso-scale modeling of concrete brings about volumetric strain related to hydration and drying, and the composite material based strain is forwarded to post-cracking structural analyses as shown in Fig.32. Here, the time-dependency of tension stiffening and softening after cracking is indispensable for most macroscopic analysis. As shown in Fig.33, space-averaged tensile strain under sustained forces increases with the progress of time. This nonlinearity is due to both time-dependent local bond and tensile creep of concrete continuum between cracks (Maekawa et al. 2006). Some research efforts have been addressed to the time-dependent modeling of local bond or macroscopic tension stiffening.

Fig.34 shows an example of post-cracking creep deflection of RC beams in flexure and the time-dependent creep analysis with a time-dependent tension stiffening model. The free-stress shrinkage strain is computed in space according to the loss of moisture under the drying state. The moisture migration is also computed based upon the micropore structural analysis. In flexure, the time-dependent curvature is governed by the flexural tension creep since the neutral axis is closer to the compression fiber. Generally speaking, the creep deflection is so large compared to the one of pre-cracking creep responses. Thus, the multi-scale structural analysis can be a versatile tool for prediction of long-term performance of RC members under ambient conditions.

This multi-scale analysis can be applied to the performance assessment of existing structures including initial defects (see Fig.35). It is reported that the time-dependent deflection is accelerated by the presence of initial damages around the anchorage zones and the increasing risk of creep failure is pointed out (Toongoenthong & Maekawa 2005). The potential of the multi-scale analysis is thought to be high owing to its versatility. The multi-scale approach is being applied to the nonlinear analysis of structures under high cycle fatigue loads.

It must be noted that the time-dependency is not negligible for fatigue as shown in Fig.36. As a matter of fact, the apparent fatigue life of materials and structures is also dependent on the rate of stress and/or strain. Under large amplitude of stresses, concrete is subjected to higher rate of creep. Then, the time-dependent damage is also included as well as the effect of stress repetition. On the other hand, the fatigue constitutive modeling has to include the time-factor (Maekawa & Toongoenthong 2006).

Fig.37 shows a high cyclic load response of RC beams in combined stress condition of flexure and shear. Recently, the direct path-integral scheme has been available for fatigue simulation similar to the nonlinear seismic response analysis. The simulation can be applied to the case under moving loads as well as the pulsation of a fixed point loading (Gebreyouhannes et al. 2007).

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**Fig.32 Effect of shrinkage strain on local and averaged stress profile**

- **Detailed method to use local free shrinkage strain in space**
- **Simplified method to use section-averaged shrinkage strain + equivalent tensile strength**
Fig. 33 Computed and experimental post-cracking tensile creep of RC

Fig. 34 Creep deflection of slab and the effect of shrinkage
Fig. 35 Shear fatigue response of RC beam and S-N curves for fixed pulsation and moving loads.

Fig. 36 Computed S-N diagram and stress-rate effect of fatigue compressive strength of concrete.

(a) Stress amplitude effect
(b) Stress-rate effect

Fig. 37 Shear fatigue response of RC beam and S-N curves for fixed pulsation and Moving loads.
CONCLUDING REMARKS

This paper provided an overview of mathematical models for time-dependent behaviour of cementitious materials and the following concluding remarks were obtained:

1) Since the cementitious materials have complex and multi-scale structures, a hierarchic system of at least three different levels needs to be introduced for linking the observed behaviour with the material structure and real mechanisms.

2) For linking the various aspects of the observed behaviour on different levels, conceptual modeling to integrate them into a general computational framework based on mathematical models is important.

3) By linking the observed behaviour of cementitious materials with details of the material structure and with real mechanisms, experimental results can be interpreted on a more general basis and development of various advanced technologies can contribute to the improvement of the mathematical models.

4) Mathematical models based on the material structure and real mechanisms are very useful to predict time-dependent behaviour and long-term performance of concrete structures.

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