Optimization of the structures material based on the integrated approach

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Abstract. One of priority problems of construction materials science is assignment of prescription and technological parameters of receiving materials taking into account a complex of requirements imposed to properties of concrete mix and concrete, as well as for a design and the material production is intended and formulated in this article. It is shown that this problem can be most effectively solved by methods of computer materials science.

1. Introduction

Modern trends in construction materials science are distinguished by increased requirements to the raw materials quality, obtaining construction composites technology and the operational properties of products. The basis of these requirements should be the principle of civilization sustainable development, taking into account the interests of both contemporaries and future generations. With respect to construction materials science, the priority is to ensure the environmental efficiency of the decisions made at all stages of the product life cycle — from the impact on the environment of the raw materials, technological processes and finished products used, to the utilization of the latter. Thus, obtaining environmentally safe and at the same time economical products is a complex multi-purpose and multi-parametric problem, the effectiveness of the solution, which is determined by the methodology used.

Currently, the basis of such a methodology in science and technology, in particular, construction is a differentiated approach, where the task is divided into “technological” and “design” components. In the first case, prescription and technological parameters are assigned by technologists without taking into account the peculiarities of the material work in the structure (“for brand”), and in the second, the design of products is carried out by designers according to Construction Rules and Regulations (SNiP), without taking into account the formulation and technological parameters of manufacturing the products.

Unlike the differentiated, an integrated approach provides for optimization of prescription and technological parameters for the construction materials production in accordance with a set of requirements not only for the material and technological parameters of product manufacturing, but also for the design itself, which this material is intended for.
2. Problem setup

For correct formulation and solution of the optimization task, it is necessary to determine the objective function, which assumes the cost of a unit of volume of iron-concrete structure

\[ C_{bc}(x) = \sum c_i + (\sum T_{ja} c_j)/V_b, \]

where \( V_b \) is a volume of concrete in the structure, \( \text{m}^3 \); \( c_i \) is the cost of \( i \)-th \( (i = 1, \ldots, I) \) component in concrete mix in a unit of volume of concrete, \( \text{rub.}/\text{m}^3 \); \( c_k \) is a reduced to \( 1 \text{m}^3 \) of concrete cost of \( l \)-th technological redesign \( (l = 1, \ldots, L) \), \( \text{rub.}/\text{m}^3 \); \( T_{ja} \) is a mass of reinforcement of \( j \)-th class \( (j = 1, \ldots, J) \) in the product, \( t \); \( c_{ja} \) is the cost of unit of mass of reinforcement of \( j \)-th class, \( \text{rub.}/t \); \( x \) is variable parameters (in the formula (1) and further in the symbol \( \Sigma \) the summation indices are omitted).

Peculiarities of the integrated approach methodology will be considered on the example of optimization of reinforced concrete mix structures without taking into account the technological peculiarities of their manufacturing, i.e. when only the prescription task solving. Then the contribution of technological costs in (1) will be constant and can be ignored in the variant design case of the concrete composition, and the objective function \( C_{bc}(x) \) will be the cost per unit volume of the reinforced concrete structure

\[ C_{bc}(x) = \sum c_i + (\sum T_{ja} c_j)/V_b. \]  

The task of the concrete composition optimizing, taking into account the requirements for both the properties of the concrete mix (for example, mobility, non-dissipation, volume of intergranular openings, etc.) and concrete (for example, average density, strength, frost resistance, etc,), and reinforced concrete structure, which concrete production is intended (for example, strength, rigidity, crack resistance, etc.), we formulate in the following way: to find the costs of the concrete constituents mixture \( x_i \), so, the minimum material cost per unit is ensured of the reinforced concrete structure volume \( C_{bc}(x) \), and the requirements imposed both on the properties of the concrete mixture and concrete and on the construction made of this concrete, or, in a mathematical formulation:

\[ x(x_i, \ldots, x_j), \]

at which

\[ C_{bc}(x) \Rightarrow \min \]

and simultaneously requirements are met, which are imposed on:

