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DEVELOPMENT AND VERIFICATION OF MECHANICAL CHARACTERISTICS OF A COMPOSITE MATERIAL MADE OF A THERMOPLASTIC MATRIX AND SHORT GLASS FIBERS

The paper presents the results of computer modeling and prediction of the mechanical properties of composite materials with a polycarbonate matrix filled with short glass inclusions. At the micro-level, the influence of the volume of inclusions on the mechanical properties of the designed composite based on polycarbonate matrix is studied in the DIGIMAT (France) program. It was found that with a ratio of the sizes of inclusions in the range of 468÷60, the particles have a needle shape, and the material with such inclusions has a higher stress limit and elastic modulus than with a shape coefficient less than 50. The components of the fiber orientation tensor were also determined, at which the values of computer modeling are in good agreement with experimental data. The influence of the size of the finite element grid on the characteristics of the composite at the macro level was studied, and recommendations were given for choosing the size of the face of the finite element. The adequacy of computer models was confirmed by the results of field tests. The paper presents the results of testing flat samples made by injection molding technology. Mechanical tests were carried out for three variants of samples made of composite material based on a polycarbonate matrix with 10 %, 20 % and 30 % inclusions. The discrepancy between the experimental and computer results for samples with 10 %, 20 % content of short chopped fibers is explained by the influence of technological factors on the properties of the material at the macro-level.

The conducted research allowed us to develop a computer modeling technique used at the stage of development of polymer composites based on thermoplastic matrices with short glass inclusions

Keywords: composite material, polycarbonate, short glass fibers, DIGIMAT, elastic modulus

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1. Introduction

One of the most effective ways to improve modern structures is the introduction of new high-strength and high-modulus composite materials into production. Thus, in pumping technology, polymer compositions are increasingly being used for the manufacture of impellers. An impeller with complex geometry can be made of polymer materials by technological processes of pressing and injection molding [1–3].

Despite the widespread use of filled polymers in many areas of human economic activity and numerous works devoted to the study of their physical and mechanical characteristics, the mechanical properties of these materials can hardly be considered sufficiently well-known.

The description of such materials is associated with great mathematical difficulties, since they have a high anisotropy of deformation properties, a significantly inhomogeneous layered structure and considerable shear compliance. Unlike the properties of traditional materials, the technology of which is well developed and stable, the properties of composites are quite sensitive to small changes in the technological regime, and the technological techniques themselves are very diverse. In principle, the design of the material, product and technological process should be a single whole [4–7].

In particular, there is no general theoretical approach to predict the influence of the filler on the deformation behavior and the mechanism of destruction of composites, which often creates significant difficulties in the development of new materials with specified mechanical characteristics and requires a large number of experiments that do not always give positive results. These circumstances determine the relevance of studies of the mechanical properties of filled polymers using computer-aided design systems. The main advantage of using such systems is the possibility of multi-variant design of the composition of material with specified mechanical properties, and reducing the cost of both the production process of the part from composites and its cost.

It should be noted that at present, the creation of a good competitive product, including from composite materials, is impossible without the use of computer technologies for virtual product development (or VPD technologies). Given the complexity of the task, modeling and analysis of composite structures should be carried out with the involvement of the most modern engineering analysis systems (or CAE systems) implementing the finite element method (FEM) [8–11].

2. Literature review and problem statement

Various techniques based on analytical and numerical methods of thermophysics and mechanics of composite materials are currently used to model and predict the physical properties of composite materials. In [12], the mechanical, thermal and electrical properties of multifunctional CNT/polymer nanocomposites are calculated using numerical and analytical models depending on the material parameters and processing factors. The influence of the content and size of inclusions was determined in the paper. The methods of numerical analysis created by the authors are applicable only for modeling composites containing nano-inclusions whose dimensions and shape are much different from those of glass inclusions.

In [13], the mechanical properties of composite materials made of three different types of polymer resins (namely, DM411 epoxy-vinyl ether, poly-pyrizophthalic P2000 and poly-terephthalic P115A) were studied. Such materials contained different concentrations of magnetite (Fe_3O_4) in the functional fillers and had different particle sizes. In conclusion, it should be noted that such a material exhibits anisotropic behavior, and its elastic modulus increases depending on the concentration and size of magnetite particles in the filler. The results of the study on the influence of fiber orientation on the properties of the composite material were not presented in the work.

In [14], the properties of an untreated polypropylene composite filled with wollastonite with the addition of silicone rubber and maleic anhydride were studied. In the course of the study, it was found that the addition of 5 % rubber to polypropylene composites containing wollastonite at various compositions of 10 %, 20 %, 30 % and 40 %, in general, provided increased rigidity, impact strength with incision and bending strength, but reduced impact strength without incision, tensile strength and bending modulus. The research is purely experimental in nature, although at the present stage, full-scale experiments should be preceded by multivariate computer design in order to reduce economic costs.

To evaluate the mechanical properties of highly porous ceramics, numerical calculation methods based on the application of the finite element method for modeling realistic representative fragments of fibrous structures are used in [15]. The structures presented in the form of a spatial "frame" of fibers or filamentous crystals were presented in the structure of a representative fragment, but the results of computer modeling at the macro level were not presented and the influence of particle size and shape on the mechanical properties of the composite at the macro level was not clarified.

The author of the work [16] studied the deformation-strength properties of a composite material based on an ethylene copolymer and silica gel particles of various sizes. It is found that with an increase in particle size, mechanical properties deteriorate, which is associated with the type of defects formed during particle separation. In this work, only the influence of size on the mechanical properties was studied, and the shape coefficient was not taken into account.

In [17], the influence of the filling parameter of composites with biofibers was studied. This paper presents a numerical analysis of composites reinforced with natural fiber (from renewable sources) to assess the mechanical behavior of biocomposites and elucidates the role of micromechanical analytical models.

