



## Advances in multi-scale simulation of hygro-thermo- mechanical deformation behavior of structural concrete

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### Abstract

*This paper presents theoretical and numerical state-of-the-art information in the field of hygro-thermo-mechanical deformation simulation in structural concrete. The aspects discussed include coupled hygro-thermo-mechanical performance of porous materials including concrete, multi-scale simulation of concrete properties especially the volumetric and structural deformation performance, and the multi-scale simulation of concrete under the coupling effect of multi-physics fields. The multi-scale simulation section includes the multi-scale simulation of composition and structure in concrete, the multi-scale simulation of concrete's mechanical performance, and the multi-scale simulation of durability concerned performance of concrete. This paper presents an overview of the work, of which data from early 80 recent studies, carried out on the multi-scale simulation of hygro-thermo-mechanical deformation performance of structural concrete. The relating previous studies and analysis showed that sufficient data have been obtained to give confidence in simulating hygro-thermo-mechanical performance of concrete based on the theory of heat and mass transfer in porous media, and the clear relationships have been obtained between moisture-heat transfer and hygro-thermal distribution at different scale. It is necessary to make further systematic multi-scale research on the relationship between micro-structure and property parameters of cement paste, three-phase basic properties at meso level of concrete and the performance of concrete structures, which makes important practical significance to solve the crack of large-area and mass concrete structure and improve the durability of concrete structures.*

**Keywords:** Hygro-thermo-mechanical deformation, Multi-scale, Concrete, Numerical simulation, Porous media.

### 1. Introduction

Durability of concrete structures is strongly influenced by cracking of concrete which results from the shrinkage performance of the concrete material. The volume change of concrete is unavoidable when used in concrete structure effected by external loads and other environmental (hygral and thermal) loading. Generally, there are two kinds of deformation of concrete, power deformations due to applied external loads and own deformations due to volume changes under influencing of changes in temperature and moisture content. The so-called applied external loads consist of static, dynamic loads and so on. According to statistics, only 20% of concrete crack results

from applied external loads and the own deformation induced concrete crack is over 80%<sup>[1]</sup>. One of the important factors that contribute to the cracks in concrete structure is that due to shrinkage.

The crack induced by volume stability, no matter what small it is, would remarkably increase the permeability and make the deterioration easier to occur, and thus heavily deteriorate the durability<sup>[2-6]</sup>. So it must be considered that the hygro-thermo-mechanical coupling effect in environment from the mechanism of heat and moisture transfer when investigate the deformation of concrete material and structure in their service life.

Deformation of structural concrete involves different mechanisms acting over a broad range of scales, from the nanometer to the meter level. Therefore, multiscale research on deformation of concrete is inevitable. Review of the literature shows that the most results concerning shrinkage have been at the micrometer level on micro structure of concrete, but the research on mechanical performance of structural concrete is always macroscopic. The research of macroscopic mechanical performance, neglecting the complex micro structure of concrete, fails to reveal the physical origins behind of the surface phenomenon. Many of the numerous investigations on microscopic structure of concrete have been limited to the micro level.

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Obviously, macroscopic mechanical behavior of concrete is determined by its microstructure. The macroscopic failure of concrete is also accompanied by intensive processes of damage generation and accumulation, fracture development. Thus it is very important to understand the relationship between microstructure and macroscopic behavior by multiscale investigation of the performance of concrete in micro, meso, and macro level. The rapid development of modern measuring and testing techniques and the greatly enhanced computational simulation function in concrete science make it possible for numerical multiscale simulation of the deformation and cracking of concrete under hygro-thermo-mechanical coupling effect.

Just as Professor R. de Brost<sup>[7]</sup> thought that multiple scales, multi-physics and evolving discontinuities were principle challenges in computational materials science, and progress of which is necessary to understand the materials properties and performance.

This paper reviews the previous researches relating to the multiscale numerical simulation on the deformation and crack behavior of structural concrete and other porous materials considering the coupling effect of hygro-thermo-mechanical conditions. And the reviews content comprise of two parts: coupling research of multi-physical fields (hygro-thermo-mechanical) and multiscale simulation of porous materials.

## 2. Coupled Hygro-Thermo-Mechanical Behavior of Porous Materials

A number of studies have been published on the hygro-thermo-mechanical coupling problem in porous materials. Usually, two main approaches have been used. One refers to the homogenization method to establish equations based on the laws of conservation of mass, heat and quantity of movement. The other refers to the theory of Mechanics of Porous Media based on Biot's poroelastic macroscopic model, and further developed by Coussy in the case of non-linear and irreversible behavior.

The earlier coupled hygro-thermo-mechanical researches has occurred in the field of geotechnical engineering and has been attracting comprehensive attentions as one of the research focus<sup>[8-14]</sup>, especially in the research of hygro-thermo-mechanical model of unsaturated and saturated soil.

A closed form two-dimensional fundamental solutions for a non-isothermal unsaturated deformable porous medium have been derived and verified mathematically by comparison with the previously presented corresponding fundamental solutions by B. Gatzmiri<sup>[15]</sup>. S. Oller and E. Onate<sup>[16]</sup> proposed a hygro-thermo-mechanical constitutive model appropriate for numerical simulation of multiphase composite material behavior based on the mixture of the basic substances of the composite, and which allows to evaluate the inter-dependent behavior between the different compounding constitutive models.

