Systems Approach to Analysis of Destruction of Cement Composites

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Abstract. A new approach to the creation of composite materials using system analysis methods is proposed. A composite is considered as a set of elements connected by relations generating an integrative quality. When studying the properties of materials, synergetic, informational and homeostatic approaches are implemented. It is noted that when the integrative parameters of the system approach the maximum permissible, a systemic crisis occurs: the system enters the bifurcation zone. The system attributes and methods for selecting elements and subsystems are determined taking into account the paradoxes of integrity and hierarchy; their implementation is indicated in the development of radiation-protective composite materials. Issues of paradigm shift in the development of composite materials are touched upon. The new paradigm does not include the old one. It is stressed that in a paradigm shift there is no continuity of theories; involves the formation of another system of views based on fundamentally new basic models and the change of the principle of management of initial structure formation. On identification, the principle of simulating a complex system is used (it was represented by a finite set of models that reflect a certain facet of its essence) and purposefulness (matching a complex system with many private criteria and specially developed global criteria that describe its existence as a whole). An example of the synthesis of composites based on the identification of kinetic processes of formation of their physical and mechanical characteristics is indicated. Some aspects of evaluating the durability of materials are considered; the destruction of the system is interpreted as a catastrophe associated with a violation of homeostasis. It is assumed that structural elements are formed from elementary particles, which, under the influence of external factors, are combined into molecules, clusters, globules and fibrils; associative clusters and more complex ordered packing of structural elements appear. The approaches of Benoit Mandelbrot are used, a quantum-mechanical description of the process of destruction of a solid body: a solid body is represented as a set of elementary oscillators; energy is released and absorbed by elementary portions - quanta; destruction of one structural element does not lead to destruction of the entire system; destruction is considered as a process proceeding at scale levels. An illustration is given of a systematic approach to modeling a cement composite as a complex scale-invariant system with the indication of particular models.
1. Introduction

Currently, a new approach is being actively developed to create building materials as systems using system analysis methods [1]. Namely: composite material is considered as a set of elements connected by relations generating integrative quality (in the absence of integrative quality, a complex object is not a system). From the point of view of the synergetic approach, the inherent properties of Nature are uncertainty and chance, and chaos is not only a complete disorganization and destruction of the structure, but also a potential source for the further development of a more complex and highly organized system. Information is considered as a measure of complexity, internal diversity and the probabilistic choice of one of the possible trajectories of the system. The determination of the mechanisms for maintaining, within acceptable limits, the parameters vital for the system by controlling its integral parameters and, therefore, preserving (homeostasis) systems is the basis of the homeostatic approach (with isomorphism of the structures of two systems, the results of the study of one homeostatic system can be directly used to evaluate the functioning of the other). The integrative quality of the system is maintained until the value of the system-forming parameter goes beyond the specified region, and when leaving the domain of partial homeostasis, this leads to the transition of the system to a new qualitative state without destruction of the system (systemic, general homeostasis ensures the preservation of integrative quality, and particular - specific component). As the integral parameters of the system approach the maximum permissible, a systemic crisis arises: the system enters the bifurcation zone.

2. Composite materials as systems

It is easy to notice that building composite materials are indeed systems [2,3], since they have the corresponding system attributes (Fig. 1). The selection of elements and subsystems for studying the system can be done by dividing into many component elements (systems of various nature) with the identification of system-forming inter-element connections and relations that give integrity. Another way of isolating the system is also possible - this is not a representation of the entire object under investigation, but only of its individual sides, which are essential for the problem under study. Here, each system in the same object (composite material) expresses only a certain facet of its essence. Such an application of the concept of a system allows a thorough and complete study of various aspects of a single object (fracture mechanics, wettability, capillary processes, etc.). a system-wide holistic approach. Here, all private, local goals obey the common ultimate goal.

![Figure 1. Composite material as a system](image-url)
Obtaining composite material with a given level of quality requires the development of an effective technology (with the scientific organization of production). The concept of “quality” is expanding and includes not only the requirements for the manufacture of the material (technological process), but also its compliance with operating conditions (operational properties and durability) and structure formation processes under the influence of operational factors. Naturally, the principle of adjusting the recipe and the production should be implemented not only according to the results of the initial state of production (quality after the completion of the technological cycle), but mainly taking into account transformations of the structural parameters of the product under the influence of operational factors. The material resistance potential (used to predict durability) and the kinetics of its consumption under the influence of individual or a combination of environmental factors are taken into account. The identification of the technological process and the construction of an adequate model of “recipe-technological factors - structure - quality of the material” are carried out [4,5].

