Computer materials science of electrical construction composite materials with specified properties

A V Ilyukhin¹, I I Zaripova¹, M Y Abdulkhanova¹, E V Marsova¹

¹ Moscow Automobile and Road Construction State Technical University (MADI), Moscow, 64, Leningradsky prospect, 125319, Russian Federation
E-mail: aviluhin@mail.ru, zaripovainamadi@mail.ru

Abstract. This article is devoted to computer materials science of electrical construction composite materials for obtaining materials with specified properties. The idea, principles and distinctive features of computer materials science are given. An approach to solving a number of problems is described, which makes it possible to fully take into account the presence of random elements that are present in the process of forming composite materials. Implementation of algorithms is implemented, in which results obtained in previous stages affect progress of algorithms execution in subsequent stages. The radar absorbing material is considered in detail using the example of radar absorbing concrete. It has been proved that with multi-factor dependence, it is possible to optimize the composition only using an automated computer system that calculates the composition of the concrete mixture. One possible computer material science problem has shown that in order to increase absorption efficiency, it is necessary to substantially increase the effective absorption volume, which can be achieved by increasing the non-conductive layers in order to reduce the through conductivity of the radar absorbent concrete, i.e., as if to break the material into a large number of small electromagnetic screens. In this case, the volume of interaction of the material with the electromagnetic field extends deep into the material and is made commensurate with the size of the sample. In conclusion, a possible list of tasks and directions for the development of computer materials science is presented.

1. Introduction
Studies in the field of the use of computers in modeling the electro-physical properties of inhomogeneous dielectric materials in order to identify factors affecting the properties of such materials were begun in the mid-60s of the XX century. Unfortunately, due to the low performance of computers existing at that time, these works were not widely developed, although very interesting results were obtained.

Currently, when the performance of modern computers has reached the required level, it is possible to continue this work. The intensive development of computer technology and software has led to the fact that computers began to be used in areas where their use was not even intended before. The results of such work formed a new direction in materials science of electrical composite materials – «Computer materials science of construction composite materials». The following are some of the results of this work in MADI.

2. Problem setting
Since the widespread use of composite materials, many scientists have been trying to obtain analytical
relationships linking the properties of the components and their concentration in the mixture with the properties of the finished composite. Such dependencies allow the calculation of the concentration-granulometric characteristics of mixtures for the manufacture of materials with predetermined properties. Still V.I. Odelevsky showed that many properties of the composites of the matrix structure (aggregate and binder matrix), depending on the concentration of the aggregate, are described in the same terms, which follows from the general theory of phase transitions. This work was the impetus for the appearance of a large number of formulas with the help of which they tried to describe the properties of composite materials. However, numerous experiments in physical models have shown that the fairness of such formulas extends to cases where there is relative proximity of the characteristics of the components and a small bulk concentration of aggregate. Such limitations are related to the difficulty of considering the mutual influence of individual closely spaced particles. Nevertheless, many authors continue to use such formulas, and to reduce the time for cumbersome calculations, they use computers. In this case, such calculations relate to computer materials science.

High hopes were placed by researchers on a relatively new theory of «percolation» - studying the properties of connected components of random graphs [1,2]. This theory, in relation to materials science, using the method of cluster structures, describes the behavior of heterogeneous materials depending on the concentration of components in them. By virtue of the universality and similarity hypotheses, the characteristic parameters of the «percolation» theory are considered independent of the particular nature of the phase transition, i.e., the various materials of the matrix and the aggregate. However, strict evidence in the framework of the theory of «percolation» is obtained for only a few statements. Most often, in such studies, the term computer materials science refers to the use of a computer to find numerical values in statistical processing of experimental data or Monte Carlo modeling of correct lattice problems.

Summing up the above-described tasks of the construction composite materials called by the authors, it can be stated that in all cases the computer acts as a means of computing, which, if especially necessary, can be performed manually. In our opinion, such calculations cannot be called computer materials science.

