IOP Conf. Series: Materials Science and Engineering **191** (2017) 012006 doi:10.1088/1757-899X/191/1/012006

From the experience of development of composite materials with desired properties

I A Garkina and A M Danilov

Department of mathematics and mathematical modeling, Penza State University of Architecture and Construction, 28 Herman Titov street, Penza, Russia

E-mail: i.a.naum@mail.ru

Abstract. Using the experience in the development of composite materials with desired properties is given the algorithm of construction materials synthesis on the basis of their representation in the form of a complex system. The possibility of creation of a composite and implementation of the technical task originally are defined at a stage of cognitive modeling. On the basis of development of the cognitive map hierarchical structures of criteria of quality are defined; according to them for each allocated large-scale level the corresponding block diagrams of system are specified. On the basis of the solution of problems of one-criteria optimization with use of the found optimum values formalization of a multi-criteria task and its decision is carried out (the optimum organization and properties of system are defined). The emphasis is on methodological aspects of mathematical modeling (construction of a generalized and partial models to optimize the properties and structure of materials, including those based on the concept of systemic homeostasis).

1. Introduction

Due to the complexity and diversity of the functioning processes in real systems can not get them absolutely adequate mathematical models. The developed mathematical model describing the process of formal operation of the system, is able to cover only the basic characteristic patterns. You can not specify the formal rules to select the characteristics of the studied states and parameters of real systems. The researcher has to be guided only by their own intuition, relying on the statement of the problem and applied understanding of the processes of functioning of the system. Analysis of each complex system - this is a unique problem that requires not only diverse cultures, but also the inventiveness and talent. System studies are a symbiosis of theoretical model simulations with observations, empirical studies, full-scale (laboratory) experiments. One of the main problems is to determine the general laws governing the functioning of the system based on individual private observations. This also applies to the problems of building materials [1-4].

System operation conditions are determined by the input variables $x_1, x_2, \ldots, x_n$ (factors); some of them amenable to regulation or partial management. The behavior, the result, the effectiveness of functioning of the system are characterized by output variables $y_1, y_2, \ldots, y_m$ (responses, resulting variables). Random latent variables $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_m$ (not amenable to direct measurement) reflects the impact on the value of unrecorded at the input factors (random measurement error of the analyzed indicators, residues). So at winter concreting electro-conductive concrete which durability depends on its structure is applied. The factors are: the percentage of Portland cement - x_1, sand - x_2, graphite - x_3, water - x_4; strength conductive concrete - y. The main objective is to construct a function

$$\mathbf{f}(x_1, x_2, \ldots, x_p) = \left(f_1(x_1, x_2, \ldots, x_p), \ldots, f_m(x_1, x_2, \ldots, x_p)\right)^{\mathrm{T}},$$

adopted in some sense makes the best restore the value of the $\mathbf{y} = (y_1, y_2, \ldots, y_m)^{\mathrm{T}}$ by $\mathbf{x} = (x_1, x_2, \ldots, x_p)^{\mathrm{T}}$, T - transposition symbol.

2. Formulation of the problem

The main objectives of the statistical analysis in building materials are:

- establish a statistically significant association between the variables $\mathbf{y}$ and $\mathbf{x}$ (components $\mathbf{x}$ and $\mathbf{y}$ can be: *quantitative* (for example, the percentage of component in material)**,** *ordinal* (ordering of objects analyzed according to the degree of manifestation being studied properties; for example, education worker, discharge working, etc.), *classification* (divide objects into homogeneous classes, not amenable to streamline; for example, methods for the treatment of concrete products, the availability of competing additives or fillers et al., employee profession, industry, the motive of family migration, etc.);
- outlook (recovery) $\mathbf{y}$ to $\mathbf{x}$ (determined the values of the function $\mathbf{f}(\mathbf{x})$, but not its structure);
- identification of causal relationships between $\mathbf{x}$ and $\mathbf{y}$, partial control $\mathbf{y}$ by regulation $\mathbf{x}$.