3. Paradigms in the development of composites

Within the strict framework of the existing paradigm, the most indicative facts from the point of view of the paradigm are used; theories are refined; more complex and thin equipment is being developed; in the future, the paradigm proper is being improved [6]. Due to the impossibility of explaining a number of facts within the framework of the current paradigm, there is a crisis of the old paradigm, the search and design of a new paradigm, verification and elimination of competing theories. Accepted rules are abolished, except for those suitable for the new paradigm (reconstruction of prescriptions: not just denial of the rules, but the preservation of positive experience suitable for the new paradigm). It is important to note that the new paradigm does not include the old. With a paradigm shift, there is no continuity of theories. It involves the formation of another belief system based on fundamentally new basic models and a change in the principle of controlling the initial structure formation: not the formation of a material structure with parameters that ensure initial quality (after manufacture), but the formation of a structure (organization) that ensures quality over time (during operation); acceptable decline in quality indicators. So, in particular, on the basis of cognitive modeling of materials, taking into account the hierarchical structure of quality criteria, a hierarchical structure of radiation-protective materials was developed [7]: a composite material was defined as a composite object, parts of which were considered as systems that were naturally combined into a single whole in accordance with certain principles or interconnected given relationships.

The system was divided into a finite number of parts (subsystems). Each subsystem (of the highest level), in turn, was divided into a finite number of smaller subsystems, etc., up to obtaining subsystems of the first level (elements; objectively not subject to division into parts, or regarding their further indivisibility there was relevant agreement). The properties of the system as a whole were determined not only by the properties of the elements, but also by the nature of the interaction between them. Two systems with pairwise identical elements, but with different interactions between them, were considered as two different systems. The principle of simulating a complex system was used: a complex system is representable by a finite set of models that reflect a certain facet of its essence (the ability to study a property or group of properties of a complex system using one or more simplified narrowly oriented models). They were limited to building up a lot of simplified models (the identification of new properties does not have to be accompanied by the construction of generalizing models). In the synthesis of composites based on the identification of kinetic processes of formation of their physic-mechanical characteristics [8, 9], the principle of purposefulness was also used (allowed matching a complex system with many particular criteria and specially developed global criteria that describe its existence as a whole [10]). As experience shows, including our own [11,12], the systematic approach does not exclude the possibility of obtaining sufficient accuracy for estimating unknown parameters by the method of successive approximations. The relevance of the significant development of analytical research methods based on the theory of random processes is not lost.
4. Durability assessment

Further we will consider issues of material durability from a system perspective. In [13], the destruction of the system is interpreted as a catastrophe associated with a violation of homeostasis. The ability to disaster is a family property of complex systems, it is impossible to eliminate it, it is inherent in the nature of a complex system. We can assume that complex systems always work as damaged. The system continues to operate due to many additional means of ensuring stability. Her work is an ever-changing combination of component failures and restorations. When noticeable global failures occur and several individually small harmless failures are combined, the possibility of a global system crash is created. Each of these failures provokes an accident, but only together they lead to destruction (there are much more opportunities for system failures than the emergencies that have manifested). Most of the opportunities are blocked at an early stage of development by means of protection created for this. A systemic accident occurs as a result of a combination of many errors: there is no single cause of the accident and it is often impossible to determine its root cause. A retrospective analysis of disasters, especially with expert assessment, is biased (technical misunderstanding of the nature of the failure makes it easy to find the culprit of the disaster).