B. A. Schrefler et al.<sup>[17, 18]</sup> presented a coupled thermo-hydro-mechanical model for the description of the thermal, hydral and mechanical behavior of concrete structures at

high temperatures. A fully coupled non-linear formulation is designed to predict the behavior and potential for spalling of heated concrete structures for fire and nuclear reactor applications. The presented model took concrete as a deformable solid matrix (linearly elastic) filled with liquid water, vapor water and dry air. The model has been implemented in a finite element code and has been applied to some case tests.

D. Gawin et al. have undertaken much of the recent pioneering work in this area<sup>[19-22]</sup>. For investigating hygro-thermal behavior of concrete at high temperature, a mathematical model for analysis hygro-thermal behavior of concrete, taking concrete as multi-phase porous materials and considering thermo-chemical and mechanical material degradation at high temperature, was proposed<sup>[19]</sup>. In simulation of damage-permeability coupling in hygro-thermo-mechanical analysis of concrete at high temperature, they developed a model for heat and mass transfer and damage analysis of concrete. The formula describing effects of damage on intrinsic permeability is tested numerically. A numerical example of high performance concrete structure concerning high temperature behavior is presented and discussed. The results of computer simulation of hygro-thermal and mechanical behavior of concrete wall showed the robustness of the numerical procedure and the computer code used. They thought that, according to the numerical results, the resulting gas pressures arising during heating of concrete elements, have lower, more realistic values when compared with the phenomenological solution<sup>[20]</sup>. A novel numerical model of hygro-thermo-chemo-mechanical phenomena in maturing concrete elements was presented by D. Gawin et al. when investigated the multi-physical modeling of concrete at early ages and beyond<sup>[21]</sup>. In the developments of the model, balance equations for phases and interfaces were introduced at micro-scale and then averaged for obtaining macroscopic balance equations, while the constitutive laws were directly introduced at macroscopic level. In the research of modeling of deformations of high strength concrete at elevated temperatures, a constitutive model analyzing deformations of concrete subject to transient temperature and pressures was proposed<sup>[22]</sup>.

Based on the theory of mechanics of non-saturated porous media and some simplifying assumptions, a coupling model is developed to simulate the hygro-thermo-mechanical response of porous materials. The mathematical model consists of space discretisation using Galerkin's method, time discretisation using the implicit finite difference method, and non-linear computation using Newton-Raphson's method. And two simulation cases concerning the drying and the condensation of moisture on a thin wall were analyzed as examples<sup>[23]</sup>. In order to simulate the behavior of concrete at high temperature, a new model, called THM+P, was developed based on the extension of the existing coupling thermal-hydro-mechanical coupling model (THM) for moderate temperature and the prediction of the risk of spalling of concrete and high-performance concrete subjected to fire load was validated<sup>[24]</sup>. A numerical method of

homogenization in thermo-hydro-mechanic for materials was also proposed based on the choice of a representative volume in which heterogeneities are generated in random process. The numerical model is used to predict elastic behavior as well as thermal damage behavior and the concrete permeability<sup>[25]</sup>.

Several models were proposed or developed by G. Meschke et al.<sup>[26-29]</sup>, within the framework of thermodynamics of partially saturated porous media, for finite element analyses of concrete structures based on the thermodynamics of deformable porous media in the context of the Biot-Coussy theory. The framework is also suitable for the homogenization of microscopic or mesoscopic properties to describe coupled hygro-mechanical mechanisms and damage of concrete on a macroscopic level.

An anisotropic combined plasticity-damage model in conjunction with the fracture energy concept was employed to describe the pre- and post-cracking behavior of concrete and for its non-linear material behavior under predominantly compressive stresses<sup>[26]</sup>. The model was demonstrated on the numerical prediction of drying shrinkage, non-isothermal moisture flow and the effects of cracking on the drying process comparing with two laboratory tests on concrete specimens. The results from two-dimensional simulations of a concrete panel subjected to coupled mechanical, hygral and thermal loading were also included as representative numerical examples.

Considering the degradation of stiffness and the growth of inelastic strains as a consequence of the opening of microcrack, a multisurface elastoplastic-damage model is employed to describe the nonlinear pre- and post-failure material behavior of concrete, which is formulated in the space of plastic effective stresses. A two-dimensional numerical simulation of a base restrained concrete wall subjected to both uniform drying and to rewetting at the foundation is investigated as a representative example<sup>[27, 28]</sup>.

A 3D coupled thermo-hygro-mechanical model for concrete, taking moisture and heat transport, cracking and irreversible deformations and the various interactions between these processes into account, is developed on the basis of thermo-mechanics of partially saturated porous media in the sense of the Biot-Coussy theory<sup>[29]</sup>. The numerical simulation results of an inner tunnel lining exposed to realistic seasonal changes of the humidity and the temperature were compared to the in-situ measurements on existing crown cracks in tunnel linings. It showed that the proposed element model is capable of simulating shrinkage-induced cracks and predicting the initial opening and the location of the cracks. The width and the penetration depth of the cracks were in good agreement with that of in-situ observations. The case analysis also showed that it is crucial for realistic prediction of shrinkage cracks in concrete structures to take the influence of cracks on the moisture transport into account.