In [18], the mechanical and thermal properties of polymer composites reinforced with glass microbeads were studied under temperature conditions. Lightweight microporous composites have been developed for advanced mechanical systems. The paper did not provide conclusions on how the particle shape affects the composite properties, studies were conducted only for spherical inclusions, while needle shapes give different results.

The author's work [19] was devoted to the study of the mechanical properties of composite materials based on polyolefins and mineral particles. The studies were carried out with various fillers of dispersed-filled composites based on thermoplastic polymers, depending on the concentration, size and shape of the particles of mineral fillers. The conclusions of the work were based on analytical and experimental studies.

Without suppressing the role and significance of the above works in the study of the mechanical properties of composite materials, I would like to note one drawback – the lack of a clear methodology for computer modeling of the properties of the designed composite materials. In today's rapidly developing high-tech production, the design of the material, product and technological process should be a single whole. Thanks to the appearance of CAE systems, the designer is given the freedom to effectively use materials, and the creative side of the design process is enhanced.

3. The aim and objectives of the study

The aim of the work is to design a composite material with specified properties for the production of a centrifugal wheel of a multi-stage pump. The designed material with low water permeability under loading must withstand a stress level of 85 MPa with elastic deformation of 0.03 %.

To achieve this aim, the following objectives are accomplished:

– to investigate the influence of the shape of filler particles on the deformation behavior of composite materials;

– to investigate the effect of the content of rigid particles on the change in the main mechanical parameters of composites;

– to investigate the influence of fiber orientation on the mechanical properties of composites based on a polycarbonate matrix and glass inclusions, to investigate the influence of the finite element grid splitting method on the results of modeling the mechanical properties of composites;

– to verify the mechanical characteristics of the composite material determined by numerical and physical experiments.

4. Materials and methods

4. 1. Theoretical approach

The theoretical approach to determining the mechanical characteristics of two-phase composites is based on the Eshelby theory. Eshelby proposed a method for calculating the deformation energy of systems containing inclusions. The formula obtained by him transforms the usual integration over the volume into integration over the surface of a particular form. According to the theory, the composite consists of two components. The indices *r* and *m* denote the reinforcing inclusion and the matrix, respectively.

The problems of determining the stress field in an isotropic ellipsoidal inclusion extracted from a matrix, plastically deformed and re-placed in it, were solved [20]. Later, the average stress field in the matrix was derived taking into account the mutual influence of ellipsoidal inclusions. Based on the theory [20], the elastic modulus for fibrous and dispersed-hardened composites with an isotropic matrix was calculated. This model takes into account the Young's modulus of the first and second kind, the Poisson's ratio of the filler and the matrix, and the inclusion shape coefficient $0<\zeta<\infty$. Equations (1)–(6) define five independent constants corresponding to the Young's modulus, the shear and volume modules, and the Poisson's ratio of the composite material.

$$\frac{E_{11}}{E_m}=\frac{1}{1+\left(c_r\left(A_1+2\nu_m A_2\right)\right)/\left(A\right)}; \quad (1)$$

$$\frac{E_{22}}{E_m}=\frac{E_{33}}{E_m}=$$

$$=\frac{1}{1+\left(c_r\left[-2\nu_m A_3+(1-\nu_m)A_4+(1+\nu_m)A_5 A\right]\right)/\left(2A\right)}; \quad (2)$$

$$\frac{\mu_{12}}{\mu_m}=1+\frac{c_r}{2c_m S_{1212}+\left(\mu_m\right)/\left(\mu_r-\mu_m\right)}; \quad (3)$$

$$\frac{\mu_{23}}{\mu_m}=1+\frac{c_r}{2c_m S_{2323}+\left(\mu_m\right)/\left(\mu_r-\mu_m\right)}; \quad (4)$$

$$\frac{\kappa_{23}}{\kappa_m}=$$

$$=\frac{\left(1+\nu_m\right)\left(1-2\nu_m\right)}{1-\nu_m\left(1+2\nu_{12}\right)+c_r\left[2\left(\nu_{12}-\nu_m\right)A_3+A_4\left(1-\nu_m\left(1+2\nu_{12}\right)\right)\right]/A}; \quad (5)$$

$$\upsilon_{12}=\frac{\upsilon_m A-c_r\left(A_3-\upsilon_m A_4\right)}{A+c_r\left(A_1+2\upsilon_m A_2\right)}. \quad (6)$$

Expressions for the coefficients A_1, A_2, ..., A and the components of the Eschelby tensor S_{igkl}, depending on the shape of the inclusions and the elastic characteristics of the phases, can be found in [20]. The elastic coefficients introduced in this way are effective values that determine the macroscopic elastic properties of the material.

4. 2. Method of computer modeling of the mechanical properties of the designed composite

The proposed methodology includes three main stages of modeling using the DIGIMAT software package. The DIGIMAT software package is almost the only software in the world that uses a micro-level approach to determine the characteristics of composite materials. The initial data for DIGIMAT are the properties, topology and volume/mass content of each phase, as well as the microstructure of the composite material. Based on these data, a mathematical model of the material is constructed at the micro-level, which is sensitive to the properties of each phase and microstructure, and the required mechanical, thermal or electrical characteristics of the composite material are determined (Fig. 1).

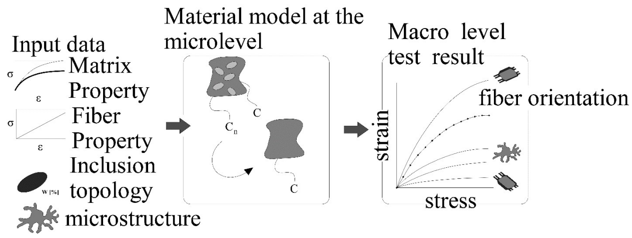


Fig. 1. Micro-level approach for determining the characteristics of composite materials

The software package allows modeling a wide range of multiphase materials and applying an integrated approach to the design of composite structures: from the development of materials and conducting virtual tests of samples, to modeling the manufacturing technology and obtaining the final characteristics of the structure.