– properties of concrete mixture and concrete

\[ \varphi_{ma}(x) \leq \mathcal{R} \{ \varphi_{ma}(x_i) \}; \]

– properties of a reinforced concrete structure

\[ \varphi_l(x_i, x_p, x_j) \leq \mathcal{R} \{ \varphi_l(x_i, x_p, x_j) \}; \]

– costs of concrete mix components

\[ x_i \leq \mathcal{R} \{ x_i \}; \]

– size of a structure

\[ x_p \leq \mathcal{R} \{ x_p \}; \]

– its reinforcement

\[ x_j \leq \mathcal{R} \{ x_j \}; \]

where \( x_i \) are variable parameters, which are the costs of the concrete mixture components in \( 1 \text{ m}^3 \) of concrete; \( x_p \) and \( x_j \) is the same, dimensions and reinforcement of the structure characterizing, respectively; \( \varphi_{ma}(x_i) \) stand for response functions, representing the properties of a concrete mixture and concrete, depending on the constituents of the concrete mixture \( x_i \); \( \varphi_l(x_i, x_p, x_j) \) – the same, being the properties of the structure and depending on the components of the concrete mixture \( x_i \), its dimensions \( x_p \) and reinforcement \( x_j \); \( \mathcal{R} \{ \varphi_{ma}(x_i) \}, \mathcal{R} \{ \varphi_l(x_i, x_p, x_j) \} \) - admissible values of the response functions \( \varphi_{ma}(x_i) \) and \( \varphi_l(x_i, x_p, x_j) \) - the same of variable parameters \( x_i, x_p \) and \( x_j \); symbol \( \mathcal{R} \) denotes the signs \( <, =, > \) or \( \leq \) or \( \geq \) used in compiling one- (for example, \( x_i \geq [x_i] \)) or two-sided (for example, \( [x_i] \leq x_i \leq [x_i] \)) constraints.
3. Methods
The solution of the optimizing problem the composition of concrete in the above formulation can be obtained by various methods, for example, on the basis of variable parameters separation [1]. In accordance with this principle, among all the variable parameters $x$, which the objective function $C_\text{m}(x)$ depends on, we distinguish the variable parameters determining the composition of concrete $x_{i_1}, \ldots, x_{i_k}$, the dimensions of the reinforced concrete structure $x_{j_1}, \ldots, x_{j_l}$, and the characteristics of its reinforcement $x_{p_1}, \ldots, x_{p_m}$. Further, we refer the variable parameters characterizing the composition of the concrete mixture $x_i$, to the 1st group, the dimensions of the construction $x_p$ – to the 2nd group of external variables, and the parameters characterizing the reinforcement of the product $x_j$ – to the group of internal variables.

In turn, for the admissible values of the concrete mixture properties, concrete and structure, external constraints (5) and (7), which contain only external variable parameters $x_i$, and internal (6), (8) and (9) constraints that contain external $x_p$ and internal or only internal variables $x_j$. Then the search for the values of the variables $x_i$ that ensure the minimum value achievement by the objective function $C_\text{m}(x)$ will represent the process of optimization, and the obtained result – the solution of the internal optimization problem. If optimization is performed for fixed external variable parameters and the solution of the external optimization problem external and internal or only external variable parameters can be changed.

The external optimization problem is solved by conducting experiments, each of which involves fixing external variables, checking external constraints, solving the internal optimization problem, and calculating the objective function. Experiments differ in the values of external variables that change from experience to experience in accordance with a particular rule is algorithm. The solution of the internal optimization problem is reduced to the calculation of the reinforced concrete construction in accordance with Construction Rules and Regulations (SNiP) 2.03.01 for concrete and reinforced concrete structures with fixed external variable parameters.