J. Kruis et al.<sup>[30]</sup> carried out the hydro-thermo-mechanical analysis of prestressed concrete reactor vessels based on the finite element method. In their research, the domain decomposition methods, which enable utilization

of parallel computers, were used to deal with efficient computer implementation of the coupled analysis. The proposed strategy was confirmed by a coupled hydro-thermo-mechanical analysis of an existing reactor vessel.

X. K. Li and R.T. Li et al.<sup>[31-33]</sup> investigated the simulation of failure process of concrete at high temperature. The constitutive models of concrete at high temperature were proposed and developed for numerical simulation of coupled chemo-thermo-hygro-mechanical processes and coupled chemo-elastoplastic-damage analysis. In their researches, concrete is modeled as deforming porous media filled with two immiscible pore fluids of gas and liquid mixture at immiscible-miscible levels. Then a hierarchical mathematical model for analysis of the coupled thermo-hygro-mechanical processes in concrete at high temperature is presented<sup>[34]</sup>. The finite element procedures were developed for corresponding non-linear coupled problems to numerically simulate thermo-hygro-mechanical behavior resulting in material failures in concrete subjected to fire and thermal radiation. Numerical simulation results demonstrate the performance and the effectiveness of the proposed model and its numerical procedures in reproducing coupled thermo-hygro-mechanical behavior in concrete. A coupled elastoplastic-damage constitutive model is developed to simulate coupled chemo-thermo-hygro-mechanical behavior in concretes at high temperature, which takes chemo-induced material elastoplastic-damage effects into account<sup>[31, 33]</sup>. The numerical results illustrate the performance of the proposed constitutive model in reproducing coupled chemo-thermo-hygro-mechanical behavior in concretes in fire and thermal radiation. A coupled chemo-thermo-hydro-mechanical (CTHM) constitutive model was also developed for the hierarchical mathematical model in CTHM analysis of concretes at high temperature<sup>[32]</sup>. The numerical results demonstrate the capability and the validity of the proposed coupled CTHM constitutive model in simulating the complex failure processes in concretes at high temperature.

A simplified coupled thermo-hydro-mechanical model, which is capable of reproducing the main features of the thermo-hydric behavior in the transient phase of concrete subjected to moderate heating, is developed with the assumption that the gaseous phase in concrete is composed only of vapor<sup>[35]</sup>. An isotropic damage model, relying on a microcrack description by applying effective-medium approximation schemes, was introduced and used to estimate the mechanical parameters, Biot coefficient and permeability evolutions as a function of damage and saturation degree. The numerical results was analyzed, commented and compared with experimental ones. The numerical study revealed that the adsorption curve affects importantly the results than others, and that certain coupling terms in the mass conservation equation of water can be neglected. The simulations also showed that the temperature gradient dominates the main cracks, and the propagation of them result from a combined action of temperature and capillary pressure gradients.

C. Davie et al.<sup>[36]</sup> proposed a detailed and fully generalized (3D) hygro-thermo- mechanical model for

concrete regarding it as a multiphase system consisting of solid, liquid and gas phases. The model captures the complex behavior of concrete through the adoption of a multi-phase material description of solid, liquid and gas. Heat and moisture transport of the fluid phases are modeled in a coupled manner such that an accurate description of the fluid transport processes in concrete is possible, illustrating in particular the redistribution of liquid and the increases in vapor content and pore pressure associated with the application of elevated temperatures. The mechanical behavior of the solid skeleton is modeled by way of an isotropic thermo-mechanical damage model considering the degradation of the material due to both mechanical and thermal loading. A further parametric study is then presented where the model is used to investigate the roles of various mechanical behaviors in the overall hygro-thermo-mechanical response of the concrete under high temperature conditions.

D. P. Chen et al.<sup>[37-40]</sup> have investigated the hygro-thermal coupling transfer and deformation based on heat and moisture transfer in porous medium. They proposed a hybrid analytic-FEA method for calculating coupling hygro-thermal deformation of concrete based on moisture

and heat transfer mechanism of porous medium. The procedure comprises of an analytical solution of heat and moisture transfer, a calculation of moisture induced stress and a finite element analysis (FEA) of hygro-thermal deformation. The methodology of a software named Combined Temperature and Moisture Simulation System for concrete (CTMSof) is introduced, in which Visual Basic program was used for the graphical user interface (GUI) and the numerical calculation was developed using Matlab and ANSYS, see Fig. 1. Meanwhile, considering that the current FEM approach is not possible to directly apply moisture loads to the nodes like temperature loads, a theoretical formula was developed for calculating the moisture induced stress transformed based on the Kelvin-Laplace equation and Mackenzie formula. Besides of above mentioned researches, considering that Knudsen diffusion should not be negligible results from the porous medium characteristic and pore distribution of cement-based materials, a theoretical formula for calculating the influence of the coefficient of Knudsen diffusion was deduced on the basis of the theoretical equivalent diameter of meso-micro pore and the kinetic theory of gas<sup>[41]</sup>.