The MSC DIGIMAT MF module was used to implement modeling on a micro-level approach. The initial data were:

– mechanical characteristics of glass fiber;
– mechanical characteristics of the matrix material;
– size of glass inclusions;
– shape of glass inclusions;
– percentage of fiber reinforcing particles.

Since the new composite material will be used for the production of centrifugal wheels of a multi-stage pump, water absorption coefficients were estimated at the initial stage of the matrix material analysis, for polycarbonate – 0.36 %.

The data for modeling are summarized in Table 1.

To date, there are a large number of companies that supply chopped fiberglass with various geometric properties. For the virtual experiment, fiber brands were used, the geometric characteristics of which are summarized in Table 2.

Based on the literature data [12–15] devoted to the study of dispersed-filled composites based on thermoplastic polymers, it can be concluded that their properties are determined by the content and shape of particles. One of the significant factors affecting the mechanical properties of the composite is the orientation of fibers in space. The indicator of this parameter is the orientation tensor *T*.

$$T=\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix},$$

where a_{ij} is the components of the orientation tensor corresponding to the directions along the *x*, *y*, *z* axes.

Table 1

Mechanical data for a numerical experiment

Parameters	Values
Elastic modulus of polycarbonate, MPa	2,360
Density of polycarbonate, kg/mm^3	$1.14\cdot10^9$
Lower yield strength of polycarbonate, MPa	75
Brinell hardness of polycarbonate, MPa	95
Elastic modulus of glass, MPa	72,000
Glass density, kg/mm^3	$2.54\cdot10^9$
Glass Poisson's ratio	0.22

Table 2

Geometric parameters of short fiberglass [22]

Fiberglass grade	Fiber diameter, microns	Fiber length, mm
ECS 11–4.5–560A	11–0.011 mm	4.5–4,500
ECS 13–3–552B	13–0.013 mm	6–6000
CS 7938	50 microns	3,000 microns

The parameters that determine the mechanical properties of composites are implemented in the program interface through the following values:

– "Mass fraction" – mass content of inclusions, cases of 10 %, 20 %, 30 were considered %;

– "Fixed aspect ratio" – coefficient determining the particle shape of inclusions, in our case, the particle length-diameter ratio $k = \frac{l_f}{d_f} = 468{,}187{,}60$;

– "Orientation tensor" – fiber orientation tensor, three cases were considered

$a_{11}=a_{22}=0.5;\ a_{33}=0,$

$a_{11}=a_{22}=0.33;\ a_{33}=0.34,$

$a_{11}=a_{22}=0.5;\ a_{33}=0,$

$a_{11}=0.8\ a_{22}=0.2;\ a_{33}=0,$

the remaining terms of the orientation tensor are zero;

– "Shape" allows you to change the shape of inclusions, we have chosen an elliptical shape of inclusions.

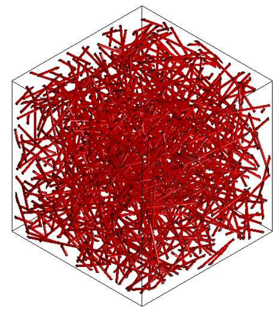
At the second stage, the results of the numerical calculation are processed and averaged over the volume of a representative fragment to obtain an estimate of the effective stiffness and strength of the material. The DIGIMAT FE module is used to generate three-dimensional models. This module is designed for modeling effective physical and mechanical properties of composite materials based on various analytical and numerical methods. The DIGIMAT FE module allows you to build three-dimensional models of inhomogeneous materials with a complex structure.

To construct a representative fragment of fibrous material in the DIGIMAT FE system, it is necessary to set the following microstructural parameters: the relative volume content of fibers, their diameter, length and orientation. It is necessary to choose the size and shape of the representative fragment. In further calculations, we will use fragments of only a cubic shape with the size of faces d. The orientation of the fibers is unchanged and can be considered equally probable in all directions (isotropic distribution) or equally probable in a given plane (for the case of transversal isotropy) or determined by a tensor whose components set the probability of orientation of the fibers in different directions. As a result of the system operation, a representative fragment is created (Fig. 2, *b*), which satisfies the initial requirements for the microstructure parameters introduced.

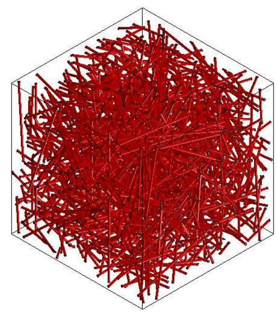
Fig. 2 shows the change in the phase structure of a representative element depending on the change in the quantitative fraction of inclusions.

The task of obtaining estimates of the statistical parameters of the distributions of local properties is associated with the need for numerous repeated calculations of the stress-strain state of the model material in the vicinity of randomly selected points with the specified parameters of the calculation scheme. In this regard, one of the main disadvantages of the finite element method becomes particularly acute, namely, significant time spent on preparing the initial data for calculation, especially on constructing finite element grids.

A total of 6 "quasi-regular" finite element grids were considered. Their main characteristics are shown in Table 3.



a



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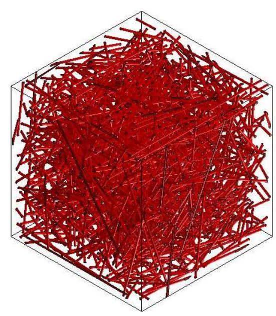

c

Fig. 2. Representative element with:
a – m_f=10 %; *b* – m_f=20 %; *c* – m_f=30 %

Table 3

The breakdown scheme of the representative level

Scheme No.	m_f	N_f	N_{fe}
1	10 %	30×30	115,000
2	10 %	50×50	125,000
3	10 %	70×70	147,000
4	20 %	30×30	27,000
5	20 %	50×50	125,000
6	20 %	70×70	343,000

In Table 3, m_f – the quantitative content of inclusions, N_f – the faces of the element of the finite element grid, N_{fe} – the elements of the grid.