In accordance with the flowchart shown in figure, we will distinguish the following tasks of optimizing concrete compositions of reinforced concrete structures:

- **task 1**: only the first group of external parameters $x_i$ vary; such a situation arises with the traditional (“from the positions of technologists”) solution of the prescription task “for brand”, i.e. taking into account the requirements for the concrete mixture and concrete properties (item 5 in figure);
- **task 2**: the first group of external variables $x_i$ varies for fixed dimensions of the structure $x_p$ and its reinforcement $x_j$; in this case, the composition of concrete is optimized for a typical design, the dimensions and reinforcement of which do not change (items 4, 5);
- **task 3**: both the 1st and the 2nd groups of external variables $x_i$ and $x_p$ vary for a fixed reinforcement of the structure $x_j$; such a situation arises, for example, with an increase in the load-carrying capacity of a structure due to a change in its dimensions (items 3-5);
- **task 4**: external (composition) $x_i$ and internal (reinforcement) $x_j$ variable parameters vary for fixed dimensions of the structure $x_p$; in this case, along with optimizing the composition of concrete, optimization of the reinforcement of the structure is carried out (items 2-5);
- **task 5**: both external $x_i$ and $x_p$, as well as internal variables $x_j$ vary; such a statement of the problem arises in the general case of an integrated approach to optimizing the costs of concrete components $x_i$ (items 1-5).

The procedure for solving tasks 1-5 is to carry out experiments. In the first experiment, the values of the external variables first group $x_1^*$ are assigned (randomly or based on the available experience) and the external constraints (7) are verified; further, the values of the response functions $\varphi_{\text{exp}}(x_1^*)$ – the properties of the concrete mixture and concrete are calculated, and external constraints (5) are verified. Then fixed values are assigned to the 2nd group of external variables $x_2^*$, the condition for the fulfillment of external constraints (8) is verified and the internal optimization problem is solved – according to Construction Rules and Regulations (SNiP) 2.03.01, the reinforced concrete structure is
calculated, and by determining the parameters $x_j$ characterizing the product reinforcement, the fulfillment of the constraints (6), (9) are verified and the value of the objective function $C_b(x)$ is calculated. At the same time, if the constraints (5) - (9) are not satisfied, new values will be assigned to the variable parameters and their search continues until the end of the experiment.

**Figure 1.** Flowchart for solving the task of optimization of concrete composition of reinforced concrete structures (RP – reinforcement package; r.c.s. – reinforced concrete structure; OT – optimization task).

The experiments are repeated the required number of times, which depends, other things being equal, on the adopted optimization method for the objective function $C_b(x)$. For example, when using the method of a deformable polyhedron experiment represents realization in the space of variable parameters $x$ the vertex of the polyhedron, the vertices number, which must be one more than the
number of variable parameters, i.e. $n = (I + P + J) + l$. The results of experiments with initial fixed values of the variable variables $x^*$ form the vertices of the original polyhedron. In the future, the initially formed polyhedron is modified [2].

With respect to the formulated optimization problem (3)–(9), the algorithm of the initial polyhedron transformation consists in calculating the objective function at its vertices and then replacing the vertex where the objective function $C_b(x)$ takes the maximum value of $C_b(x^*)_{\text{max}}$, on a vertex with a minimum value of $C_b(x^*)_{\text{min}}$. The algorithm finishes the work if the polyhedron obtained at some $k$-th step coincides with the polyhedron obtained at the previous step of the algorithm, or degenerates to a point. The calculated values of the concrete components costs $x_i^k$, as well as $x_p^k$ and $x_j^k$ at the vertex of the polyhedron with the minimum value of $C_b(x^k)_{\text{min}}$ are optimal.

For practical implementation of the described optimization methods, there is a problem of the response functions adequate representation $\varphi_{\text{opt}}(x_i)$ – properties of concrete mixture and concrete (for the response functions $\varphi_i(x, x_p, x_j)$ – strength, rigidity and crack resistance of the constructions there are no fundamental difficulties, as they are determined by calculation in accordance with Construction Rules and Regulations (SNiP) 2.03.01), depending on the consumption of concrete constituents $x_i$. Such a representation can be performed using experimental statistical models obtained by methods of experiment planning or regression analysis [3].

