

INFORMATION MODELING OF CONCRETE: CURRENT STATUS AND DEVELOPMENT PROSPECTS

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Abstract: The paper addresses the challenges posed by the digitization of building materials science. It highlights the importance of developing a digital model of concrete for optimizing the design and synthesis of its structure and improving the technology used in its production. It is demonstrated how this model will enable building experts to better calculate and clarify methods for creating sturdy and efficient structures. The paper also examines the evolution of information modeling of concrete within the context of the various stages of development in system-building materials science and technology.

A review is presented of the primary contemporary techniques used in computer modeling of concrete structures in both domestic and foreign scientific research. It is worth noting that these methods fail to consider the intricate composition of concrete. The article explains that concrete can be characterized as a conglomerate composite that boasts a hierarchically organized structure with dimensions ranging from 10⁻¹⁰ to 10⁻¹ meters. It is comprised of no fewer than 5-6 distinct scale levels and three distinct types of substructure design. Substructures vary in scale, origin, and manifestation of properties. The first type of substructure is observed at macro, meso, and micro scales. It is composed of a two-component structure consisting of a spatially continuous matrix and deterministically and stochastically distributed discrete inclusions. The second type of substructure pertains to the sub-micro, ultra-micro, and nanoscale levels. It is believed that the cementing substance takes the form of a microscale spatial structure resulting from the consolidation of individual crystalline differences. The third type corresponds to the atomic-molecular structure of newly formed cementing substance.

The characteristics of each substructure type are presented based on the component scale, formation features, mechanics of property manifestation, design criteria, and means of synthesis. A default assumption is made regarding the unique modeling of the three concrete substructure types and their consolidation into a unified digital model. The objective is to create an information platform for this purpose. The platform should consist of a knowledge base rooted in theory, an empirical database, a database consisting of analytical, numerical, and statistical models, algorithms for the purpose of designing and synthesizing structures, optimization criteria and boundary conditions, and specific terms of reference for computer modeling of concrete.

Keywords: design of structures, synthesis of materials with specified properties, digitalization of building materials science, digital model of concrete, information platform

ИНФОРМАЦИОННОЕ МОДЕЛИРОВАНИЕ БЕТОНА: ОБЗОР СОВРЕМЕННОГО СОСТОЯНИЯ И ПЕРСПЕКТИВЫ РАЗВИТИЯ*

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Аннотация: Публикация относится к проблемам цифровизации строительного материаловедения. Показана актуальность разработки цифровой модели бетона для решения оптимизационных задач конструирования и синтеза его структуры, уточнения методик расчета строительных конструкций, совершенствования технологии их изготовления. Анализируется эволюция информационного моделирования бетона в контексте этапов развития системно-строительного материаловедения и технологии.

* Содержание статьи было частично доложено на VIII международном симпозиуме «Актуальные проблемы компьютерного моделирования конструкций и сооружений», 17-21 мая 2023 г., Тамбов

Приводится обзор основных современных методов компьютерного моделирования структуры бетона в отечественных и зарубежных научных исследованиях. Отмечается, что эти методы не учитывают всю сложность строения бетона. В статье бетон представлен как конгломератный композит с иерархически организованной структурой размерностью от 10^{-10} до 10^{-1} м. Он обладает минимум 5-6 масштабными уровнями и тремя типами конструкции подструктур. Подструктуры отличаются по своему масштабу, генезису и механике проявления свойств. Первый тип подструктуры характерен для макро-, мезо- и микромасштабного уровней. Принимается в виде двухкомпонентной «конструкции» из пространственно непрерывной матрицы и детерминировано-стохастически распределённых в ней дискретных включений. Второй тип относится к субмикро-, ультрамикро- и наномасштабным уровням. Полагается в виде «микромасштабной пространственной конструкции» новообразований цементирующего вещества из консолидированных индивидуальных кристаллических разностей. Третий тип соответствует атомно-молекулярному строению новообразований цементирующего вещества.

Дается характеристика каждого типа подструктуры по: масштабу компонентов; особенностям формирования; механике проявления свойств; критериям конструирования; средствам синтеза. Формулируется предположение о специфичности моделирования каждого из трех типов подструктур бетона и их интегрирования в единую цифровую модель. Ставится задача разработки информационной платформы такой модели. Платформа должна включать: базу теоретических знаний; базу эмпирических данных; базу аналитических, численных и статистических моделей; алгоритмы конструирования и синтеза структур; критерии оптимизации и граничные условия; техническое задание на компьютерное моделирование бетона.