Fig. 3 shows representative elements with different partitioning schemes into a finite element grid according to the data in Table 3.

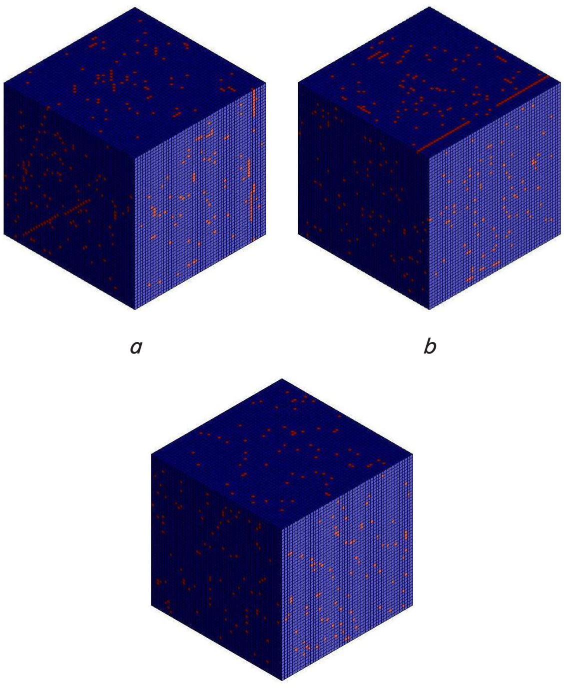

Fig. 3. Representative elements with partitions: *a* – dimensions of the FE grid element 30×30×30; *b* – dimensions of the FE grid element 50×50×50; *c* – dimensions of the FE grid element 70×70×70

In Fig. 3, it is seen how the element of inclusions changes from the size of the partition, and in the future the size will affect the rigidity of the entire representative volume.

5. Results of the study of the mechanical characteristics of composite materials

5. 1. Influence of the inclusion shape coefficient on the mechanical properties of composites based on a polycarbonate matrix

According to the raw materials of short glass chopped fibers available on the market, the dimensions of which are shown in Table 2, a numerical analysis was carried out at the micro-level, the properties of composites from a polycarbonate matrix with a filling of 10 %, the parameter of the fiber length-diameter ratio was the value k_r=467.187.60. Fig. 4 shows the diagrams of the deformation resistance of the composite material with the data given above.

When the polycarbonate is filled with 10 % glass fiber, with a particle shape coefficient k_r=467, the upper limit of stress during deformation is 0.03 % σ=92 MPa, at k_r=187, σ=91 MPa, at k_r=60, σ=91 MPa.

Considering that the maximum stress values are achieved with a shape coefficient k_r=467, further virtual and experimental studies are carried out with a composite of polycarbonate matrix and short glass fibers with a particle size ratio "Fixed aspect ratio" equal to the value k_r=467.

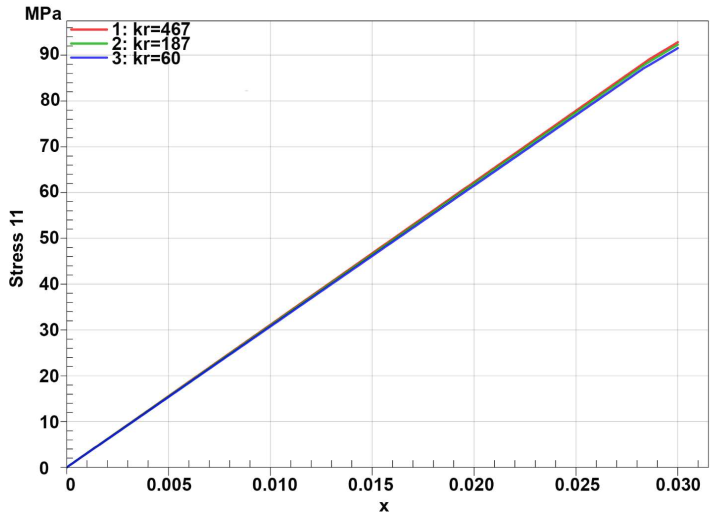

Fig. 4. Stress-strain diagram for composites based on a polycarbonate matrix with inclusions of 10 %, size ratio: k_r=467.187.60

5. 2. Influence of the filler volume on the mechanical properties of composites based on polycarbonate matrix and glass inclusions

Using the MF module and the data given in Table 1, the results obtained with the deformation curves of composite materials with polycarbonate and filled with short chopped glass fibers with a particle size ratio k_r=467 are shown in Fig. 5.

According to the results of modeling the properties of a composite made of a polycarbonate matrix with a glass fiber content of 10 %, the upper limit of stresses during deformation of 0.03 % reaches the value of σ=90 MPa, the elastic modulus of the first kind has the value of E=3,200 MPa, the elastic modulus of the second kind G=1,156 MPa, Poisson's ratio μ=0.35. For the 20 % percentage of fibers, the upper limit of stresses during deformation of 0.03 % reaches the value σ=120 MPa, the elastic modulus of the first kind E=4,029 MPa, the elastic modulus of the second kind G=1,498 MPa, Poisson's ratio μ=0.33. For the 30 % content of inclusions, the upper limit of stresses during deformation of 0.03 % reaches the value σ=150 MPa, the elastic modulus of the first kind E=5,060 MPa, the elastic modulus of the second kind G=1895, Poisson's ratio μ=0.32.