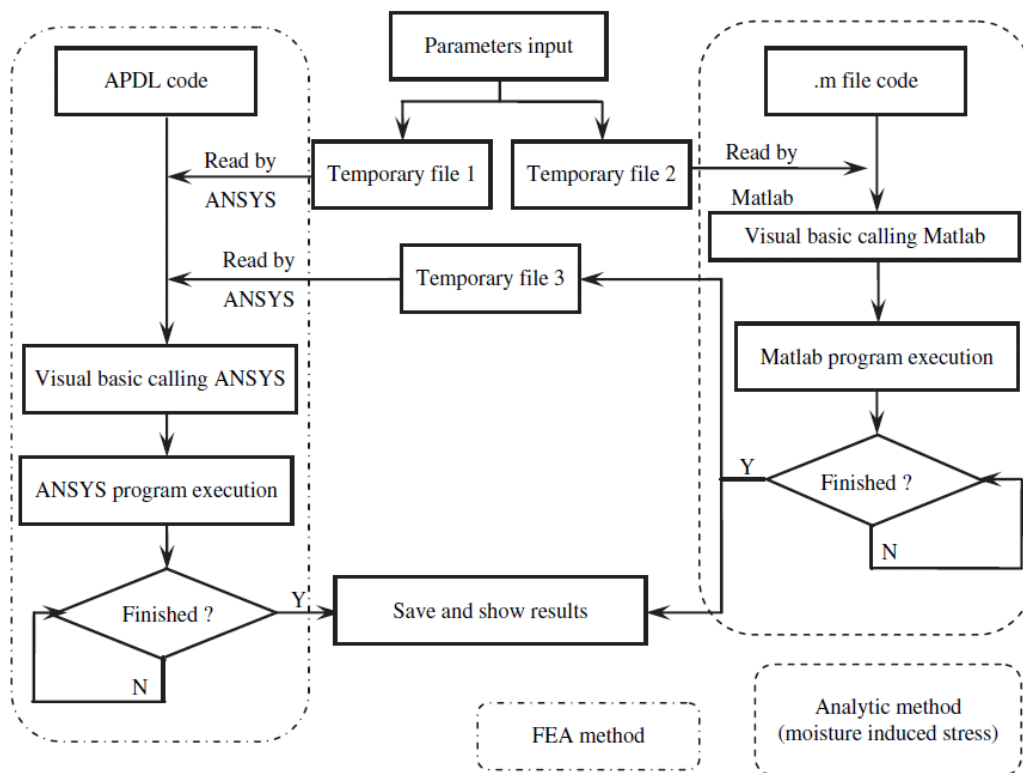


Fig. 1 The holistic structure of CTMSof<sup>[40]</sup>

According to the researches on coupled hygro-thermo-mechanical deformation of concrete mentioned above, the shrinkage or cracking of concrete, especially the hygro-thermal transfer and induced deformation were mostly investigated at high temperature to analyze the behavior of concrete in fire<sup>[15-25]</sup>. Some studies based on thermodynamics of partially saturated porous media will benefit the future research of hygro-thermal-mechanical

performance of structural concrete<sup>[29]</sup>. While some research of concrete performance in fire using phenomenological theory of heat and mass transfer would be not fit for concrete materials. Many researchers didn't take the coupling effect in the process of interaction of heat, moisture and load, especially the coupling hygro-thermo process, let alone the hygro-thermal effect of concrete structure in real service environment. The authors

have investigated the coupling effect of interaction process, presented the hybrid analytic-FEA method and developed software named CTMSOFT, by a mix programming of Visual Basic, Matlab and ANSYS, for simulating the coupling hygro-thermal deformation of concrete. The approach was inapplicable when used to analyze the cycle hygro-thermal effect by transfer function method.

### 3. Multi-Scale Simulation of Concrete's Properties

The amount of published materials on multi-scale simulation of concrete is burgeoning rapidly. Many of the numerous investigations of concrete multi-scale simulation have been focused on the following three aspects: composition and structure; mechanical performance; and properties relating to the durability of concrete. It must be mentioned that quite a few papers in journals and conferences concerned with more than one of the aspects mentioned above.

#### 3.1. Multi-scale simulation of concrete's composition and structure

A series of investigations of micro-structure and relevant properties of concrete have been carried out by D.P. Bentz and E.J. Garboczi et al.<sup>[42-47]</sup>. The composition and micro-structure of concrete were systematically studied and the multi-scale composition was simulated by the aid of digital-image-based structural models for the C-S-H at nanometer level, the hydrated cement paste at the micro meter level, and a mortar or concrete at the millimeter level. Computations performed at one level provide input properties to be used in simulations of performance at the next higher level. As a first step in a multi-scale approach to computing the drying shrinkage of model cement-based materials, a set of structural models for C-S-H gel and computational techniques for their validation have been developed<sup>[43]</sup>. The basic nanostructure of C-S-H gel was conceived as a self-similar agglomeration of spherical particles at two levels (diameters of 5 nm and 40 nm). Computational techniques were presented for simulating transmission electron microscopy images and computing sorption characteristics of the model nanostructures. Such an approach provided a better understanding of the relationships between microstructure and the shrinkage behavior of cement based materials. The ionic diffusivity and drying shrinkage of concrete were analyzed by the methodology<sup>[43, 44, 46, 47]</sup>.

