STRUCTURAL APPROACH FOR NUMERICAL INTERNAL STRAIN MODELLING OF CONGLOMERATE STRUCTURES

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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.

The research is carried out in accordance with research activities plan NIR No. 7.546.2011 “Development of fundamental basis and practical principles applicable to creation of engineering structures with improved serviceability and security" under government task (Reg. No. 01201257464).

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-
The next stage of numerical model creation is implementation of FEM processes that allow to represent the cement stone pore space. 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 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
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.

**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 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.

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

<table>
<thead>
<tr>
<th>Model Scale</th>
<th>Porosity, %</th>
<th>Modulus of Elasticity, GPa</th>
<th>Poisson Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>General</td>
<td>Model</td>
<td></td>
</tr>
<tr>
<td>nano-</td>
<td>a 24.0</td>
<td>24.0</td>
<td>35.1</td>
</tr>
<tr>
<td></td>
<td>b 36.0</td>
<td>15.8</td>
<td>15.0</td>
</tr>
<tr>
<td></td>
<td>c 39.2</td>
<td>5.0</td>
<td>13.1</td>
</tr>
<tr>
<td>micro-</td>
<td>a 34.4</td>
<td>1.5</td>
<td>14.2</td>
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<td></td>
<td>b 30.9</td>
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<tr>
<td></td>
<td>c 26.7</td>
<td>0</td>
<td>17.3</td>
</tr>
<tr>
<td>meso-</td>
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<td>3.4</td>
<td>21.3</td>
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<tr>
<td></td>
<td>b 19.4</td>
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<tr>
<td></td>
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<td>2.4</td>
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</tr>
</tbody>
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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).
References