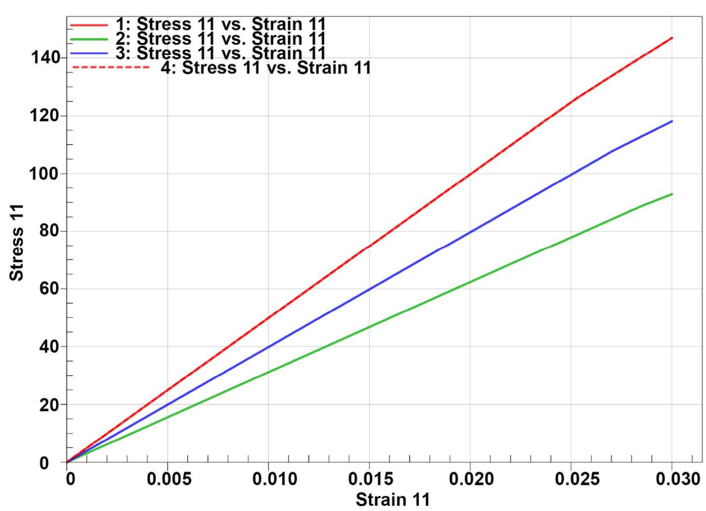

Fig. 5. Stress-strain diagrams for a composite material based on a polycarbonate matrix containing: green line – 10 % inclusions; red line – 20 % inclusions; blue line – 30 % inclusions

5. 3. Influence of fiber orientation on the mechanical properties of composites based on a polycarbonate matrix and glass inclusions

Taking into account the fact given in the literature review that there is no clear methodology for modeling adequate models of the mechanical behavior of composite materials based on polycarbonate matrix and glass fibers, the researchers proposed to study three options out of nine combinations of choosing a component of the fiber orientation tensor. The choice was based on the rule of invariance of the tensor terms, as well as the geometric dimension of the model.

The study on the influence of fiber orientation was modeled for a polycarbonate matrix with inclusions whose particle size ratio "Fixed aspect ratio" is equal to k_r=467, the mass content is 30 %. The simulation results are shown in Fig. 6.

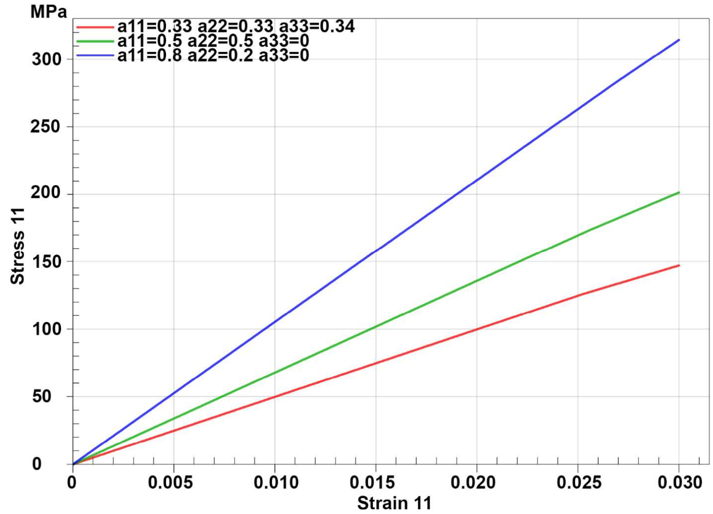

Fig. 6. Stress-strain diagrams for a composite with a polycarbonate matrix, with inclusions with different fiber orientations: red line – with a volumetric orientation a_{11}=0.33, a_{22}=0.33, a_{33}=0.34; green line – with a flat orientation a_{11}=0.5, a_{22}=0.5, a_{33}=0; blue line – with a flat orientation a_{11}=0.8, a_{22}=0.2, a_{33}=0

Since there is no clear methodology and recommendations for determining the orientation of fibers in the literature and in studies on the creation of computer models describing the mechanical properties of composite materials based on a polycarbonate matrix and chopped glass short fibers, modeling was carried out for flat, volumetric and uniaxial directions. The diagram shown in Fig. 6 shows a large spread of the results of the mechanical characteristics of the composite. In the future, it is necessary to verify the simulation results with the results of field experiments.

The resulting solutions of the field of parameters characterizing the stress-strain state of the selected fragment of the structure allow us to calculate its effective mechanical characteristics (Fig. 7).

The results presented in Fig. 8 show that the distribution of the calculated local characteristics of the stress-strain state in the calculated domain, in contrast to the locally effective ones, significantly depends on the type of partitioning into finite elements.

In Fig. 8, the diagrams of the deformation resistance of the composite material, modeled at the macro-level, indicate the effect of the size of the partition on the magnitude of the elastic modulus, so for a grid with a size of 30×30×30 and 50×50×50, the value of the elastic modulus is the same, for a grid with a size of 70×70×70, the value of the elastic modulus differs by 20%. The latter value shown in Fig. 8 correlates with the value of the elastic modulus determined in the MF module at the micro-level.