When assessing the durability of cement composites as complex systems, it was assumed that structural elements are formed from elementary particles, which, under the influence of external factors, are combined into molecules, clusters, globules and fibrils; associative clusters and more complex ordered packing of structural elements appear (cubic, hexagonal, octahedral, etc.; [14]). With the change in the energy state of complex systems, the forms of structure formation also change. Now, in place of the hypothesis of a continuous medium (in classical mechanics, a deformable solid), ideas about the discrete structure of the medium have also formed. According to Benoit Mandelbrot, many forms in Nature are so irregular and fragmented that, in comparison with Euclidean objects, not only a higher degree is demonstrated, but a completely different level of complexity (particular as a whole; adherence to the principle of scale invariance; at each scale level, structures are formed that can be considered similar to structures at adjacent material levels [15]). In a quantum - mechanical description of the process of destruction of a solid body, the hypothesis is valid: the discrete structure of matter (a solid body is represented as a set of elementary oscillators), on the discrete nature of the release and absorption of energy (energy is released and absorbed by elementary portions - quanta); the destruction of one structural element does not lead to the destruction of the entire system (translates it into a new energy state; [16]). Here, destruction is considered as a process proceeding at scale levels (an integral manifestation of the simultaneous occurrence of processes taking into account the activation energy, critical stress level, and relaxation time).

In the classical theory of resistance of materials, the tensile strength is considered as the ultimate stress corresponding to the beginning of the progressive destruction of the material and is calculated on the basis of data on atomic bonds in crystal lattices; depends on the type and number of defects in its structure (in metals - dislocations, distortions of atomic-crystalline spatial lattices; in composites - pores, inhomogeneities, inclusions). Usually, to increase the strength, elimination or reduction of the number of dislocations, the creation of metals with the correct atomic crystalline structure are used; an increase in the number of heterogeneities, the creation of dampers to absorb the energy of destruction.

The destruction of a solid from the standpoint of the theory of complex systems can be considered not as a critical event of the limiting state of a system, but as a process related to different scale levels. The process of destruction of solids begins from the moment of power, temperature, chemical, radiation and other energy effects. At the first stage, plastic loosening accumulates in the material structure, the smallest cracks and other structural defects are formed; at the second stage, the formation of new cracks is possible, the formation of a main crack (described by the laws of mechanics of fracture of solids; [15, 17]). The growth of the main crack to critical sizes leads to the destruction of fractals (structural elements) and, finally, with the progressive development of the crack, the destruction of the solid occurs [17]. Destruction begins at the microdimensional scale level (kinetic-fluctuation approach of description; [18]). As a result of microdestruction, loosening, softening of the material occurs; prerequisites are created for the growth of technological cracks (the release and absorption of energy by
individual quanta; discrete fractures of individual or associative fractals). During the destruction of microcracks, structural defects or damping elements appear, stopping the development of cracks until another portion of the fracture energy is accumulated.

5. Prediction of cement composite strength

As an illustration, we present a systematic approach to predicting the strength of a cement composite as a complex scale-invariant system [14 ... 19]. The hierarchy of its structure was determined on the basis of the principle of self-similarity at any scale level of the structure of the composite (cement composites at each level are represented by a matrix and a filler). An integral component of the internal structure was considered structural defects: pores, cracks, cavities. Filler and aggregate particles were considered defects. The adhesion of the matrix with the filler was attributed to the pores. The fractal dimension was considered a quantitative measure of the order of fractal structures (for structural elements of composites it has the same fractional value at any scale level; for cement composites was determined by Mandelbrot-Richardson).

The compressive strength of concrete was evaluated by the relation [19]:

\[ R_b = \frac{R_l}{1 - \left( \frac{E_2}{E_1} \cdot \frac{\mu_2}{\mu_1} \right) (1 - \theta)} \left( \frac{q_1 + E_2}{q_2} \right) \]

\( R_1, \mu_1, E_1 \) - strength, Poisson and Young modulus of the matrix; \( \mu_2, E_2 \) - Poisson and Young modulus of the placeholder; \( q_1, q_2 \) - relative volumetric contents of the matrix and placeholder; \( \theta \) - the relative length of the zone of external adhesion of the matrix with a placeholder.

The fractal dimension of the pore space and other heterogeneities of the considered composites is close to 1.5; the linear size of the structural defect (cracks, pores) at scale level \( \delta \) was determined as:

\[ L(\delta) = a \delta^{d-d_n} = l_0 \delta^{d-d_n} l_0 \delta^{-0.5} \]

\( d_n \) - fractal dimension; \( d \) - Euclidean dimension; \( a \) - a factor equal to half the length \( l_0 \) of the crack.