The computer, as a means of automating the process of searching for the optimal composition of composites, should be used to obtain the latter with predetermined properties. Programs should ensure that the final result is obtained using not algorithms that implement calculations according to predetermined analytical expressions, but only limiting criteria that should direct the calculations in the desired direction. This approach, as applied to construction materials, will be understood by the term computer materials science, which allows to fully realize the random elements necessarily present in the process of forming composite materials, since as the algorithms are executed, the results obtained in the previous stages affect the progress of the algorithm in subsequent ones. Therefore, the distinguishing feature of programs implementing such algorithms should be the absence of initial parameters and the presence of limiting criteria set by the researcher.

In our country, a new radio absorbing material has been developed, called «Radio Absorbing Concrete» (RAC). This material can be advantageously used both to prevent the effects of electromagnetic radiation on instruments, equipment and maintenance personnel, i.e. to ensure the radio tightness of buildings and structures, and to provide protection against electronic means of detecting and tracking objects of a terrestrial, long-term nature. Unlike traditional radio-absorbing and radio-shielding materials, RAC has a significant spread of efficiency absorption (EA) values from sample to sample, which is a consequence of the dependence of its electro-physical properties on a significant number of parameters [3].

3. Materials and methods.
As is known, the loss power of electromagnetic waves by nonlinear dielectrics that do not have magnetic properties (to which RAC belongs) is described by the Landau-Lifshitz formula

\[ P = \frac{\alpha''}{2} V_{\text{mol}} |E|^2 \]  \hspace{1cm} (1)

where: \( \alpha'' \) – imaginary component of electrical polarizability of phase interface of two-component
material of matrix type;

\[ V_{\text{kon}} \] – volumetric concentration of conducting phase;

\[ E \] – electric field of absorbed wave.

By analyzing the expression (1), it can be concluded that in order to increase the absorption efficiency of electromagnetic waves in the RAC, it is necessary to have the maximum content of the conductive phase in the material and only a small content of thin interlayer films, which ensure the bonding of the conductive phase particles into a single whole. However, such a conclusion is erroneous. The fact is that when the \( V_{\text{kon}} \) increases, the amount of dielectric gaps between the conductive particles decreases and, as a result, the value of potential barriers at the boundaries of these particles decreases. This leads to the fact that although cement layers are a dielectric with very low intrinsic conductivity, nevertheless, in the form of thin layers (on the order of several tens of angstroms) they can have great transparency for electrons due to the tunnel effect. This increases the homogeneity of the material, in which case the material must already be considered as an electromagnetic shield, and according to the theory of electromagnetic shielding, the volume in which the effective absorption of electromagnetic energy is observed is limited by the size of the skin-layer. As a result, the reflectance of the material is increased, which is unacceptable for RAC. To improve absorption efficiency, it is necessary to significantly increase the effective absorption volume, which can be achieved by increasing the non-conductive layers to reduce the through conductivity of the RAC, i.e., as if to break the material into a large number of small electromagnetic screens. In this case, the volume of interaction of the material with the electromagnetic field extends deep into the material and is made commensurate with the size of the sample.

According to the reasonings given above can seem that the internal contradiction consists in expression (1). Actually, there is no contradiction as with increase in \( V_{\text{kon}} \) layers between the carrying-out particles decrease that leads to reduction of interlaminar polarization, i.e., \( \alpha_{\text{E}} \) and vice versa.

Thus, with the set properties it is necessary to make optimization for receiving RAC, both on conductivity, and on frequency characteristics of electromagnetic fields.

Besides, as RAC is composite material, its properties have to depend on its structure, concentration of the carrying-out phase and its particle size distribution.

Therefore, by drawing up concrete mix RAC it is necessary to consider a factor of conductivity of components, their particle size distribution, concentration in mixes and frequency of the electromagnetic field at which ready RAC has to work, and all these parameters are closely interconnected with each other, and change of one of them results in need to change also others under difficult laws [3].

At such multiple-factor dependence optimization of structure, perhaps to carry out, only using the automated computer system making calculation of composition of concrete mix RAC.

In [4-6] it is shown that electro-physical characteristics of conductive composites are well described by the theory of «percolation». However, application of this theory encounters the insuperable difficulties connected with impossibility of the calculations, due to the lack of ways of obtaining values of fundamental coefficients called by «critical indexes». The way out was for the first time offered in [7] where it is shown that there is no need to be engaged in search of values of «critical indexes» of the theory of «percolation», and it is possible to use some formulas of «the effective environment» within the theory of «the generalized conductivity», imposing on them restrictions of the theory of «percolation».