The solution of these tasks to determine the physical meaning of the statistical relationships (for example, depending on the properties of the materials studied on factors). *Standard techniques and methods to determine the structure of the model (the general form of the function* $\mathbf{f}(\mathbf{x})$*) does not exist.* In the staging phase of statistical analysis each elementary object of research is associated with a set of analyzed parameters $\{x_1, x_2, \ldots, x_p, y_1, y_2, \ldots y_m\}$; determined the final purpose of the study, the type of study dependencies, the shape and the degree of accuracy of statistical conclusions. Information step is to collect the results of measurement of statistical information

$$\{x_1^{(i)}, x_2^{(i)}, \ldots, x_p^{(i)}, y_1^{(i)}, y_2^{(i)}, \ldots, y_m^{(i)}\},\ i = \overline{1,n}.$$

The structure of connections and their tightness (class $\mathbf{F}$ of feasible solutions; view, the desired connection between the structure $\mathbf{x}$ and $\mathbf{y}$ the (family of functions $\mathbf{f}$) between the study variables) are determined based on the correlation analysis. Calculates an estimate of the parameters in the test equation the statistical relationship. If the class $\mathbf{F}$ is defined as a parametric family of functions $\{\mathbf{f}(\mathbf{x},\mathbf{\Theta})\}$, the problem boils down to the selection of (statistical estimation) Θ values of the conditions for an extremum of a functional (for example, the method of least squares). Of course, it provides an analysis of the accuracy of the constraint equations.

In a dynamic system, there is an interaction between its heterogeneous parts*,* and formed observed (output) signals. All other signals are considered as perturbations (input signals, measured and is not measured noise). *The totality of the alleged links between the observed signals and is a model (in the broad sense).* The model can take different forms and degrees of mathematical detail (or at all without using the language of mathematics). Ambiguous choice of identification method (the incompleteness of knowledge about the object, limitations in the observations of the object in time, the inaccuracy of the measurement signals at the input and output of the object, and so on.).

The adequacy of the system model and the object of study can not prove: model can be accepted or rejected on the grounds that obtained the assessments and conclusions contradict the observed facts. System model will always be different from the original; we can talk about the asymptotic approximation to it under certain conditions for each practical task. Asymptotic convergence is ensured by the fact that the object of the simulation is a concrete system with inherent only to her autonomous operation of law (peculiar and unique to this system). The adequacy of the system model is achieved by narrowing the scope of its use *(limited practical applicability of the model). Model experiments provide an 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. Today is no unified theory of constructing system models, to fully implement the concept of systemic homeostasis. System modeling studies are always iterative. In assessing the effectiveness and reliability of the model be used quantitative criteria;

qualitative criteria allow us to estimate a model in terms of its clarity, usability, testability, applications in other areas of concern (an intermediate position between the quantitative and qualitative criteria is the criteria with point scale). Model experiments precede full-scale and direction information collection point in the process of observation (the leading role modeling). At the same time, the results of modeling studies need to be the actual source of data and require experimental verification. A systematic approach can reduce or even eliminate the uncertainty inherent in the problem at hand; reconstruct it in the models that meet the objectives of the study; identify objects, properties and relationships of the studied system, taking into account the mutual influence of the external environment. It allows you to understand the connections between individual facts and on a higher level to carry out the study. The theoretical value of the systems approach is that it allows you to define general patterns that are isomorphic for different classes; the most important of them is isomorphic backbone factor.

3. Synthesis of materials for special purposes as the complex systems

The approach the authors used effectively in the development of materials for special purposes as the complex systems. The role and place of the identification in the synthesis follow from Fig. 1.