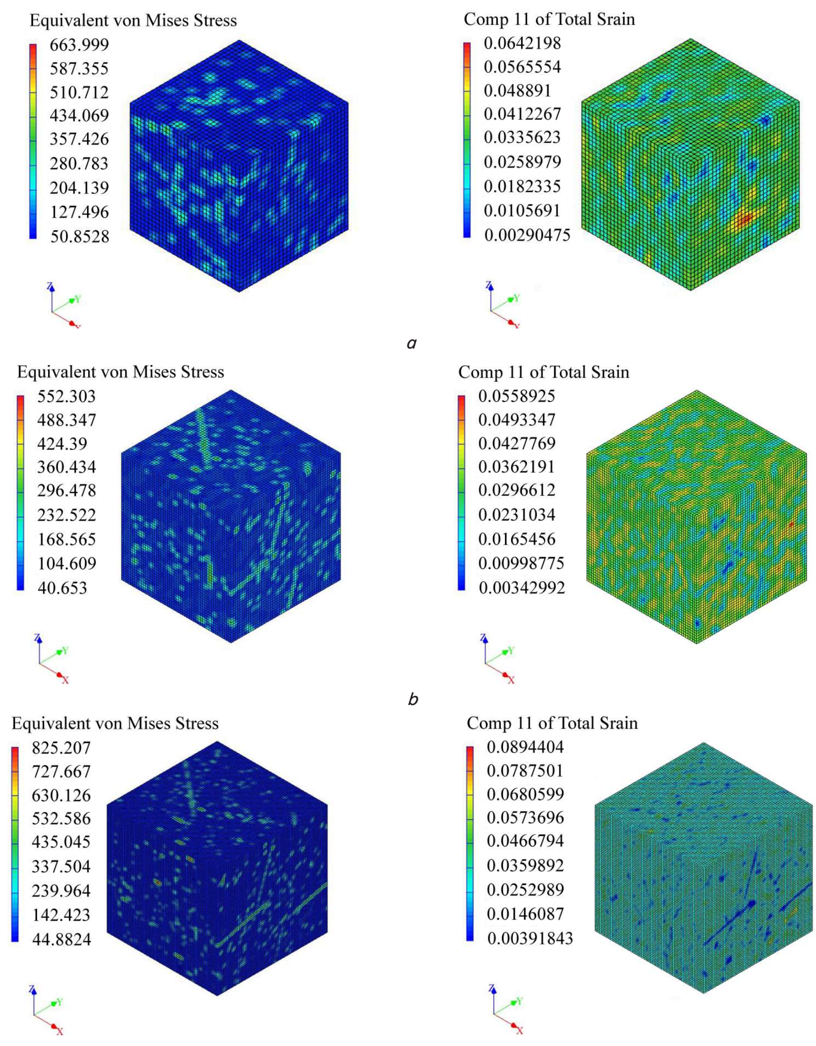

Fig. 7. Diagrams of the stress-strain state of representative elements made of a composite material based on a polycarbonate matrix with chopped short fibers from finite element grid dimensions of the elements: *a* – dimensions of the FE grid element 30×30×30; *b* – dimensions of the FE grid element 50×50×50; *c* – dimensions of the FE grid element 70×70×70

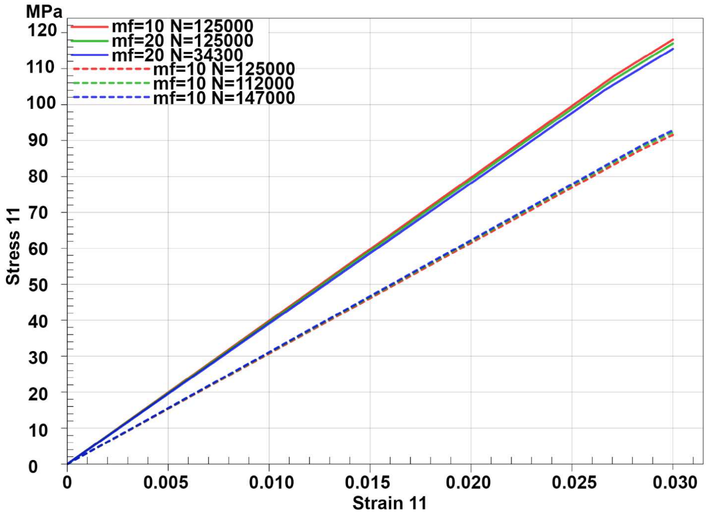

Fig. 8. Diagram of deformation resistance of 10 % occupancy with the dimensions of the grid elements: red line – 30×30×30; green line – 50×50×50; blue line – 70×70×70

5. 4. Experimental studies of the properties of composites and verification with mechanical characteristics determined by numerical results

Polymer mixtures were prepared on a single-screw extruder with a diameter of 45 mm, L: D=25. The heating is electric. The temperature is regulated by thermocouples and a thermostat. The extrusion temperature regime is as follows: Zone I – 260 °C, Zone II – 265 °C, Zone III – 270 °C, Zone IV – 260 °C.

Polycarbonate (data are given in Table 1) and glass fibers of the CS7938 brand (data are given in Table 2) were used in the experiment. After drying the starting materials at 105 °C for 4 hours, mixtures of 400 g of polycarbonate (PC) and short glass fibers (SGF) with the composition shown in Table 4 were prepared.

Table 4

Composition of the prepared polycarbonate composites

No.	PC, %	SGF, %
1	100	0
2	90	10
3	80	20
4	70	30

For each variant of the filling capacity of the composition, several samples were tested, the average values of the strength limits are shown in diagram 9.

During the tests, it was noticed that the formation of the neck occurs only in the first sample, so only there ey is set, i.e. the flow deformation. In all other places, elongation occurs at break, since there is no yield deformation.

Table 5 shows that with an increase in the number of short glass fibers, the characteristics of composites improve and reach values significantly exceeding the requirements.

Knowing the experimental curves of the stress-strain dependence, the elastic modulus of composites for different filling options of samples were determined by a technique based on the geometric interpretation of this value $E = \mathrm{tg}\frac{\sigma}{\varepsilon}$. The results of the experiment are shown in Table 5.

Table 5

Test results of composites based on polycarbonates and short glass fibers

Indicator	1	2	3	4
E_t, MPa	1,970	5,240	5,250	6,190
σ_m, MPa	63.1	125	128	150

The data of the numerical and physical experiments were compared and summarized in Table 6.

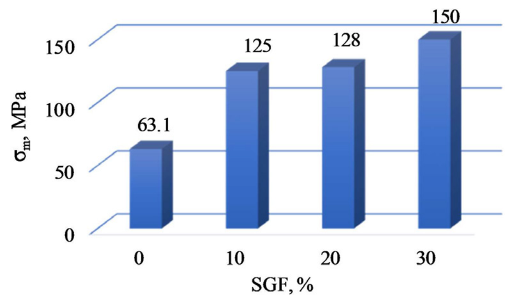

Fig. 9. Change in tensile strength (σm, MPa) of polycarbonate composites filled with different amounts of SGF (%)

Table 6

Comparison of numerical and field experiment results

Indicator	1		2		3		4	
Type of experiment	natur	model	natur	model	natur	model	natur	model
E_t, MPa	1,970	–	5,240	3,200	5,250	4,029	6,190	5,060
σ_m, MPa	63.1	–	125	90	128	120	150	150

The table shows discrepancies in the results of computer and field experiments, which require explanations.