Ключевые слова: конструирование структур, синтез материалов с заданными свойствами, цифровизация строительного материаловедения, цифровая модель бетона, информационная платформа

INTRODUCTION

Currently, the methods of design and calculation of structures, buildings and facilities rely on computer modeling of their stress-strain state, loads and impacts. Information technologies are used in experimental and field studies [1, 2].

The transition to computer modeling of construction objects, in our opinion, forms a favorable situation for the involvement of material scientists in this process. Their task is to design optimal structures of concretes with specified properties. Structure construction is a speculative, virtual procedure of "filling" the volume of the designed building structure that takes into account its configuration, peculiarities of reinforcement, etc., with structural elements forming the material. The outcome is the creation of a spatial and geometric "structure design" capable of maximizing the use of force structural bonds under the conditions of destructive impact of the operating environment on the building structure. Based on the results of the design, a set of control actions is assigned during the synthesis of the structure. This is a chemical-technological procedure for the implementa-

tion of the compiled project of spatial-geometric "structure design" in the production process of a building product [3].

However, the opportunities for interaction and mutual understanding between specialists in the calculation of building structures ("mechanics") and material scientists have been limited so far. They were confronted with the "watershed" between the used concepts, methods, passing through the scale boundary of 10^{-1} m in the "space and world" of construction science. Objectively, it turned out that "mechanics" deal with bodies on the scale of 10^{-1} m and larger. The material structure of such a body (structure) is modeled as a continuous homogeneous iso-tropic medium with some averaged "effective" characteristics [4]. The degree of compliance of these characteristics with the real values predetermines the predictive value of the calculation results. The potential deviations are compensated by the assignment of overestimated material reserve coefficients. Material scientists "work" with structured solids, which are a complex construction of elements with dimensions from 10^{-1} to 10^{-10} meters. In most cases, such a structure is perceived as a "black box" - an

experimental-statistical model relevant in a strictly limited factor space [5].

The lack of adequate models limits the possibilities of designing and subsequent synthesis of concrete structure with a given level of quality. It is known that the method of designing concrete mixture composition for concrete of a given strength was developed in the late 19th century. Nevertheless, the efficiency of concrete property management is still much lower than that of metals or polymers. This is clearly demonstrated by the difference in the values of the reserve coefficients of the compared materials.

In our opinion, a digital model of concrete can overcome the "barrier" between mechanics and material scientists. It should, first, describe identification universals and qualitative-quantitative attributes of concrete structure at all its scale levels. Secondly, it should reveal cause-and-effect links and relations in the system "technology" - "composition, structure, state" - "properties at the moment of production and unfolded in time in the operational environment".

The usage of a digital model of concrete in the design and calculation of building structures is aimed at clarifying the real pattern of their stress-strain state [6]. In system-structural materials science, the numerical model is intended for the development of fundamental principles of design and formation of an arsenal of means for synthesizing optimal concrete structures with predetermined characteristics. This model is most relevant for obtaining variable structures of new generation concretes (construction composites): super dense, especially high-strength, ultra-lightweight, ultra-resistant to the action of the operating environment, etc.

Applied goal of the digital model of concrete is to solve the problems of optimization design of concrete composition and structure depending

on the operating conditions in building structures. The result of this is the assignment of rational modes and parameters of manufacturing of structures. In the future, the digital twin of concrete (reinforced concrete) structures should be integrated into BIM-technologies. Here it will manage the automated manufacturing process of the product, and then monitor its condition during operation with the forecast of residual resource.

Let us consider the evolution of system-structural concrete science in the context of digital approach.

EVOLUTION OF CONCRETE INFORMATION MODELING

Optimization of the structure and technology of concrete lies in the context of the system-wide task of creating a methodology and a comprehensive quality management system for industrial products. The development of solutions for quality management is based on a quantitative description of the phenomena of substance and energy transformations in the procedures of production. The highest form of such description is an information model of phenomena, for the creation of which it is necessary to formalize the transition from the real sides and relations of the object to their symbolic designation. In turn, formalization is feasible only after appropriate identification (recognition for display in human consciousness [7, 8]).

Academician of RAACS E.M. Chernyshov carried out a retrospective analysis of the "parallel" chronology of the development of basic scientific knowledge in the field of concrete science [9] and the stages of development of the methodology of the quantitative approach [10]. Table 1 presents the results of the analysis.