Properties of cement paste and concrete such as creep and shrinkage was dominated by the smallest gel pores associated with the calcium-silicate-hydrate (C-S-H) phase. Multi-scale modeling has proven to be a promising approach for correlating the nanometer-level structure of C-S-H to the bulk properties of cement paste and concrete<sup>[48, 49]</sup>. According to F.-J. Ulm et al.<sup>[49]</sup>, the microstructure of cement-based composite materials can be classified into four levels (i) LEVEL I (C-S-H): two types of C-S-H with different elastic properties is estimated at a scale of  $10^{-8}$ - $10^{-6}$ m; (ii) LEVEL II (Cement

paste): including C-S-H matrix, large CH crystals and cement clinker, and is at a scale of  $10^{-4}$ - $10^{-3}$ m; (iii) LEVEL III (Mortar): at a scale of  $10^{-4}$ - $10^{-3}$ m composing of sand particles embedded in a cement paste matrix, and interfacial transition zone (ITZ); (iv) LEVEL IV (Concrete): at a scale of  $10^{-1}$ - $10^1$ m, considering aggregates with ITZ embedded in a mortar matrix and gradation of aggregates/sand inclusions embedded in a cement paste matrix.

F. Jennings et al.<sup>[50]</sup> investigated the nanoporosity of cement paste by the aid of experimental techniques such as small-angle neutron scattering (SANS), equilibrium drying, and nanoindentation. The experimental results give a more complete and detailed picture of the nanostructure of the C-S-H gel phase as a function of aging, drying, and heating. And a quantitative structural model of the C-S-H gel was extended to account for new experimental data. A new constitutive model was developed, by decomposing a boundary value drying problem, to predict the elastic shrinkage due to capillary stresses during drying of a porous material<sup>[51]</sup>. The proposed mathematical model was different from the models developed based on either the concept of average pore pressure or equivalent pore pressure. The predictions of the new model were demonstrated by the experimental results of linear drying strains and the implications to the poromechanics and the effective stress of partially saturated porous media were also discussed<sup>[52]</sup>. Taking into account finite air (gas) pressure, finite external load, and variables that are absent during simple drying under atmospheric conditions, a novel and quantifiable form of effective stress in partially saturated materials was proposed. A primary shortcoming of the classic Bishop effective stress expression was overcome by the proposed framework and a novel way incorporating important morphological features was given. In their opinion, the existing micromechanical homogenization techniques aided by basic descriptions of material morphology can be used to inform the study of elastic deformations in the partially saturated media, the reason of which was also explained. The proposed effective stress framework remarkably reduces to a volumetric average pressure form which is commonly encountered in literature<sup>[52]</sup>.

B. Bary and S. Be'jaoui<sup>[53]</sup> proposed a simplified multi-coated sphere assemblage model, which is capable of assessing the diffusive and mechanical properties of hardened cement pastes, for the description of the microstructure of cement based materials. According to the multi-coated sphere assemblage model, where the core is constituted of the anhydrous cement grain (if it exists) and the first and second layers represent inner and outer C-S-H, respectively. The other major hydrated products such as CH and AF, together with the capillary porosity, are homogeneously distributed through the C-S-H layers as spherical inclusions.

Based on the quantitatively characterize of multi scale capillary porosity and entrained air content in hardened cement paste by advanced ultrasonic techniques, an inversion procedure based on a theoretical attenuation model is used to predict the average size and volume

fraction of entrained air voids in each specimen was proposed by W. Punurai et al.<sup>[54]</sup>. The validity of the model was demonstrated by the results obtained by standard petrographic methods and by gravimetric analysis.

### 3.2. Multi-scale simulation of concrete's mechanical performance

B. A. Schrefler et al.<sup>[55]</sup> Proposed a mathematical and numerical model to predict the non-linear behavior of concrete as multiphase porous material. All the important phase changes of water and chemical reactions such as adsorption-desorption, condensation evaporation, hydration-dehydration, and the related heat and mass sources or sinks are considered. Temperature and pressure changes, damage or carbonation motivated material properties and coupled thermal, hygral and mechanical effect are taken into account. The numerical simulation of young concrete properties, self-desiccation process, and deformation in high temperature environments were investigated by the aid of the proposed model.

In the researches of F. Grondin et al.<sup>[56]</sup>, a micro-mechanical model was developed by coupling the effective moduli approach with a finite element model based on the representation of the heterogeneous materials random

microstructure. They also carried out numerical simulations in order to localize damage on the microstructure scale and to analyze the effective behavior of confined concrete samples subjected to high temperatures and compressive loads. They also found that there is so-called "transient thermal strain" during experimental tests and thought it should be result from the thermal damage of concrete.

F. Bernard et al. proposed a 3D multi scale modeling approach of mechanical properties of cement-based materials considering the eventual changes in the microstructure<sup>[57]</sup>. This approach is illustrated in Fig. 2. In this proposed approach, two numerical tools are used successively for fulfilling the multi-scale simulations. First, a 3D model called CEMHYD3D, which was developed by National Institute of Standards and Technology (NIST), is used to generate a realistic 3D Representative Volume Element of cement-based materials at two different scales (cement paste, mortar). Then, the voxelized images are converted to Finite Elements Meshes compatible with the FE software Abaqus and the mechanical behavior of cement-based materials is calculated. The outcome of a lower scale is used as input at a higher scale.