6. Discussion of computer modeling and experimental results

Analyzing Fig. 5 for a polycarbonate matrix modeled at the micro-level, it can be concluded that the mass content of inclusions affects the mechanical properties of composites such as strength and stiffness. When studying the influence of the inclusion shape coefficient on the mechanical properties of composites based on a polycarbonate matrix, it turned out that if the shape coefficient varies within k_r=487 60, the glass inclusions have a needle shape, and below k_r=50, the inclusions take an elliptical shape, which will significantly reduce the values of stresses and elastic modulus. When studying the influence of fiber orientation on the mechanical properties of composites based on a polycarbonate matrix and glass inclusions, the diagram in Fig. 4 shows a large variation in the results of the mechanical characteristics of the composite. Verification of the numerical calculation with a physical experiment indicates the correctness of the choice of the volume orientation a_{11}=0.33, a_{22}=0.33, a_{33}=0.34 for plates with a thickness of 3 mm.

A comparison of the data given in Table 6 shows that the discrepancy in the values of the elastic modulus is explained by the scaling parameters of the breaking equipment, as well as the influence of technological factors in the manufacture of samples, for which there are many confirmations in the literature. For example, in [23], the results of the tensile strength and elastic modulus of composite materials obtained with different parameters of the technological process are presented, the discrepancy of the elastic modulus under different modes is 66 %, while the discrepancy of the tensile strength values is 5 %.

According to the comparison of the results of numerical and full-scale experiments, the average difference between the elastic moduli was 40 %, the average difference between the strength limits was 7 %. When modeling the effective mechanical characteristics for a fragment of the structure of a model material at the macro level, it is shown that the distribution of the calculated local characteristics of the stress-strain state in the computational domain, in contrast to the locally effective ones, significantly depends on the type of division into finite elements. The value of the elastic modulus for a grid with a size of 70×70×70 correlates with the value of the elastic modulus defined in the MF module at the micro-level, as well as with the values of experimental data. Small differences in the results for 20 % and 10 % of the composite are explained by the influence of technological factors on the structure of the material at the macro level. When constructing computer models of composites at the macro level, it is recommended to choose the size of the finite elements ($d/A<0.1$), where d is the length of the side of the square column element, A is the size of the larger fiber axis.

The paper did not investigate the influence of the modes of the injection molding process on the orientation of fibers and, ultimately, the effect on the mechanical properties of the designed composite. To determine these parameters in the future, it is necessary to simulate and predict the parameters of casting processes in the Digimat-RP/Moldex3D module with an assessment of the strength of parts from a polymer composition at the macro level in a nonlinear NASTRAN/MARC solver. The adequacy of the results obtained should be confirmed by experimental data.

7. Conclusions

1. The coefficient of the shape of glass inclusions does not significantly affect the value of the elastic modulus if its change is in the range k_r=468÷60. In this case, the shape of the inclusions is close to needle-shaped and if $k_r<50$, the inclusion takes the form of a pronounced ellipsoid and the change in mechanical characteristics is significant.

2. For a polycarbonate matrix with a glass fiber content of 10 %, the upper limit of stresses during deformation of 0.03 % reaches the value of σ=90 MPa, the elastic modulus of the first kind has the value of E=3,200 MPa, the elastic modulus of the second kind G=1,156 MPa, Poisson's ratio μ=0.35. For the 20 % percentage of fibers, the upper limit of stresses during deformation of 0.03 % reaches the value σ=120 MPa, the elastic modulus of the first kind E=4,029 MPa, the elastic modulus of the second kind G=1,498 MPa, Poisson's ratio μ=0.33. For the 30 % content of inclusions, the upper limit of stresses during deformation of 3 % reaches the value σ=150 MPa, the elastic modulus of the first kind E=5,060 MPa, the elastic modulus of the second kind G=1,895, Poisson's ratio μ=0.32.

3. Based on the results of numerical calculation of mechanical characteristics and their verification with the experimental results, the components of the fiber orientation tensor a_{11}=0.33, a_{22}=0.33, a_{33}=0.34 were determined, at which the computer results are most consistent with the experimental results of the mechanical characteristics of the designed composite material. The influence of the parameters of the finite element grid on the mechanical properties of the composite at the macro level is determined. It is recommended to choose the size of the finite elements ($d/A<0.1$), where d is the length of the side of the square column element, A is the size of the larger inclusion axis.

4. The conducted experimental studies have confirmed the correctness of the created computer model, which allows us to obtain both reliable estimates of the locally effective characteristics of a structurally inhomogeneous composite material and acceptable estimates of the distribution of local parameters of the stress-strain state. According to the comparison of the results of numerical and full-scale experiments, the average difference between the strength limits was 7 %.

Taking into account all the results of the study, it can be concluded that the developed method of computer modeling of the properties of composite materials based on polycarbonate matrix and short glass fibers can be used to predict the properties, and its application will reduce the number of experiments and the cost of products made of these materials.

