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Materials as Complex Systems

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Abstract: It is proposed methodological principles for the development of building materials on the basis of their representation as a complex system with the relevant system attributes. The effectiveness of the approach was confirmed in the design of a number of composites with desired structure and properties. An example of implementation.

Key words: Building materials, complex systems, hierarchical structure, system model, private models, quality assessment

INTRODUCTION

It is proposed approach to the creation of building materials based on their representation as complex systems (Bazhenov *et al*., 2012; Budylina *et al*., 2015) which allows for the analysis and synthesis of full use of methods of system analysis. It is assumed:

- A holistic vision of the material as a complex object
- The existence of a dominant role of whole over the private
- The impossibility of knowing the main characteristics of the material by studying only the characteristics of its elements (the system properties can not be reduced to the sum of the properties of its components)
- The number of properties of the material is greater than the sum of the properties of elements (relationship between of the elements is given a new special quality a systemic, integrative)
- The system is represented as a set of elements, connected relationships that generate integrative quality; in the absence of an integrative quality of a complex object it is not a system

MATERIALS AND METHODS

Statement of the problem and methods of solution: Construction materials have the appropriate system attributes and they can be considered as a system. Easily detected internal contradictions and paradoxical in the study of building materials as systems. The paradox of the integrity lies in the fact that the full description of the construction material is possible only with the "integrity" of its splitting apart (in the description of a certain integrity); knowledge as a building material integrity is impossible without analyzing its parts. With regard to the paradox of hierarchy, a description of the building material as the system is only possible if its description as part of the super-system (broader system) and back again, the description of the building material as a super-system element is possible only with the description of the actual building material.

There are two ways of decomposition of integrated system the "building material". In the first method, after the breaking of an integrated system elements are obtained parts which do not bear the holistic properties of the original system. Thus, when designing concrete (system) natural to the system partition on the individual components. However, this view does not allow with the necessary certainty to predict properties of concrete on the basis of studying the properties of the components (elements). This is also true for the decomposition of the material on the basis macro and microstructure in polystructural theory (V. Solomatov). The second method involves the allocation of such parts (elementary education) which preserves the integrity of the specific form of the properties of the material ("holistic" partition). Thus, the material properties of the sample (elementary education) are determined by the properties of the components and the integrative properties of the entire system (material).

Without a holistic system approach it is impossible to study the material for the purpose of forecasting the possibility of its practical use. However, even the integrative property of system (as part of the structure) can be qualitatively examined outside the system (for example, surface wettability filler determined in a separate experiment). The results can serve as a qualitative description of structure formation process but does not allow a complete description of the entire system.

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The difference between the composite materials and of the mechanical mixture of the components (the properties of which are defined as the sum of the properties of the components) is the presence of the phase boundary (determines the intensity of the processes of structuring and properties of the material (system). At the phase boundary is formed by the contact layer: it is provides traction components (adhesive strength, a new integrative properties that do not have the elements included in the system). Combining of the components at the phase boundary form a layers with altered properties. They influence on the properties the system which are different from the characteristics of components (for example, processes of curing cement in bulk and in thin layers at the phase boundaryare different). As see, at the study of building materials have the paradox of integrity.

On the one hand, assessment and analysis of building materials can be made only on the basis of consideration of the material as an integrated and unified system; on the other hand impossible to study the material without analyzing its parts. That is why the study of the structure and properties of the material should be made on the basis the study of elements and of inter-element links while maintaining the integrity of the system (such as study kinetic processes of the formation of physical and mechanical characteristics of the material (Garkina, 2015). The quality of building materials is estimated taking into consideration their place as an element in the hierarchical structure of an integrated super system. Criteria of subsystem quality must be part of criteria quality of system (defined by integrative properties).

A complex system is divided into subsystems of different nature (decomposition of the system); are determined inter-element connections and relationships that give integrity. There is another way of extracting a system: description of individual aspects of the object not a whole object). Here, each system in one and the same object (building material) expresses only a certain facet of his nature. This use of the concept of the system allows a thorough and integrally study different aspects or facets of a single object (such as surface phenomena: wetting, capillary processes, etc). Note, in many cases, a change in any element of the system has an effect on other components and it leads to a change in the whole system. Therefore, it is often impossible to produce of the building material decomposition (as a whole system) into individual components without loss of integrative properties.

Further the complexity and diversity of the processes of operation of real systems including building materials, do not give a completely adequate mathematical models. A describing mathematical model the formal process of functioning of the system is able to cover only the basic characteristic patterns. If the problem is formulated in mathematical language, it is completely solved by mathematical methods. Theoretical modeling is a method of scientific knowledge from a practical point of view is a technology solutions applied scientific and technical problems. The role of mathematical modeling and computer simulation greatly increased if full-scale experiment is impossible or difficult.