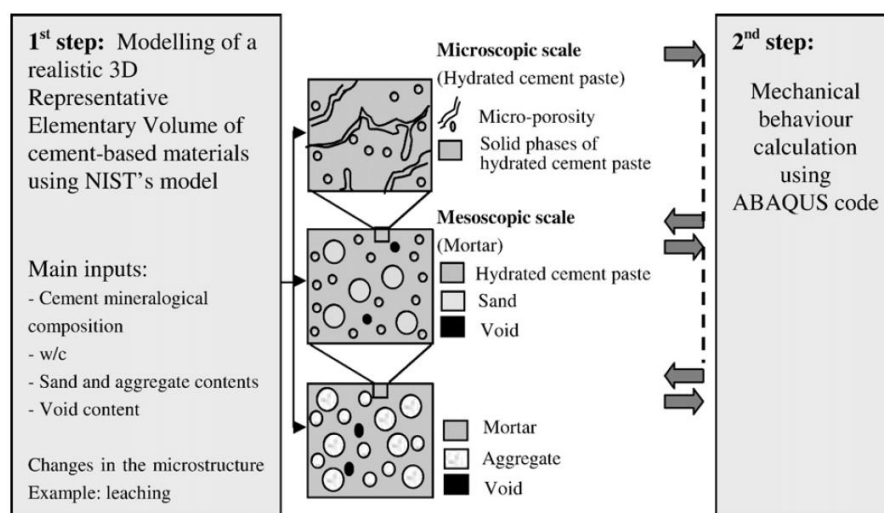


Fig. 2 Illustration scheme of the proposed 3D multi-scale numerical modeling approach<sup>[57]</sup>

In the opinion of F. -J. Ulm et al.<sup>[48]</sup> cement-based materials are poromechanics materials that are sensitive to the pressure that develops in the porosity of these materials at multiple scales. And the poroelastic properties of cement-based materials can be rationally estimated through the Continuum Micromechanics analysis, advanced microstructure modeling of cement chemistry and advanced micromechanical testing. S. Avril et al.<sup>[59]</sup> proposed a multi-scale approach to model the mechanical behavior of a cracked RC beam with externally bonded composite plates when loaded in flexure. This multi-scale approach, in which the structural behavior of the beam is assessed from numerical computations conducted over a relevant representative volume element, makes the input parameters have a physical meaning and the results are consistent with full-field measurements conducted on

repaired beams. P. Wriggers and M. Hain<sup>[60]</sup> have investigated the behavior of concrete, using the concept of representative volume elements (RVE) and homogenization, on three different scales: the hardened cement paste (hcp), the mortar and finally the concrete. The micro-structure of hardened cement paste, constitutive equations, homogenization and thermo-mechanical coupling have then been studied. S. Ghabezloo<sup>[61]</sup> used the results of a macro-scale experimental study performed on a hardened cement paste in association with the micromechanics modeling and homogenization technique to investigate the poroelastic properties. A multi-scale homogenization model, calibrated on the experimental results, is used to extrapolate the poroelastic parameters of cement pastes prepared with different water-to-cement ratio. A new method of modeling the fracture of concrete

is proposed by J. van Mier<sup>[62]</sup>, based on its disordered material structure, by using fracture potentials (F - r relations) at various observation scales (atomistic, molecular and macroscopic). The simple lattice approach was used to mimic the micro structure of concrete, and then the correlating mechanical performances of concrete were investigated using the newly proposed model.

### 3.3. Multi-scale simulation of concrete's durability

Deterioration of concrete is governed by coupled diffusion processes such as heat conduction, moisture transfer, and chloride ion penetration. The interactive diffusion processes in concrete can be characterized by multiscale modeling. Z. P. Bazant and E. P. Chen<sup>[63]</sup> reviewed the progress achieved in the understanding of scaling and size effect in the failure of structures. Three main types of size effects were discussed, namely the statistical size effect due to randomness of strength, the energy release size effect, and the possible size effect due to fractality of fracture or microcracks. In their opinion, the size effect in these materials is due to stable growth of large fractures prior to the attainment of maximum load, and in particular to stress redistributions and the release of stored energy engendered by such large fractures. A multiscale model is proposed by Xi and Jennings<sup>[64, 65]</sup>, according to multiscale effective homogeneous theory, for

modeling the shrinkage of cement paste and concrete that links properties at multi-scale level (nanometer, micrometer and millimeter). H. Chemmi et al.<sup>[66]</sup> have investigated the impact of multi-scale moisture transport on durability of hardened cement pastes by longitudinal relaxation NMR experiments of hardened Grey CEM I paste with two controlled degree of relative humidity. The comparison between these two aged materials evidences that the moisture transport only occurs on the meso and capillary scales. G. Mounajed et al.<sup>[25]</sup> have developed a simulation tool, the Digital Concrete, integrated into the general F.E.code SYMPHONIE of the Centre Scientifique et Technique du B'atiment. It allows characterizing the concrete homogenized behavior under a thermo-mechanical load by a multi-scales approach. The elastic behavior as well as thermal damage behavior and the concrete permeability were predicted using the proposed numerical model.