Table 1. Stages of development of information modeling of concrete and basic scientific knowledge of concrete science

Stage	Period	Content of the stage	Personalities, schools
I	the first third of the nineteenth century - first third of the 20th century	The formation of the paradigm of quantitative approach, the emergence and development of the science of processes and devices of engineering technologies as a field of scientific and applied knowledge [11-13]. Introduction of physical and mathematical analogies; physical analog modeling; modeling based on the theory of similarity [14-16].	F.A. Denisov, V. Badger, N.D. Zelinsky, A.A. Kirov, V.L. Kirpichov, A.K. Krupsky, V. Luis, W. McAdams, W. McCabe, D.I. Mendeleev, I.A. Tishchenko, W. Walker, etc.
		Obtaining the first scientific data on the influence of technology on concrete properties and processes of its structural formation [17-20].	D. Abrams, I.P. Alexandrin, A.A. Baikov, N.A. Beilyubsky, N.M. Belyaev, I. Bolome, O. Graf, N.A. Zhitkevich, V.A. Kind, I.G. Malyuga, E. Freysine, R. Fere, E.G. Cheliyev, A.R. Shulyachenko, V.V. Ewald and etc.
II	first third of the XX century - middle of the XX century.	Establishment of fundamental principles of the general theory of systems [21-23]. Formation of the methodology of system analysis of engineering and technology objects. Application of mathematical modeling for solving engineering problems [24].	N.A. Belov, A.A. Bogdanov, L. Bertalanffy, W. Ross-Eshby, T. Kotarbiński, M. Petrovic, A. Espinas, et al.
		Identification of regular relations in the system "formulation-technological factors" - "composition, structure, state, properties" of concrete. The beginning of the formation of the structural approach in concrete science [25-28].	V.V. Mikhailov, N.A. Popov, B.G. Skramtaev, A.E. Sheikin, V.N. Jung et al.
III	second half of the 20th century	Implementation of the cybernetic approach to systems as an object of control according to the "black box" principle [29-31]. Development of probabilistic-statistical methods of active planning and design of experiments [32-34]. Application of experimental-statistical models in construction materials science and technology [35-37].	Y.P. Adler, P. Ahnazarova, N. Wiener, V.A. Voznesensky, V.V. Kafarov, R. Fischer, et al. Kafarov, R. Fischer, etc.
		Development of the foundations of system-structural building materials science with active use of the provisions of natural science disciplines [38-42]. Qualification of concrete as a composite material, experimental study of its composition and struc-	I.N. Akhverdov, Y.M. Bazhenov, J. Bernal, I.I. Bernay, P.I. Bozhenov, S.S. Gordon, I.M. Grushko, A.E. Desov, G.I. Gorchakov, A. Grudemo, I.A. Ivanov, F.M.

		ture on the basis of new quantitative physical and chemical methods [43-47]. Development of the foundations of the mechanics of manifestation of structural and functional properties of concrete [48-51].	Ivanov, J.L. Kalousek, P.G. Komokhov, D. Conrad, R. Lermi, F.M. Lee, P.A. Melnichenko, O.P. Mchedlov-Petrosyan, T.P. Pauers, T. Pauers, R. Lermi, F.M. Lee, P.A. Melnichenko. Komokhov, D. Conrad, R. Lermi, F.M. Lee, P.A. Melnichenko, O.P. Mchedlov-Petrosyan, T. Powers, V. Reichel, P.A. Rebinder, A.I. Rybiev, V.I. Solomatov, M.M. Sychev, H.F.W. Tay-lor, V.V. Timashev, A.V. Ushero-Marshak, M.M. Kholmyansky et al.
IV	Since the end of the 20th century	Mathematical and computational optimization problem solving in construction materials science and technology. Development of "computer material science" of concrete on the scientific basis of classical concrete science [5, 52-54]. Attraction of mathematical physics models and simulation modeling. Validation of neuro-computing application in construction materials science [55-58].	A.A. Askadsky, V.V. Belov, V.A. Voznesensky, V.A. Vorobyov, B.V. Gusev, V.I. Kondrashchenko, E.V. Korolev, T.V. Lyashenko, A.S. Ovchinsky, V.P. Selyaev, S.V. Fedosov et al.
		Development of a scientific platform for the development of breakthrough innovative solutions in system-structural materials science and high technologies of concrete with a new level of quality. Staging and realization of special researches of cause-effect relations according to the formula "4C" [7, 59-62]. Development and generalization of provisions of mechanics of concrete properties manifestation as composites [4, 63-66]. Development of methodology and theory of design and synthesis of optimal structures of conglomerate building composites [3, 8, 67, 68].	T.K. Akchurin, O.V. Artamonova, V.N. Vyrovoy, A.M. Danilov, V.T. Erofeev, S.S. Kaprielov, N.I. Karpenko, D.N. Korotkikh, V.S. P. Lesovik, N.I. Makridin, V.I. Morozov, A.P. Proshin, Y.V. Pukharrenko, G.S. Slavcheva, E.M. Chernyshov, V.I. Shevchenko, V.P. Yartsev et al.