The process of understanding reality in the practical development of the system can not always be explained from a scientific point of view. Here is dominated by the level of mathematical rigor; mathematical language is considered as the best means of reporting systems. In most studies are limited to only a statement and investigation of mathematical problems and does not provide meaningful and practical aspects of human identity. Note, the task of identifying characteristics of the system can be regarded as a dual (conjugate) in relation to the problem of control system. You can not operate the system if it is not identified either in advance or in the management process. Structural identification determines the form of a mathematical model of the system (general identification problem). After the mathematical model of the system is determined, conduct parametric identification (private identification task); is determined the numerical parameters of the mathematical model (constant values must not contradict the physical sense and theoretical considerations). The role of the structure of the model can not be overestimated: a bad choice negates all parametric identification. Models can be formalized in different ways but always without distorting the overall picture. The totality of the alleged links between the observed signals is a model in the broadest sense of the word. The choice of method of identification is not uniquely defined: in the very formulation of the problem presupposes uncertainty (incomplete knowledge about the object, limitations in the observations of the object in time, the inaccuracy of the measurement signals at the input and output objects, etc).

Creating an adequate model is possible only when the properties and interactions of the simulated object sufficiently studied. The model is postulated on the basis of empirical data (available to the researcher) without justification The adequacy of the system model can not be proved: model is accepted or rejected based on experimental data. System model will always be different from the original, we can only speak about the asymptotic approximation to it under certain conditions for each practical task. Adequacy achieved by narrowing the of use of the considered system model, limiting the practical applicability; it is enhanced by the model experiments: there are new intuitive knowledge of nature which can be used to adjust the model taking into account the properties of the object being studied. The simulation allows a deeper insight into the essence of the original object and modeling studies led to the discovery of new properties and the laws of the functioning of the system under study.

System modeling is iterative: It is impossible to obtain a comprehensive description of the object being studied. The challenge is, how well the level of knowledge allows to solve the problem posed. On the basis of qualitative criteria model is estimated in terms of its clarity, usability, testability, development opportunities as well as use in other problem areas. The criterion is quantitative, when it makes sense to compare values. An intermediate position between quantitative and qualitative criteria are criteria with a scale. Of course, when analyzing and solving multiobjective optimization problem is only necessary to apply the definitions and concepts, methods and procedures, which result in appropriate conclusions and recommendations.

System studies are a symbiosis of theoretical model simulations with observations, empirical studies, full-scale (laboratory) experiments. The leading role of the simulation is that the model should be preceded by a full-scale experiments and to indicate the direction of the collection of information in the process of observation. At the same time, the results of modeling studies need to be the actual source of data and require experimental verification. This systematic approach allows to understand the connections between individual facts and on a higher level to carry out the study. The theoretical value of a systems approach is to determine the general laws (isomorphic for different classes); this applies especially to the backbone factors.

This approach was used effectively in the development of materials for special purposes as a complex system. At cognitive modeling was used principle of simulated. Composite material (complex system) was presented as a finite set of models that reflect the essence of a particular facet of the system (Garkina and Danilov, 2013; Danilov and Garkina, 2015). Each of the properties of the material is investigated in one or more simplified (narrowly focused) models. Building the set of simplified model allows to identify new properties and often without building generalizing model. The composite material is defined as the result of the interaction of simplified models.

RESULTS AND DISCUSSION

Annex to the development of radiation-shielding materials: This approach was used in the development of radiation-shielding materials (Bazhehov *et al*., 2012). By methods of mathematical planning of the experiment were determined the analytical dependences of quality criteria (porosity q_1, %, compressive strength q_2, Mpa, the density q_3 (hereinafter, it has been possible to exclude from consideration)) from volume fractions $x_1 \in [0.5;0.6]$, $x_2 \in [0.35;0.4]$ aggregate and filler:

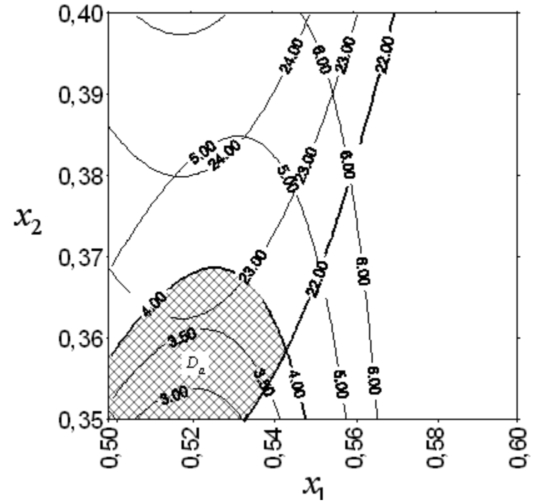

Fig. 1: Search area

$$q_1(x_1,x_2) = 196,9\text{-}1217x_1\text{+}623,6x_2\text{-}1064x_1x_2\text{+}1532x_1^2$$
$$q_2(x_1,x_2) = \text{-}305,3\text{+}1188x_1\text{+}57,20x_2\text{-}1148x_1^2$$

Optimization by the method of successive concessions showed that the minimum value of porosity is achieved at the point M_1 (0.519; 0.35)for which q_1 (0.51; 0.4) = 2.735% and the maximum strength corresponds to the point M_2 (0.518; 0.4) for which q_2(0.51; 0.4) = 25.14 MPa. Later in the synthesis of the material basis of the conditions $q_1 \leq 4\%$, $q_2 \leq 22$ MPa (area D_a, Fig. 1).

CONCLUSION

- It is proposed methodological principles of a systematic approach to the development of composite materials
- Is given the application of developed approach to the synthesis of materials with special properties
- The efficiency of the proposed the methodological principles is confirmed in the design and optimization of composite materials for protection against ionizing radiation

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