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STRUCTURAL APPROACH FOR NUMERICAL INTERNAL STRAIN MODELLING OF CONGLOMERATE STRUCTURES

Aleksey Kharitonov

Saint Petersburg State University of Architecture and Civil Engineering
Vtoraja Krasnoarmejskaja ul. 4, St. Petersburg, Russia

peepdv@mail.ru

Abstract

The paper defines the principles for structure-simulation modelling of conglomerate material properties by an example of cement compositions. The constitutive essence of the principles consists in generation of hierarchical models of individual structural levels (including a sub-microstructural level) based on material structure data. Parameters of properties, determined for models of the previous structural level, are used as input data of continuum environment, which forms a matrix element for models of the following level.

Detailed development of a general model for a composition makes it possible to correlate structural features at the level of a nanometer with material macro properties. Algorithms simulating physical and mechanical processes and phenomena, typical of cement systems individual properties (dry shrinkage, straining under load), are implemented based on the finite element method by determination of corresponding external and internal loads.

Application of the finite element method makes it possible to completely maintain geometrical and physical “reality” of the model describing specific features of the structure under study; and enables solutioning, with a high degree of confidence, of theoretical and practical issues related to determination of quantitative effect of structure discrete parameters on various material properties.

Keywords

Concrete, Dry Shrinkage, Simulation Modeling, Finite Element Method.

Introduction

It is known that properties of conglomerate materials are directly attributed to their structure. Meanwhile, upon development of materials exhibiting the required values for individual properties a situation may occur when structure parameter requirements are in conflict with other structure parameters. Thereby, a problem is originated concerning development of a system with required property values that correspond to a defined set of operating conditions.

Solving of the said problem is complicated with the fact that investigation of conglomerate system properties (e.g., concretes or soils) is mainly based on empirical approaches which are not always suitable for determination of quantitative relation between the discrete parameters of the structure and various properties of the material. Experiments, as a rule, provide an integral estimate of structure impact on the property under investigation.

The required relation expressed in mathematical terms could be obtained by computer simulation modeling which involves creation of composite structure simulation models (Bentz, 2011; Buffo-Lacarrière et al., 2007).

This publication is devoted to methodologies for cement conglomerate material properties forecasting and control on the basis of structure-simulation modeling which consists of presentation of the structure components distribution, mutual orientation and integration, as well as their combined action at different levels using numerical methods.

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Background

Analysis of the research results in the field of mathematical representation of composite material properties in conjunction with their structure allowed to select a main line for solving a problem of cement system properties forecasting. The solution involves generalization of known regularities in a form of numerical simulation models (Garbocz et al., 2000; Haecker et al., 2005; Jennings et al., 2007; Kharitonov, 2007; Kharitonov, 2008). The advantage of such models as compared with statistical and phenomenological concepts is in possible explicit consid-

eration of structure parameters and simulation of physical nature of phenomena using numerical methods. The most advanced and proven method for solution of differential equations describing continuous medium behaviour is finite element method (FEM).

In order to implement the abovementioned line, it is required to develop a methodology for cement composition properties modeling based on presentation of material structure in a form of hierarchical model of individual structural levels that simulates physical and mechanical processes and phenomena (Sychev, Badin, 2016).

Two main approaches in development of computer model of cement system structures and investigation of properties based on such model can be pointed out at the present period:

- development of a kinetic simulation model for cement hydration and application of FEM based on this model in order to describe main properties attributed to material at individual time segments of structure formation;
- application of discrete structure models, the construction algorithm for which is based on stochastic filling of some volume with geometric features according to pre-determined distribution of their form, size and orientation. Further composite properties modeling is related to implementation of the effective medium theory or FEM.

Both given modeling lines consider cement grains as the smallest structure elements at best, without considering the cement gel. The mentioned disadvantage is attributable to attempts to simultaneously include structural inhomogeneities of wide-range size into the model, thus making calculations more complicated and roughening the results of material properties modeling.