The fractal model of the cement composite was represented by a complex system consisting of flat structural elements, each of which contains a crack-shaped defect in length \( L(\delta) \) (Fig. 2). The model was built under the assumption of validity of hypotheses during the manufacturing process, many congenital (technological) cracks are formed in the cement composite; the conditions of scale invariance and self-similarity are satisfied for the system; orientation of cracks in space - random; the strength of cement composites at various scale levels depends on the size of the cracks.

The tensile strength of the primary fractal (structural element) was determined based on the Griffiths model:

\[ R_{Gr} = \frac{4 \gamma E}{\pi \delta} \cdot \delta^{0.5(d-d_n)} = k_1 \delta^{0.5(d-d_n)} \]

The compressive strength of \( R_G \) cement composite, taking into account the condition of the Coulomb - Navier strength, was calculated by the relation [2]:

\[ R_G = \frac{4 k_1 k_2 \delta^{0.5(d-d_n)}}{\sqrt{\pi \delta} (1 - \beta)} \]

\( k_1, k_2 \) - stress intensity factors under tension and shear; \( \beta \) - coefficient of friction.

The strength of cement composites at various scale levels of the structure was described taking into account the previous one in the form:

\[ R_G(\delta) = R_{GU} \alpha_n \delta^{0.5(d-d_n)} \]

\( R_{GU} \) - the strength of the structural element, the reference sample of specific sizes \( \delta \); \( \alpha_n \) - cast coefficient.
Figure 2. Fractal model of concrete structure: a) is the primary fractal; b) - calculation model of the fractal; c) - chain fractal; d) - a flat fractal; 1 ... 5, - structure levels.

If the structural element is represented by a cube with the size of the edge \( \delta = 15 \text{ cm} \) at \( d = 1, d_m = 1.5 \) then according to the previous one:

\[
\frac{R_s(15)}{R_{SU}} = \alpha_u \cdot \delta^{-0.25} = 1
\]  

At \( \delta = 15, \alpha_u = 1.97 \), the change in strength, taking into account scale invariance, will be described by the relation:

\[
R_G(\delta) = R_G(15) \cdot 1.97 \cdot \delta^{-0.25}
\]
The calculation results are shown in Table 1 and in Figure 3.

**Table 1. Values of** $\frac{R_{bi\alpha}}{R_{bi0}}$ **depending on the size of the rib (scale factor** $\alpha$ **)**

| No | $\alpha_i$ | Numerical values |
|----|-------|------------------|
|    | $R_{bi\alpha}$ | $R_{bi0}$ |  |
| 1  | $\alpha_i$, m | $1 \cdot 10^{-5}$ | $1 \cdot 10^{-4}$ | $1 \cdot 10^{-3}$ | $1 \cdot 10^{-2}$ | $1 \cdot 10^{-1}$ | $1.5 \cdot 10^{-1}$ | $2.0 \cdot 10^{-1}$ | $4.0 \cdot 10^{-1}$ |
| 2  | $1.97 \alpha_i^{-0.25}$; $\alpha_0 = 15$ | 11,1 | 6,23 | 3,5 | 1,97 | 1,1 | 1,0 | 0,93 | 0,788 |
| 3  | $0,58 + 0,42\left(\frac{\nu_0}{\nu}\right)^{1/\beta}$ | - | - | 42,58 | 4,78 | 1,0 | 0,86 | 0,79* | 0,685 |
| 4  | $\alpha_i$, cm | 0,001 | 0,01 | 0,1 | 1,0 | 10 | 15 | 20 | 40 |
| 5  | $1,75\alpha_i^{-0.25}$; $\alpha_0 = 10$ | 10,0 | 5,6 | 3,16 | 1,77 | 1,0 | 0,89 | 0,84 | 0,7 |

If the fractal dimension $d_m = d = 1$ (homogeneous defect-free structure, the linear dimensions of which are described by the Euclidean geometry), then the strength of the samples does not depend on the size; no scale effect.

**Figure 3.** The dependence of strength on the size of the cube: curve 1 - according to V.V. Bolotin, curve 2 - according to relation (1).