As part of the theory of «generalized conductivity» the properties of heterogeneous systems (composite materials) combined under the general name «generalized conductivity» (electrical conductivity, thermal conductivity, dielectric and magnetic permeability, etc.) are calculated. This combination is based on the known formal coincidence of differential equations of scalar and vector fields for stationary heat, electric current, electrical and magnetic induction flows. There are a large number of formulas describing the generalized properties of heterogeneous systems depending on the properties of the components and their concentrations (for example, Lawrence, Maxwell, Mosotti-Lorenz, Lichteneker, Odelevsky, Landauer-Bruggeman), all of them describe with approximately the same accuracy the concentration behavior of the properties of composites outside the critical region of
aggregate concentrations for matrix systems (critical refers to the value of the concentration of electrically conductive aggregate at which a sharp, threshold change in the electrical conductivity of the entire composite occurs). None of these formulas includes absolute particle sizes, only volumetric phase concentrations appear in them. This circumstance is by no means accidental, and can be generalized to all cases in which surface, linear or point effects are absent or excluded from consideration. However, none of these formulas allows us to obtain values of the properties of composites in critical areas that mainly interest us, since it is here that the maximum dependence «composite property - the concentration of electrically conductive aggregate» comes.

Based on the methodology set forth in [3,4,7], it is possible to obtain a solution of the Landauer-Bruggeman formula in the framework of the theory of an «effective medium» when superimposing the conclusions of the «percolation» theory on it, given that, due to the theory of «generalized conductivity» the dielectric constant $\epsilon$ and the specific conductivity $\sigma$ are described by the same expressions:

$$\begin{align*}
\sigma_{ef} & \approx \frac{\sigma_k(1 - V_{kon})}{k \cdot V_{kon}(1 - V_{kon})} \\
\sigma_{y} & \approx \frac{k \cdot V_{kon}(1 - V_{kon})}{k \cdot V_{kon}(1 - V_{kon})} \\
\varepsilon_{ef} & \approx \frac{V_{kon} - V_{kon}}{V_{kon}^k - V_{kon}} \\
\varepsilon_{c} & \approx \frac{V_{kon}^k - V_{kon}}{V_{kon}(1 - V_{kon})} \\
\end{align*}$$

(2)

where:

- $\sigma_{ef}$ – effective value of specific conductivity of composite (conductivity characteristic of the whole material);
- $\sigma_y$ – specific conductivity of carbon (aggregate);
- $\varepsilon_c$ – specific dielectric constant of cement stone (material of binding matrix);
- $V_{kon}$ – current value of volume concentration of carbon in composite;
- $V_{kon}^k$ – critical volume concentration value (percolation threshold);
- $\omega$ – angular frequency of electromagnetic field acting on material;
- $\tau$ – relaxation time of the double electric layer at the interface of carbon-cement substances ($\tau = \frac{\varepsilon_c}{\sigma_y}$).

Using the proposed expression, it is possible to obtain «effective» values of conductivity and dielectric constant of the entire RAC by multiplying the right and left parts by $\sigma_y$ and $\varepsilon_c$. Therefore, knowing the electro-physical characteristics of the carbon and cement used in the manufacture of the material, it is possible to select a value of the volume concentration of carbon that will provide a given loss (absorption) power of the electromagnetic field in the material.

On the basis of the given theoretical conclusions the «CritConc» program which allows to study influence of conductivity of carbon and dielectric permeability of a cement stone on extent of absorption, to vary particle size distribution and volume concentration of carbon, to define values «critical volume» concentration of filler of any composite material and also to accumulate data for the further statistical processing that allows to count optimum composition of material for specific objectives was developed.