The first approach obviously has great importance for understanding and practical application for modeling of physical and chemical processes of cement hydration. Currently, development of this approach is at the stage of concept implementation.

This article is concerned with investigations made in the view of the second approach related to creation of models based on data on hardened cement stone (within 28 days). Prior information is required for this purpose, pertaining compositional analysis, quantitative and geometry parameters of structure elements, as well as consideration of stochastic nature of their distribution within the material volume. At that, kinetic aspect of structure formation becomes insignificant, but mixed results of hydration process simulation are excluded.

Methods

For the purpose of this paper, modeling is based on two-dimensional presentation of structure components. But this approach also demands for the trade-off between the intent to represent component shapes, structure peculiarities and computer capabilities. Nevertheless, two-dimensional task allows to investigate internal stresses under various factors, with consideration of stochastic nature of structure components mutual location and their links.

At the first stage of such simulation, a nanostructural model of cement stone, corresponding to C-S-H phase, was developed. The model is based on the results of physical and chemical investigations of 28-days cement stone, with consideration of various technology factors (hardening conditions, water-cement ratio, additives availability). The following were considered as main parameters: total porosity and pore size-distribution. Porosity is determined as per the methods based on proton magnetic resonance (PMR), benzene desorption and mercury porosimetry.

Size-distribution of cement gel pores determined with PMR showed that, irrespective of technology factors, considerable volume of cement stone pore space is represented with pores with the radius of about 0.85 nm.

The factors under investigation showed their influence over the volume of such pores by changing the degree of cement hydration. However, quality of C-S-H structure (concerning pore parameters) remains unchanged. Total volume of pores with the above stated size equals 18% of the cement stone volume on the average, and 65% of all pore volume.

Availability of pores with the radius of about 0.85 nm points out to the size of individual elements of gel structure, which is about 4-5 nm. Similar results for the gel hard phase size evaluation are obtained with small angle neutron scattering (Leitea et al., 2004).

Investigation of cement stone porosity with benzene adsorption and mercury porosimetry methods allowed to determine large volume of pores with the radius of 3-5 nm. This fact, in its turn, proves a suggestion of agglomeration of gel individual elements: clusters of 40-50 nm provide for origination of pores with the stated radius; and this corresponds to experimental data (Pucharenko et al., 2013).

With regard to large-size pores (5-10 nm), no unambiguous conclusion could be made, but it is possible to name pore size ranges common for all investigated compositions: 7-10 nm, 12-16 nm, 21-26 nm, 41-44 nm, 70-73 nm.

Case history

Modeling of properties, phenomena and processes typical for cement systems presents independent tasks. The reason for this is that algorithms describing appropriate properties and their mechanisms are implemented at the final stage of model development. For example, algorithms describing strength properties are completely different from those for shrinkage deformation.

The stage of creation of various structural level models is a common stage at modeling of any property. A source model is being created at this stage, which approximates elastic properties and links between individual components, as well as entire cement system.

At the first stage material structure levels are established and physical and mechanical parameters of individual level components are determined. Then, with consideration of applied mathematical tools and computer capabilities, geometry models of various scale are created for the structure with consideration of stochastic nature of structure components location.

The next stage of numerical model creation is implementation of FEM processes that allow to represent the model as an integrated system consisting of components

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with different physical and mathematical parameters (modulus of elasticity, Poisson ratio, etc.). General elasticity characteristics used as parameters of a continuous medium (matrix) for each subsequent scale approximation are determined for each model. Creation of a model of the largest scale is considered as completion of the first stage. Validity of structure level models is verified by comparison of design parameters with experimental results.

The second stage of modeling is associated with investigation of particular properties of cement systems under consideration, i.e. development of algorithms for material properties presentation, that are based on conventional theories and ideas. In the context of simulation modeling, these algorithms are related to determination of loads effective within models of different levels, evaluation of load effect results and initial modeling transformation, if required. An integrated response corresponding to the property under investigation is considered as a result.