6. **Conclusions**

1. Implemented a new approach to the creation of composite materials using methods of system analysis; the composite is considered as a set of elements connected by relations generating an integrative quality. The system attributes and methods for selecting elements and subsystems are determined taking into account the paradoxes of integrity and hierarchy.
2. The author's implementation of synergistic, informational and homeostatic approaches in the development of radiation-protective composite materials is indicated.
3. Issues of paradigm shift are investigated: when changing paradigm there is no continuity of theories; it is supposed to form another system of views based on fundamentally new basic models and a change in the principle of managing the initial structure formation.
4. An illustration is given of a system approach to modeling a cement composite as a complex scale-invariant system with an indication of particular models.
References

[1] Irina Garkina and Alexander Danilov, “Mathematical Methods of System Analysis in Construction Materials“, IOP Conf. Series: Materials Science and Engineering, vol.245, pp. 062014, 2017.

[2] Irina Garkina and Alexander Danilov, “Mathematical Methods of System Analysis in Construction Materials“, IOP Conf. Series: Materials Science and Engineering, vol.245, pp. 062014, 2017.

[3] I.A. Garkina, A.M. Danilov V.P. Selyaev, “Materials as Complex Systems“, Journal of Engineering and Applied Sciences, vol.11(11), pp. 2461-2464, 2016.

[4] Garkina I., Danilov A., “Composite Materials: Identification, Control, Synthesis“, IOP Conference Series: Materials Science and Engineering, vol.471, pp. 032005,2019.

[5] I.A. Garkina and A.M. Danilov, “From the experience of development of composite materials with desired properties“, IOP Conf. Series: Materials Science and Engineering, vol.191, pp. 012006, 2017.

[6] Garkina I.A., Danilov A.M., Korolev E.V., “The evolution of ideas about composite materials from the standpoint of changing paradigms“, Construction materials, № 1-2, pp. 60-62, 2018.

[7] Grishina A.N., Korolev E.V., “New radiation-protective binder for special-purpose composites“, Key Engineering Materials, vol. 683, pp.318-324, 2016.

[8] Irina Garkina, Alexander Danilov, “Parametric identification and optimization of properties of building materials as complex systems“, J. Ponte, vol. 73, pp.119-12, 2017.

[9] Garkina Irina, Danilov Alexander, “Experience of Methods of Rank Correlation“, Key Engineering Materials, vol. 777, pp.8-12, 2018.

[10] Danilov A.M., Garkina I.A., “Control of Properties of Composite Materials - Quality Functional“, Defect and Diffusion Forum, vol. 394, pp.15-19, 2019.

[11] Irina Garkina, Alexander Danilov, Vladimir Selyaev, “Principles of Optimal Control in the Synthesis of Composite Materials“, Key Engineering Materials, vol. 723, pp.32-36, 2016.

[12] Danilov A.M., Garkina I.A., “Systems approach to the modeling and synthesis of building materials“, Contemporary Engineering Sciences, vol. 8 (5), pp. 219-225, 2015.

[13] Garkina I., Danilov A., “Property Modelling and Durability of Composite Materials“, IOP Conference Series: Materials Science and Engineering, vol. 471(3), pp.032004, 2019.

[14] Selyaev V.P., Kupriyashkina L.I., Korovina O.Yu., Kechutkina E.L., “Application of the Bose-Einstein model to analyze the time dependence of the strength of composite materials under the combined action of aggressive media, temperature and mechanical stresses“, Proceedings of higher educational institutions. Building. №8, pp.21-27, 2010.

[15] Selyaev V.P., Selyaev P.V., Kechutkina E.L., “The evolution of the theory of strength of concrete. From simple to complex“, Construction Materials. Scientific, technical and production journal, №12, pp. 70-78, 2016.

[16] Selyaev V.P., Kupriyashkina L.I., Neverov V.A., Selyaev P.V., “Fractal models of concrete destruction“, Regional architecture and construction, №1, pp. 11-23, 2015.

[17] Selyaev V.P., Selyaev P.V., Sorokin E.V., Kechutkina E.L., “Forecasting of the durability of reinforced concrete bent elements by the method of degradation functions“, Housing construction, №12, pp. 8-19, 2014.

[18] Travush V.I., Selyaev V.P., Selyaev P.V., Kechutkina E.L., “On the possible quantum nature of deformation and destruction of composites“, Industrial and civil construction, №9, pp.94-100, 2016.

[19] Selyaev V.P., Selyaev P.V., “Physico-chemical fundamentals of fracture mechanics of cement composites“, Monograph, Publishing house Mordov. University, Saransk, 203 p., 2018.