It must be mentioned that K. Maekawa et al.<sup>[67-70]</sup> have systematically investigated the multi scale modeling of concrete materials and structure, involving micro structure of concrete materials, mechanical performance and durability of concrete materials and structure. Please find the schematic representation of the targeted multi-scale modeling of material science and structural mechanics in Fig. 3.

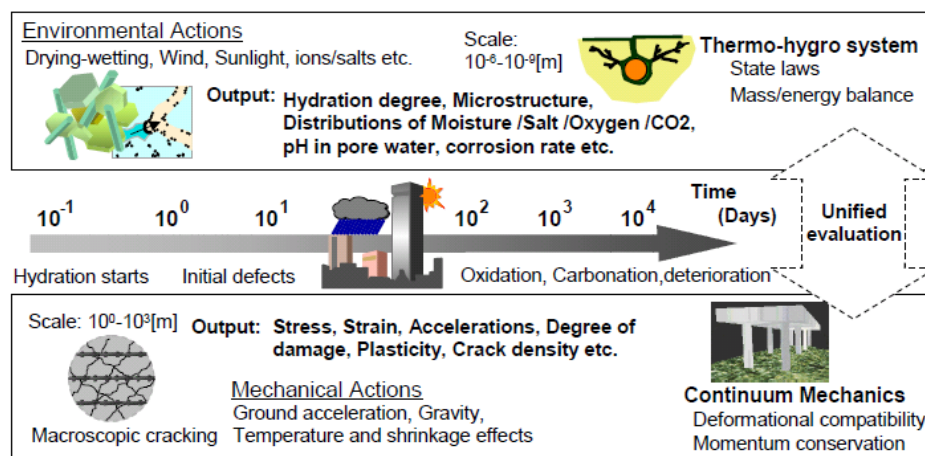


Fig. 3 Multi-scale scheme and lifespan simulation for materials and structures<sup>[67]</sup>

Besides of the above mentioned researches, F. Sanchez and A. Borwankar<sup>[71]</sup> have investigated the multi-scale performance of carbon microfiber reinforced cement-based composites exposed to a decalcifying environment by scanning electron microscopy, energy dispersive X-ray spectroscopy, and derivative thermogravimetric analysis.

Few domestic researches relating to the multi-scale simulation on cement-based materials has been carried out. But the multi-scale simulation has captured more and more attention from many researchers. Y. L. Bai et al.<sup>[72, 73]</sup> deemed that the multi-physics and multi-scale coupling is a new challenge in solid mechanics, and the fundamental difficulty in these multi-scale nonequilibrium problems is due to the hierarchy and evolution of microstructures with various physics and rates at various length levels in solids.

Y. Y. Li et al.<sup>[74]</sup> proposed an iterative multi-scale finite element method for predicting the equivalent mechanics parameters of the concrete with multi-graded aggregate based on the porosity property of concrete. Reasonable multi-scale model is important to carry out multiscale analysis of structures. X. Z. Lu et al.<sup>[75]</sup> presented a newly developed multiscale finite element model by implanting a precise microscopic finite element model into a macro frame structure one. The newly developed methodology can meet the deformation compatibility well at the interface between different-scale models.

Z X. Li and her research group<sup>[76-79]</sup> have worked on the multi-scale modeling and analyses of long-span bridges many years and have made many important outcomes: the methodology and strategy for concurrent

finite element modeling of long-span bridges at the different scale levels have been developed for the purposes of analyses on structural deteriorating; the model updating techniques with concurrent multi-objective and multi-factor optimization technique were developed for concurrently updating the multi-scale model of the bridge; the proposed procedures of multi-scale model modeling, updating and verification were applied to the model verification in several long-span bridges as actual

engineering practices of the proposed procedures; the method of numerically simulating structural deteriorating and damage involution in multiple temporal and spatial scales was developed based on the previous developed multi-scale model and was applied to analyze the performance of long-span bridges under service loading. The physical description of the proposed concurrent structural multi-scale model is illustrated in Fig. 4. The mixed structural multi-scale modeling is shown in Fig. 5.

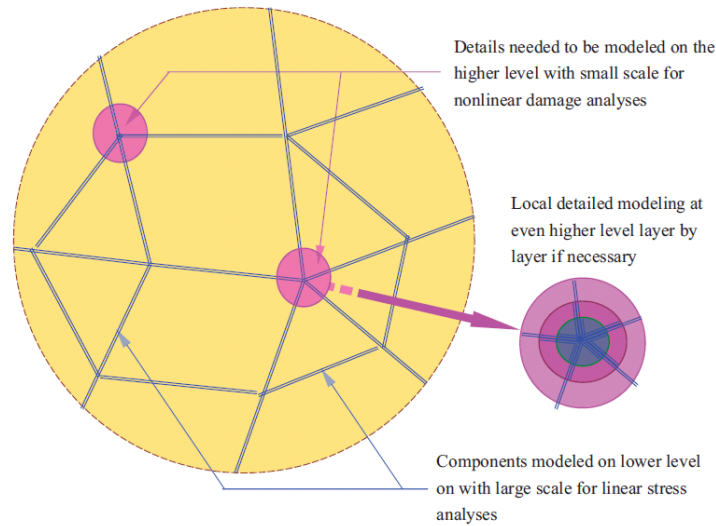


Fig. 4 Physical description of the concurrent structural multi-scale model<sup>[77]</sup>

