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The Volume contains works of young researchers - participants of the XVI International Forum-Contest of Students and Young Researchers “Topical Issues of Rational Use of Natural Resources”, which was held at St. Petersburg Mining University on June 17-19, 2020. The Volume can be of great interest for a wide range of researchers, scientists, university lecturers, specialists and managers of industrial enterprises and organisations as well as for businesspeople involved in exploration, prospecting, development and processing of minerals.

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COMPUTER SIMULATION OF THE STRUCTURE OF ARTIFICIAL CONGLOMERATES

Today, there is the problem of controlling the dangerous state of an array of rocks [1]. The materials studied actively form their properties during operation, and the changes that occur have both positive and negative effects on their structure at different scale levels. When studying the formation of internal defects of agglomerates, it is important to pay attention to its structure. The authors created a virtual model of the structure of the cement composite tested in [2].

Actual studies show that a significant impact on the change in the strength and deformation properties of concrete is exerted by micro-destruction of its structure under the influence of force factors. It has been established that the process of micro-destructions begins when the stresses in concrete are much lower than its tensile strength and can decay or develop over time [3]. It is believed that the cause of the first microcracks is the concentration of stresses near structural defects: pores, inclusions, dislocations. The study of the physical processes causing the development of micro-destruction is of both scientific and practical interest.

According to modern concepts, microcracks appear at low stress levels - **σc = 0.3fcm.** The destruction of concrete begins with the development of cracks in the contact zone (matrix - aggregate) with their subsequent exit into the matrix. Contact cracks develop under the action of shear, and cracks in the matrix develop tensile stresses [4]. All these cases are caused by expansion or contraction of the intra-pore phase, which leads to deformations of the structure, then to stresses, at a critical value of which cracks form in the structure [5].

Considering the structure of cement stone, V.N. Jung [6] called it micro-concrete, in which the resulting cement gel acts as a binder, and unhydrated clinker grains as a filler. Structural models of cement stone look like porous concrete. They contain cement grains with unhydrated cores and shells of neoplasms that grow together in contacts.

To simulate the microstructure of concrete was used Virtual Concrete and Cement Testing Laboratory (VCCTL) [7]. This program was developed by the National Institute of Standards and Technology (NIST), USA. The program models 3D - microstructures of cement systems and allows predicting the final properties of the resulting composite.

The hydration of these microstructures can be modeled according to different hardening conditions, and the resulting hardened material can be analyzed for a number of properties, including linear elastic moduli, compressive strength and relative diffusion coefficients. 3D - packaging of small and large aggregates in mortar and concrete mixtures can also be created.

The authors created a virtual model of the structure of the cement composite (W/C = 0,4). Also, 3D packaging of the final solution was created by converting 3 planes into one cube. The final structure is shown at Figure 1.

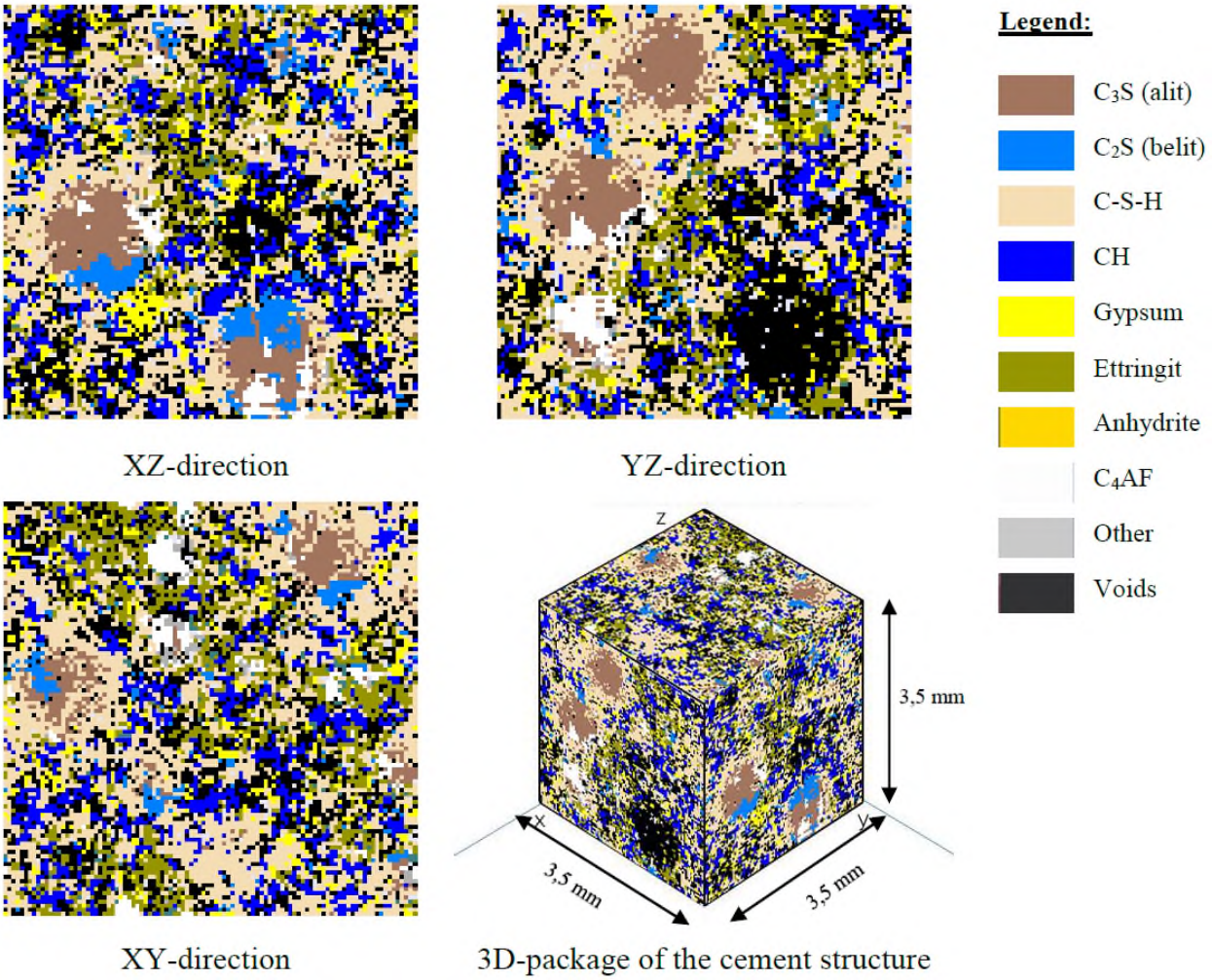

Fig. 1 – Virtual modelling of the cement solution structure (after 28 days)

Studies carried out in [2] should be supplemented with computer simulation results, which will give a broader picture of the processes occurring in concrete structures and will allow optimizing the data already obtained taking into account their structure at various levels of organization. Further tests are planned to be carried out in accordance with the most promising areas of concrete structure simulation.

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