Figure 1 shows the experimental and model average concentration relationships of the uptake efficiency of the RAC at the voltage of the electric component of the electromagnetic field $E = 1$ V/m and a frequency of 1 GHz. The gap in characteristics is due to the fact that in the zone of «critical» carbon concentrations during the experiment there is a rapid heating of the RAC, as a result of which there is a significant drift of readings and an increased probability of destruction of the material sample (carbon burnout). Experimental data were captured in an echo-free chamber. To obtain data, 150 RAC samples were produced with an increasing volume concentration. The value of $EA$ for each volumetric concentration was taken as an average of 150 samples. Model dependence is obtained as the average for 35 implementations of the program.
The sharp decrease in absorption efficiency in the «after critical» area is due to the increase in homogeneity of the material and its gradual transition from the radio absorbing material to the radio shielding one. In addition, the strength characteristics of the RAC in the «after critical» region are also sharply reduced, since the volume concentration of carbon increases so much that the cement matrix is not able to effectively bond its individual particles. For this reason, for real products from RAC, a volumetric concentration of carbon 0.25... 0.3 is used.

4. Results
Unfortunately, it is not possible to describe all aspects of the work carried out within the framework of the submitted materials. Note only that the values of the «critical» concentration themselves are determined using mathematical modeling using a bipolar (bispherical) coordinate system and are a function of variation in the particle size distribution of the aggregate (carbon).

Characteristics and dependencies similar to those shown in Figure 1 are given in [8-10] for aggregate compositions of nickel, chromium, niobium, molybdenum, etc. As can be seen from Figure 1, experimental and model dependencies have a good coincidence in the precritical region (divergence of not more than 15%) and a slightly worse coincidence in after critical, which can be explained by the absence of a mechanism in the model that allows modeling the reflection of an electromagnetic wave.

The results of the production tests showed that with the traditional (experimental) technology for selecting the composition of the RAC, only the 20% of products with a 10%-th variation in absorption efficiency from the expected value established by technical standards are absolutely suitable. When using the program «CritConc» the absorption efficiency of all products fits into the 10%-th range of the tolerance for scattering values, and the average maximum deviation from the expected values is 9.7... 9.8%.

5. Conclusion
Thus, it can be concluded that the use of the developed method for calculating the composition of the RAC allows us to provide the 100% yield of finished products suitable for use.

Further research in the field of computer materials science of electrical construction composite materials with given properties made it possible to determine the range of problems that can be solved by the methods described above:
- Modeling of composites structure,
- Modeling of composite structure with edge effects,


- Modeling of low-filled and highly filled composites,
- Study of clustering processes,
- Study of the mutual coordination and kinetics of the formation of the skeleton of composites,
- Modeling of strength characteristics of composites,
- Modeling of electro-physical properties of composites,
- Simulation of thermal conductivity of composites,
- Modeling of formation, development and quenching of cracks and pores in composites,
- Modeling of gas-liquid permeability of composites,
- Modeling of filtering properties of porous composites.

These are briefly the tasks of modeling and studying the properties of building composites in the framework of computer materials science.

Consider possible options for research and the use of a generalized problem of calculating and designing composites with optimization by their properties.

As already noted, the scope of these tasks is the development of a software product with a convenient interface, designed not for researchers, but for a practical user. Therefore, the purpose of such programs is to optimize the given properties of composites in order to obtain materials with specific parameters. The development of such applications can be based on two approaches. In the first approach, the initial data for the programs are only the specified properties of the composite and the data bank for existing source materials. In this case, the computer «informs» how much and what aggregate is to be taken, the range of its particle size distribution and the type of binder used. With the second approach, it is possible to realize the now popular trend in construction, aimed at using local raw materials or waste from other industries. In this case, a specific aggregate material and a specific binder type are specified, and the task of the program is to optimize only the concentration-particle size characteristics of the aggregate. This approach makes it possible to obtain a cheaper material, but at the same time the probability that it will not be possible to provide the given properties of the composite increases. Therefore, on a case-by-case basis, the user must decide whether or not to take a particular approach.

Based on all of the above, it is possible to formulate possible, at the moment, tasks of software development to optimize composites:

- Strength optimization,
- Electro-physical optimization,
- Thermal conductivity optimization,
- Minimization of crack formation,
- Porosity optimization,
- Optimization by moisture and gas saturations,
- Optimization by filtering properties.

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