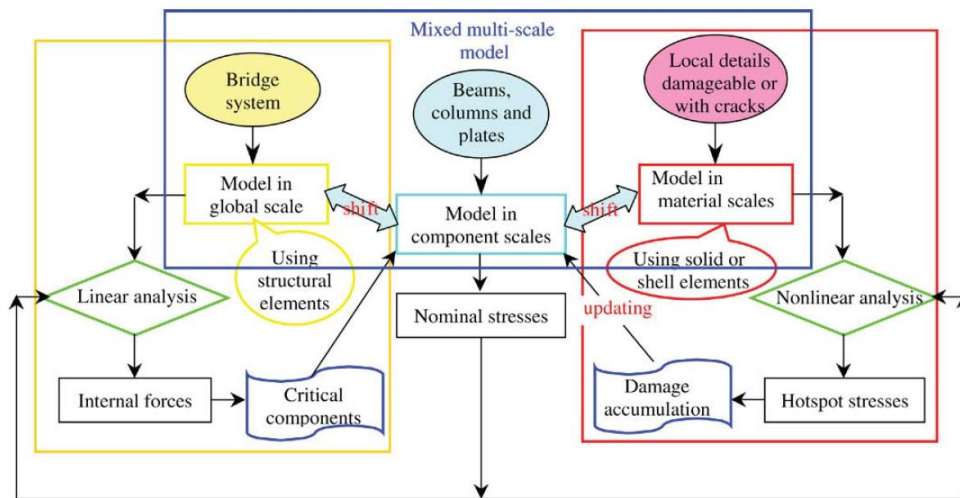


Fig. 5 Flow chart for separated and mixed structural multi-scale modeling<sup>[76]</sup>

According to the multiscale researches of deformation of concrete materials reviewed forward, concrete prosperities were usually investigated at micro-meso scale<sup>[25, 48, 55-58, 61-64]</sup>, the macro damage performance were also studied at component and structure scale in Chinese<sup>[71, 4-75, 78-79]</sup>. While the symmetric study of the relationship of mesoscopic basic prosperities of concrete materials and macro performance of concrete structure is rare. The meso-mechanism of macroscopic performance of concrete structure is not clear. So there are some important key problems must be solved before studying the coupling hygro-thermo-mechanical deformation and crack

performance. Some researches on multiscale simulation of mass concrete structure mainly at the component and structure scales, which considering the multiscale relationship between partial details and whole structure, and the coordination between different scales.

It must be mentioned that the hygro-thermo-mechanical and multi-scale simulation of concrete structure performance are not isolated, in spite of the relating researches were review respectively in this paper. The authors and other researchers will benefit from the previous researches of multi-physics and multi-scale coupling of porous materials, of course the cement paste and concrete is included.



#### 4. Conclusions

The studies of coupled hygro-thermo-mechanical behavior of porous materials, multi-scale simulation of the properties and performance of concrete, which are relating to the multi-scale simulation of hygro-thermo-mechanical deformation and cracking behavior of structural concrete, were reviewed in this paper. The various aspects on multi-scale simulation of hygro-thermo-mechanical deformation behavior of structural concrete, presented in this paper could be summarized and concluded as:

(1) Studies and analysis from nearly 80 references concerning the multi-scale simulation of hygro-thermo-mechanical deformation of structural concrete have shown the interesting progresses in nearly every respect, especially in the multi-scale simulation on the composition of concrete and the hygro-thermal performance of concrete in fire or at high temperature.

(2) In previous studies, coupling hygro-thermo-mechanical shrinkage or cracking of concrete, especially the hygro-thermal transfer and induced deformation were mostly investigated at high temperature to analyze the behavior of concrete in fire. However the similar research at normal temperature was rare.

(3) In the modeling of multi-scale structure of concrete, the random aggregate method concerns of composition of hardened concrete structure, has the advantages of simple principle and easy realization. Some previous structural multi-scale modeling of large engineering structure mainly emphasized the structural performance of components or whole structure, which considered to construct the global model at the structural level and to incorporate the local concerned details models of constitutional relationships for analytical purposes. The "scales" in these researches can be ranked as component level and structure level, both of which belong to macro-level according to the three multi-scale systems of micro-meso-macro scales which is emphasized in this paper and also is the concept accepted by most researchers in multi-scale studies. The investigation of hygro-thermo-mechanical deformation and cracking behavior of structural concrete will be carried out from micro level cement paste composition to three phases of aggregate-cement paste-interface transition zone, and to concrete specimens, components and concrete structure levels.

(4) Almost no researches of multi-scale simulating on the deformation and other performance have been investigated considering the coupling hygro-thermo-mechanical effect in service environment of concrete materials and structures. It is necessary to make further the systematic research on the relationship between micro-structure and property parameters of cement paste, three-phase basic properties at meso level of concrete and the performance of concrete structures.

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