The stages presented in Table 1 reflect the vector of movement on the way from phenomenological (factual, empirical) knowledge to essential (system-structural, conceptual) knowledge in materials science of construction composites.

This movement is accompanied by the evolution of concepts and methodology of information modeling of concrete in the form of deepening and detailing of aspects of identification and formalization of its structure.

It follows from Table 1 that the current state of basic scientific knowledge and information modeling of concrete can be evaluated as an exit to digitalization of construction materials science and technology. Setting and solving problems of designing and synthesis of optimal structures today should be carried out on the basis of formalization and computer modeling of cause-and-effect relations in the system "technology - material - construction - building (structure) - operating environment". Digitalization here should be understood as a transition from physical, in-situ models (concrete samples) to work with its mathematical image. Digitalization makes it possible to perform control actions with a virtual object (a digital twin of a building structure) with the help of a computer. In this case, the computer is used not so much as a means of processing information and calculations, but as a direct "productive force" in obtaining the final result.

REVIEW OF CURRENT METHODS FOR COMPUTER MODELING OF CONCRETE

The goals of digitalization have become achievable due to the emergence of universal shells and increasingly powerful algorithmic programming languages, computational and information resources for applied mathematical modeling. Supercomputer technologies and hybrid architecture computing systems using traditional and advanced algorithms have become commonplace.

The method of neurocomputing ("machine learning" in foreign terminology) has received a particularly rapid development in this respect. Neurocomputing provides the creation of systems and algorithms for information processing capable of autonomously generating adaptive responses of the "cause-effect" type for a specific information environment. Neurocomputing is considered as an alternative to programmed computing due to its ability to "learn" to process information while acting in an informational environment [55, 69]. Since the 90s of the last century, neural networks have been used in the development of concrete

composition selection and property prediction [70-77]. Unfortunately, and this is noted by the researchers themselves [78], such developments are reduced to neural network programming of cause-effect links and relations in the system "formulation-technological factors" - "properties" of concrete. Machine learning is carried out on the basis of empirical data according to the "black box" principle, without taking into account structural factors. That is, in their methodological bases and statements such works lie in the context of the III stage of evolution of construction material science and concrete technology (see Table 1). Moreover, according to Lyashenko [79], machine learning models are "more passive" than experimental-statistical models. She argues that the initial data for them are not generated according to a special plan, but in an arbitrary way.

A review of foreign sources shows that the most common method of computer modeling of concrete structure today is mesoscale modeling. According to this method, concrete is considered as a composite material made of aggregates of different shapes and sizes included in the cement matrix. It should be noted that in the domestic materials science terminology, the macroscale level of concrete structure corresponds to this interpretation.

In most cases, mesoscale modeling is based on the formation of pseudo-random 3D packing of particles according to their computer-generated locations and radii [80, 81]. The nonlinear behavior of the simulated structure is investigated by numerical methods using its finite element discretization [82], including the use of general-purpose software such as ANSYS [83].

It is noted that "classical" mesoscale modeling often shows significant discrepancy with the results of physical experiments, as it does not consider microstructural levels of concrete. To refine the mesoscale models, for example, matrix-inclusion contact zone modeling is used [84], microstructure visualization using X-ray computed tomography [85], machine learning [86], including for image analyzer data processing [87].

Computer modeling of atomic and molecular structure of cement stone neoplasms by molecu-

lar dynamics methods has become a separate independent direction of digitalization of building materials science. These methods combine quantum-mechanical description of objects and models of "classical forces" [88-90].

In Russian science, Vorobyov should be considered as the founder of the calculation of the composition and prediction of concrete properties using computer modeling of their structure. His methods combine the probabilistic-geometric concept with the theory of percolation and the theory of effective media [91]. Modeling of the structure of building composites today is carried out on a large scale by the leading Russian scientific schools [53, 58, 61, 63, 67, 67, 92, 93].

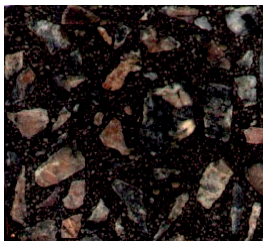
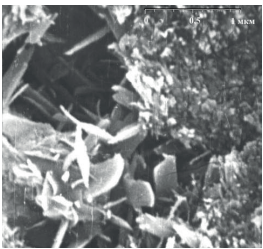
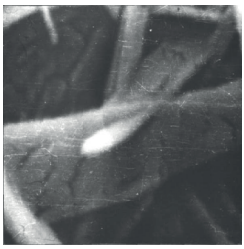
DISCUSSION OF THE CURRENT STATE OF COMPUTER MODELING OF CONCRETE AND FUTURE PROPOSALS

Despite significant successes, the methods of computer modeling of concrete listed in the previous section do not take into account the com-

plexity of the structure of this material. The applied approaches are differentiated by scale structural levels and do not provide a holistic adequate digital model of concrete. In our opinion, these methods require integration on the basis of modern concepts and data on identification and formalization of concrete structure.