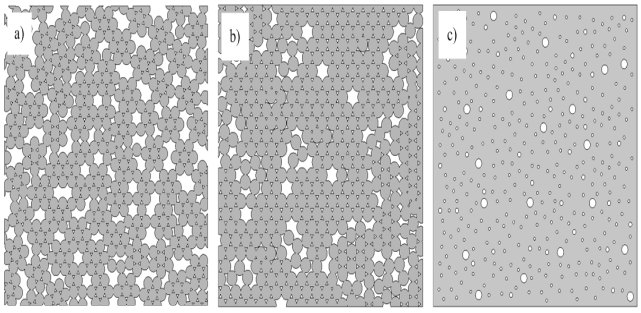

Figure 1. Geometry model of nanostructure. Model sizes a) 200×200 nm; b) 800×800 nm; c) 5×5 μm

Results

We developed a flat three-level numerical model of cement stone nanostructure (the cement stone is of normal moist curing) (Figure 1).

The first level model gives an idea of gel as a system consisting of particles with diameter of 4.4. nm and pores primarily having the radius of about 0.85 nm (Figure 1a).

This does not preclude laminated nature of individual particles interior, but this fact is not considered in calculation due to extremely small size of interlayer space.

The model of the second level structure (Figure 1b) represents a formation of aggregate individual particles with the diameter of 40 nm. The model covers the pore size range of 5 to 30 nm. Pores having the radius of 30 to 80 nm and distributed within the matrix are considered as elements of the third level (Figure 1c).

In order to obtain stochastic distribution of structure elements within created simulation models, we developed "PoreSolution" software which implements Monte Karlo method (Pucharenko, Morozov, 2013).

When creating a microstructure model, we considered portlandite, ettringite and also unhydrated clinker as the most important structural elements. Content of portlandite (~20%) and ettringite (~10%) within the cement stone

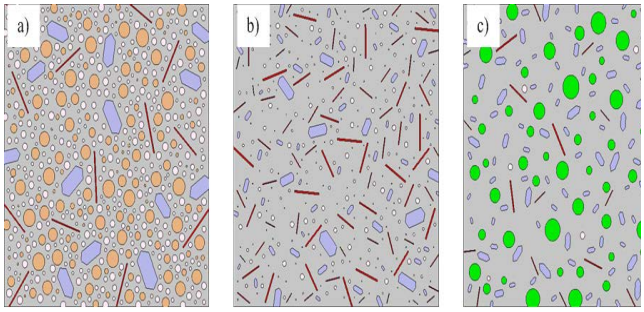

Figure 2. Cement stone microstructure model. Model sizes: a) 50×50 μm; b) 100×100 μm; c) 200×200 μm
Needle-like elements – ettringite; hexagonal elements – portlandite, circles – clinker and pores (white color)

under modeling was determined by quantitative X-ray phase and thermographic analysis.

Figure 2 shows the microstructure model of a cement stone (water-cement ratio = 0.28), consisting of three different scale approximations.

The meso-level model (Figure 3) shows four phases: matrix (cement stone), sand grains, contact zone with the thickness of 20 μm and pores.

Pores distribution within real concrete was determined stereometrically. Sand grain content equals 48%, that is about 1:2.5 ratio of cement and sand weight in concrete.

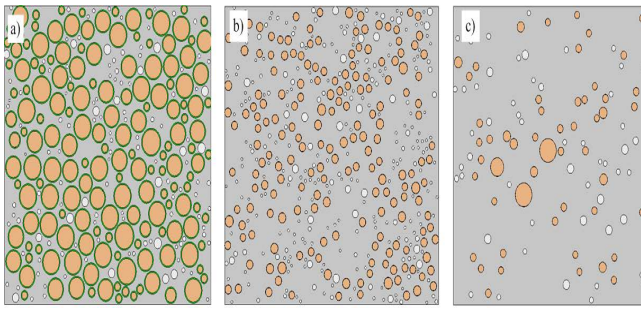

Figure 3. Concrete meso-level model. Model sizes: a) 5×5 mm; b) 25×25 mm; c) 50×50 mm

One of the stages of design model creation at each scale was implementation of FEM algorithm. When assigning elastic properties for a model, it was taken into account that physical properties of the next level matrix would inherit properties of the entire previous level system.