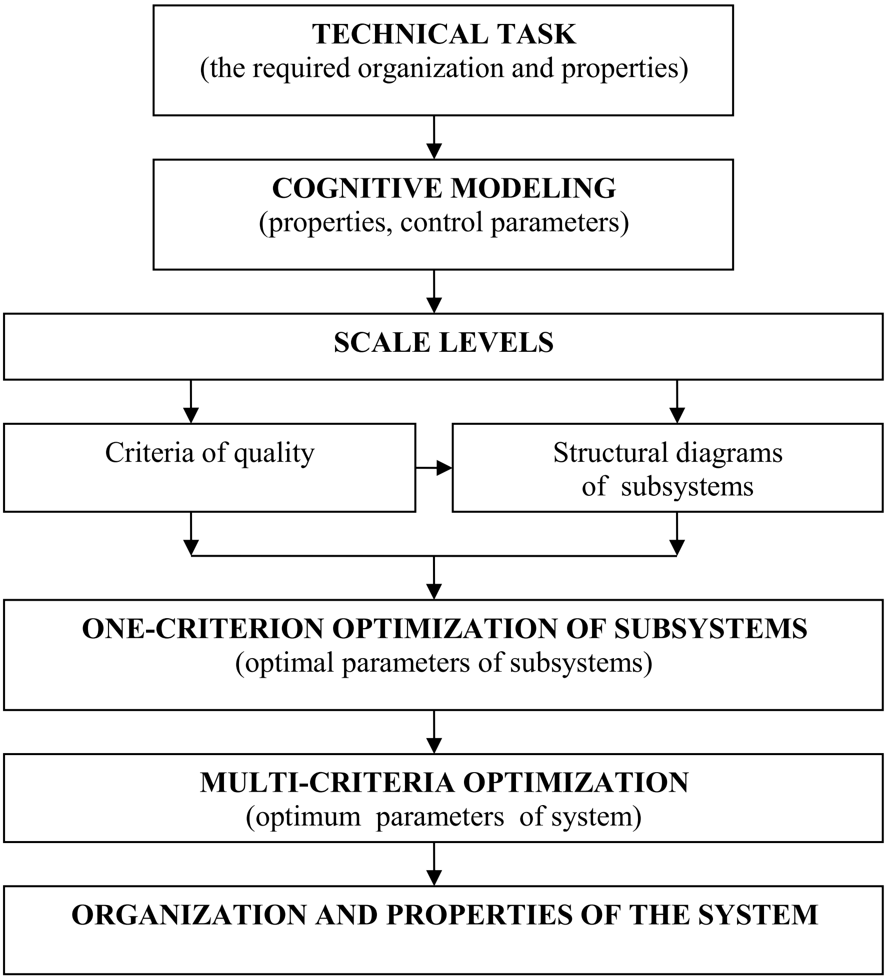

Figure 1. Synthesis of complex system

The synthesis began with a cognitive modeling. Identification is interdisciplinary. Therefore, in the composition of the expert group to develop terms of reference included experts of various fields (materials scientists, physicists, chemists, mathematicians, managers, experts in the field of system analysis, etc.). Each of the representatives played a dominant role in determining the individual pieces of the system; inter-element connections are established by the whole group. The cognitive model has allowed to produce material decomposition (synthesis of an integrated system reduces to solving the problems of synthesis of subsystems). Class of mathematical models of radiation-protective composites was selected; later they were used to optimize the structure and properties (fragments were seen as a subsystem; identify ways of measuring their properties). In drawing up the cognitive map is important not to miss the connection, which is determined by the considered property; «... quite insignificant reason escapes us by its smallness, it is a significant action that we can not foresee, and then we say that this phenomenon is a result of the case» (A.Poincare; a violation of the principle of transitivity). Linked to this is the difficulty of determining the number of partial criteria that are determined by the required performance of the material.

If the material is multi-layered structure, the construction of a mathematical model is almost impossible. Therefore, postulated the existence of a mathematical model to replace the identified object. Material properties were seen as particular criteria; structure of the material defined as the totality of their.

According to the results of cognitive modeling (using simulated principle) a complex system (composite) was represented as a finite set of models that reflect the essence of a particular facet of the system. Each of the properties of the material investigated by one or more simplified (narrowly focused) models. Building the set of simplified models revealed new properties (often without building a model generalizing). In other words, the composite material is determined by the interaction of simplified models [5, 6].