Let us characterize concrete as an object of mathematical modeling. "Concretes are composites of conglomerate type, which are structured solids endowed with the features of substance, multiphase, polystructure, scale multiscale, deterministic, stochastic and dialectic" [94]. E.M. Chernyshov identified these features as universals of structure [95]. The universals of polystructure and scale multilevelness show that, despite the diversity of concrete varieties, their structure is a spatial-geometric construction of characteristic dimensionality from 10^{-10} to 10^{-1} meters. The structure has at least 5-6 structural levels and three types of substructures in the integral structure of concrete. Substructures are distinguished by their scale, genesis and mechanics of properties manifestation (Table 2).

Table 2. Characterization of substructures in the polystructure of concrete

Characteristic feature	Substructure type		
	I (conglomerate composite)	II (microconstruction)	III (continuous medium)
Visualization			
"Occupied" levels of the holistic structure	macro-, meso- and microscales	sub-micro-, ultra-micro- and nanoscale	nanoscale and atomic molecular
Dimensional range of structural elements, m	$10^{-1} - 10^{-(4\div5)}$	$10^{-(4\div5)} - 10^{-(8\div9)}$	$10^{-8} - 10^{-10}$

Description of the structure	two-component "construction" of a spatially continuous matrix and deterministically stochastically distributed discrete inclusions; a continuous heterogeneous body	"Microscale spatial construction" of cementitious matter neoplasms from consolidated individual crystalline and hidden crystalline differences	solid-phase substance of individual hidden crystalline or crystalline neoplasms; solid monophasic body endowed with imperfections (defects) in the form of vacancies, substitutions, dislocations.
Genesis	a product of the formation of the "addition system"	a product of the interaction between the "addition system" and the "growth system"	a product of the evolution of the "growth system"
Regularities of property mechanics	mechanics of composites	construction "micromechanics"	thermofluctuation theory, crack mechanics
Design criteria	control of the stress field by parameters of their concentration and localization	Load bearing capacity	kinetic strength, fracture toughness
Scientific basis for synthesis tools	Mechanics and mechanochemistry of granular media, physicochemistry of dispersed systems	physicochemistry of dispersed systems, theory of structure of matter, solid state chemistry, crystal chemistry, nanochemistry	
Volume in the composite space, %	100	15-20	6-10

Each of the identified types of substructures has its own specific formalizations and mathematical model. The first type is a probabilistic-geometric model of granular particle packing, the second type is a finite element model of stochastic structure, the third type is a discrete model of crystal lattice. To obtain an adequate numerical model of concrete, the disclosure and integration of these models is necessary.

In this case, it is most difficult to formalize the substructure of the second type. It has a pro-

nounced stochasticity and variability. It is a structure of morphologically crystalline (or hidden crystalline) lamellar, fibrous-needle, etc. differences of neoplasms. The mathematical model of the second type of substructure can be correlated with the corresponding models of spatial systems of building macroscale structures (rod, rack-and-beam, shell structures, etc.) [96]. However, with this approach we will have to face the problem of determinization of stochastic systems.

CONCLUSION

In our opinion, the proposed approach to the development of a digital model of concrete as a polystructural material requires preliminary creation of an information platform. Such a platform will include:

- 1) theoretical knowledge base,
- 2) empirical data base,
- 3) base of mathematical and computer models of concretes and processes occurring in them during production and operation,
- 4) algorithms for construction and synthesis of structures,
- 5) optimization criteria and boundary conditions,

6) terms of reference for computer simulation. Generation of the knowledge base in the information platform implies a system identification and formalization of concrete polystructure. This should result in a system of quantitative parameters of the structures of each of the three types of substructures.

These parameters with their estimates and characteristics will be a function (output) in mathematical models of the type "formulation-technological factors - composition, structure, state" and "operational factors - composition, structure, state", and then serve as arguments (input) in models of the type "composition, structure, state - properties".

Numerical solution of inverse problems on the basis of these models is the essence of optimization design and technological synthesis of concretes with characteristics specified depending on the conditions of their operation in building structures.

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