Table 1 gives designed properties for model discrete levels.

Modulus of elasticity (E) and Poisson ratio (μ) are taken on the basis of the following data (Pukharenko, Aubakirova, 2016) and equal to: for C-S-H elements, E=84.5 GPa, μ =0.45; for portlandite, E=42.3 GPa, μ =0.324; for ettringite, E=25.0 GPa, μ =0.25; for clinker, E=117.6 GPa, μ =0.314; for sand, E=72.8 GPa, μ =0.167.

We formulated calculation methods for modeling of dry shrinkage behavior. This behavior is based on thermodynamic equilibrium between the system and medium; also capillary pressure and change in free surface energy are taken into account (Shahsavari, 2011). The calculation method involves determination

of water-filled pore radius and capillary pressure in such pores under appropriate relative humidity. Capillary pressure acts as a load applied to finite elements along pore surfaces. Then change in surface energy and appropriate deformations due to this energy are calculated. Obtained deformation values are set in the matrix of the structure model. In addition to deformations at each designed humidity level, determined for a discrete model, model deformations of the previous level are added.

Table 1. Physic and mechanical properties of discrete models

Model Scale		Porosity, %		Modulus of Elasticity, GPa	Poisson Ratio
		General	Model		
nano-	a	24.0	24.0	35.1	0.38
	b	36.0	15.8	15.0	0.30
	c	39.2	5.0	13.1	0.29
micro-	a	34.4	1.5	14.2	0.29
	b	30.9	0	15.4	0.29
	c	26.7	0	17.3	0.29
meso-	a	18.0	3.4	21.3	0.28
	b	19.4	4.4	22.0	0.27
	c	20.3	2.4	21.1	0.27

Conclusion

Comparison of design and experimental data on shrinkage dependence from relative humidity (Figure 4) proves validity of the suggested cement stone model and shrinkage calculation algorithm.

The design shrinkage values also correspond to the results obtained by other authors (Smirnova, 2012; Sychev, Badin, 2016; Tennis, Jennings, 2000; Wittmann, 1984).

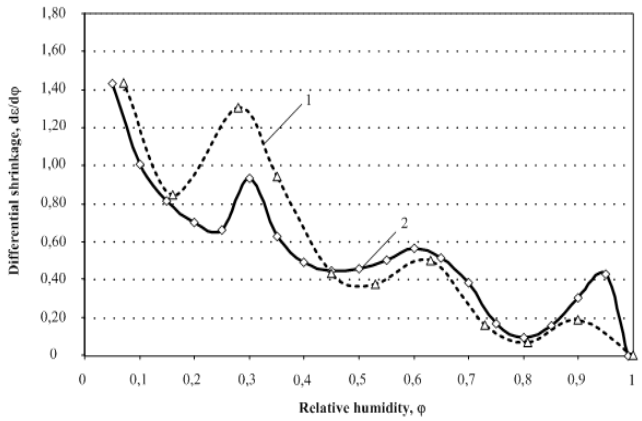

Figure 4. Differential shrinkage.
1 – experimental work; 2 – calculation

The developed two-dimensional models of concrete structure which explicitly include structural elements at different scales of 25 nm to 5 mm describe real material properties.

The advantage of the suggested modeling method is in possible quantitative evaluation of material properties with consideration of close relation between different structure levels – from nanometer to millimeter. This approach allows to investigate the degree of effect of various structure-determining factors on material properties that are of investigator's interest.

The algorithm of dry shrinkage behaviour modeling, which considers capillary pressure and deformations attributed to change in free surface energy depending from environmental relative humidity, shows a real situation with own concrete deformations in view of comparison of modeling results with experimental determination results for dry shrinkage.

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