Structural identification is carried out (selection-end models) the solution of the general problem of identification in the selected class of models, as well as the decision of private problems of identification (parametric). Accordance with the basic requirements for the model: ease of interpretation of the physical meaning of the coefficients included in the model. Thus, the regression models are illustrative and are not used for the prediction and purposeful change factor values.

Each of the operating characteristics of the material was considered as an asymptotic value of the solution of the differential equation (kinetic process of the formation of physical and mechanical characteristics). Such representation is not the sole (test class may be replaced if necessary). Unfortunately, as a rule, there is a problem of correctness. We need the correct formulation of the problem with the involvement of additional information on the desired solution (or should use the classic control algorithms for ill-posed problem). The main kinetic processes (set of strength, changes in the modulus of elasticity, contraction and shrinkage, the increase of internal stress, heat resistance, chemical resistance, water absorption and water resistance) were modeled in a class of ordinary fourth-order differential equations with constant coefficients and real roots of the characteristic polynomial [5-7]. Concentrations and granulometric characteristics were determined by the material ingredients depending on the requirements (critical concentration, dependence of the critical volume concentration of the mean aggregate size distribution, the averaged effective strength of the material).

Proceeding from the above, we propose the following synthesis scheme:

- modeling of individual properties;
- selection of main parameters of models;
- determining of model parameters from composition, technological characteristics;
- determining a plurality of partial criteria;
- ranking the properties of materials;
- minimizing of dimension of the criterions space;
- multi-criteria optimization of the quality of the material and the corresponding prescription and process parameters.

Multi-criteria optimization was to optimize the vector of the objective function $\mathbf{q}(\mathbf{x}) = (q_1(\mathbf{x}), q_2(\mathbf{x}), \ldots, q_m(\mathbf{x}))$, if the criteria adopted are equally significant. In some cases, multi-criteria problem of minimization of the vector $\mathbf{q}(\mathbf{x})$ (using weighted sums of the strategy) was reduced to a scalar problem (accepted $q(x) = \sum_{i=1}^{n} \alpha_i \cdot (q_i(x))^2$). Definition of integrative properties of systems at

IOP Conf. Series: Materials Science and Engineering **191** (2017) 012006 doi:10.1088/1757-899X/191/1/012006

a qualitative level was made on the basis of independent studies of separate subsystems (with a certain degree of autonomy). Combining separate subsystems into a single system carried with allowance for interconnections. Each element in the hierarchical structure of the quality system was defined autonomously (without all the interconnections). Interconnections eliminated by introducing customizable reference models with a simultaneous decentralization of modules for inputs. Selection of parameters was done using the experimental samples.

4. Conclusions

Given the experience in the development of a number of composites developed a scheme of synthesis of building materials with predetermined properties and structure. It is proposed methodological principles of creation of materials (as complex systems) using a system approach.

References

[1] Korolev E V, Smirnov V A 2013 Using Particle Systems to Model the Building Materials (Advanced Materials Research Vol 746) pp 277-280
[2] Grishina A N, Korolev E V 2016 Influence of Nanoscale Barium Hydrosilicates on Composition of Cement Stone (Key Engineering Materials Vol 683) pp 90-94
[3] Loganina V I, Makarova L V, Tarasov R V 2016 The Effect of Filler Based on Calcium Silicates on Strength of Lime Composites (Applied Mechanics and Materials Vol 835) pp 531-534
[4] Kiselev D G, Korolev E V, Smirnov V A 2014 Structure Formation of Sulfur-Based Composite: The Model (Advanced Materials Research Vol 1040) pp 592-595
[5] Danilov A M and Garkina I A 2015 Systems approach to the modeling and synthesis of building materials (Contemporary Engineering Sciences Vol 8) pp 219-225
[6] Budylina E A, Garkina I A, Danilov A M 2015 Control of multi-objective complex systems (Contemporary Engineering Sciences Vol 8) pp 441-445
[7] Garkina I A 2015 Modeling of kinetic processes in composite materials (Contemporary Engineering Sciences Vol 8) pp 421-425