4. Results
Let’s give an example of the differentiated and integrated approaches application for optimization of high-strength slag-pumice concrete compositions. It has been experimentally established that there is a sufficiently wide variation range of such concrete properties when the flow rate of the components varying, which reaches 36% for the axial extension strength, the initial modulus of elasticity is 16%, the average density in the dry state is 220 kg/m$^3$ for a fixed concrete strength on compression [4]. With the integrated approach to optimizing the compositions of high-strength slag-pumice-concrete, this avoids an increase in the compressive strength of concrete with no rigidity and / or crack resistance of the reinforced concrete structure due to an increase in the tensile strength and / or the modulus of concrete elasticity by varying its composition.

In the process of the composition of such concrete “for brand” selecting, the optimum composition was obtained with a cement flow of 380 kg in 1 m$^3$ of concrete mix, and taking into account the work of the same strength concrete in the slab of PC 4.5-88.12 designed under the action of a short-term strength load, rigidity and crack resistance, with a flow rate of 402 kg [4]. The difference in the cost of cement is due to the need to produce a concrete of increased elasticity to ensure the required slab rigidity. If long deformations are taken into account, even for such a brittle material as concrete, an even greater difference in the consumption of its constituents should be expected when considering the work of the material in the structure.

5. Conclusion
The idea of assigning concrete compositions according to a set of requirements not only for the properties of a concrete mix, technological parameters for the manufacture of reinforced concrete products, the properties of concrete, but also for structures was apparently not only formulated for the first time, the justification of the ways to solve it was given, but it was also practically realized in [4]. In the future, the idea of combining the construction materials science tasks and building structures was formulated in the form of an integrated approach to the solution of concrete science optimization problems. It was applied in [5] with reference to the definition of rational compositions and technological parameters for obtaining not only heavy concrete (a rational technological regime definition of rotational technology), but concrete on porous aggregates (for example, reinforced concrete pre-stressed sleepers made of high-strength slag-pumice concrete), wood plastic (technology for producing wood pressed cross-beam and composite sleepers), and the composition and processing parameters to receive bioplastic.
The problem of the integrated approach is touched upon in [6] in a different aspect where the optimization of the material is considered in accordance with the power circuit of the design. Therefore, the size of the fibers, their shape, concentration and position should change in the section of the structure according to the force calculation for fiber-reinforced concrete. The stressed state of the structure will determine the “integrated material” with a variable modulus of deformation along the product cross-section [6].

The term “integrated” can be referred both to the unification of tasks from one or several scientific areas into certain “over task”, in order to the unification of methods for their solution into a universal “over method”. With regard to construction, the combination of tasks can be performed at the level of the optimality criterion for a particular design, fragments of a building or a structure as a whole. Concerning the choice of the “universal” method, the situation is less definite because of the extremely complex structure of the material and the mechanisms variety for its formation at different levels of matter organization. However, it can be assumed that the development of such a unifying technique lies in the way of applying computer technology, computational experiment, the development of information technologies and methods of computer material science.

One of the promising areas in computer material science is the structural method, imitated modeling (SIM-method) and the technology of simulation experiments based on it (SIM-technology). The SIM-method means the process of forming on the computer information about individual structural elements of the modeled system (material and / or technology) and the conditions of their interaction with subsequent reproduction on the processes computer occurring in the system with changes in external influences, while SIM -technology provides for a number of steps to conduct a computational experiment, such as setting the problem, describing the conceptual model, writing and debugging the program, checking the model reliability and some other procedures. Apparently, there are sufficient grounds for evaluating the SIM-method as a powerful and effective means of solving material science problems [7-9].

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