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References

1. Volkov, A. V., Parygin, A. G., Vikhliantsev, A. A. (2018). Analiz perspektivnykh napravlenii sovershenstvovaniia nasosnykh agregatov neftekhimicheskikh i neftepererabatyvaiuschikh proizvodstv. KHimicheskaia tekhnika, 10. Available at: http://chemtech.ru/analiz-perspektivnyh-napravlenij-sovershenstvovanija-nasosnyh-agregatov-neftehimicheskih-i-neftepererabatyvajushhih-proizvodstv1
2. Cárdenas, D., Escárpita, A. A., Elizalde, H., Aguirre, J. J., Ahuett, H., Marzocca, P., Probst, O. (2011). Numerical validation of a finite element thin-walled beam model of a composite wind turbine blade. Wind Energy, 15 (2), 203–223. doi: http://doi.org/10.1002/we.462
3. Rabochie kolesa nasosov iz polimernykh kompozitsii (2016). Stroitelnii resurs. Available at: http://spb-sovtrans.ru/polimernye-kompozicii/963-rabochie-kolesa-nasosov-iz-polimernyh-kompoziciy.html
4. Ponomareva, N. R. (2010). Strukturno-mekhanicheskie osobennosti deformatsionnogo povedeniia kompozitsionnykh materialov na osnove poliolefinov i mineralnykh chastits. Moscow, 153. Available at: https://freereferats.ru/product_info.php?products_id=667

5. Dong, X., Sui, G., Yun, Z., Wang, M., Guo, A., Zhang, J., Liu, J. (2016). Effect of temperature on the mechanical behavior of mullite fibrous ceramics with a 3D skeleton structure prepared by molding method. Materials & Design, 90, 942–948. doi: http://doi.org/10.1016/j.matdes.2015.11.043
6. Eshelby, J. D. (1957). The determination of the elastic field of an ellipsoidal inclusion, and related problems. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 241 (1226), 376–396. doi: http://doi.org/10.1098/rspa.1957.0133
7. Jagath Narayana, K., Burela, R. G. (2019). Multi-scale modeling and simulation of natural fiber reinforced composites (Bio-composites). Journal of Physics: Conference Series, 1240, 012103. doi: http://doi.org/10.1088/1742-6596/1240/1/012103
8. Jiang, C. P., Chen, F. L., Yan, P., Song, F. (2010). A four-phase confocal elliptical cylinder model for predicting the effective thermal conductivity of coated fibre composites. Philosophical Magazine, 90 (26), 3601–3615. doi: http://doi.org/10.1080/14786435.2010.492767
9. Liu, Q., Lu, Z., Hu, Z., Li, J. (2013). Finite element analysis on tensile behaviour of 3D random fibrous materials: Model description and meso-level approach. Materials Science and Engineering: A, 587, 36–45. doi: http://doi.org/10.1016/j.msea.2013.07.087
10. Muktinutalapati, N. R., Benini, E. (2011). Advances in gas turbine technology. Gas Turbines. doi: http://doi.org/10.5772/664
11. Povetkin, V. V., Isametova, M. E., Isayeva, I. N. Bukayeva, A. Z. (2018). Dynamic modeling of ball mill drive with regard to damping properties of its elements. Mining Informational and Analytical Bulletin, 5, 184–192. doi: http://doi.org/10.25018/0236-1493-2018-5-0-184-192
12. Tserpes, K., Tzatzadakis, V. (2019). Computation of mechanical, thermal and electrical properties of CNT/polymer multifunctional nanocomposites using numerical and analytical models. MATEC Web of Conferences, 304, 01013. doi: http://doi.org/10.1051/matecconf/201930401013
13. Lara-González, L. Á., Guillermo-Rodríguez, W., Pineda-Triana, Y., Peña-Rodríguez, G., Salazar, H. F. (2020). Optimization of the Tensile Properties of Polymeric Matrix Composites Reinforced with Magnetite Particles by Experimental Design. TecnoLógicas, 23 (48), 83–98. doi: http://doi.org/10.22430/22565337.1499
14. Singh, U. P., Biswas, B. K., Ray, B. C. (2009). Evaluation of mechanical properties of polypropylene filled with wollastonite and silicon rubber. Materials Science and Engineering: A, 501 (1-2), 94–98. doi: http://doi.org/10.1016/j.msea.2008.09.063
15. Lurie, S. A., Rabinsckiy, L. N., Solyaev, Y. O., Buznik, V. M., Lizunova, D. V. (2016). Methodology of numerical modelling of mechanical properties of porous heat-shielding material based on ceramic fibers. PNRPU Mechanics Bulletin, 4, 263–274. doi: http://doi.org/10.15593/perm.mech/2016.4.15
16. Desiatkov, A. V., Ponamareva, N. R., Goncharuk, G. P., Obolonkova, E. S., Budnitskii, Iu. M., Serenko, O. A. (2009). Vliianie razmera chastits na mekhanicheskie svoistva kompozitov na osnove odnorodnodeformiruschegosia polimera. Uspekhi v khimii i khimicheskoi tekhnologii, XXIII (5 (98)), 32–35. Available at: https://cyberleninka.ru/article/n/vliyanie-razmera-chastits-na-mehanicheskie-svoystva-kompozitov-na-osnove-odnorodno-deformiruyuschegosya-polimera
17. Skvortsov, Iu. V., Glushkov, S. V., Khromov, A. I. (2012). Modelirovanie kompozitnykh elementov konstruktsii i analiz ikh razrushenii v SAE-sistemakh MSC.Patran-Nastran i ANSYS. Samara.
18. Ozawa, Y., Watanabe, M., Kikuchi, T., Ishiwatari, H. (2010). Mechanical and thermal properties of composite material system reinforced with micro glass balloons. IOP Conference Series: Materials Science and Engineering, 10, 012094. doi: http://doi.org/10.1088/1757-899x/10/1/012094
19. Matveeva, U. A., Van Khattum, F. (2011). Razrabotka i analiz strukturnykh modelei kompozitnykh materialov na osnove uglerodnykh nanotrubok.
20. Nazarov, S. A. (2009). Teorema Eshelbi i zadacha ob optimalnoi zaplate. Algebra ianaliz, 21 (5), 155–195. Available at: http://www.mathnet.ru/links/b4ab83583efec8059ed7924e3cec2ada/aa1157.pdf
21. Rublenoe steklovolokno. Available at: https://glass-tex.ru/index.php/49–carousel/2015–10–23–08–17–23/151–rublenoe-steklovolokno
22. Mashkov, Iu. K. (2010). Mekhanicheskie i tribotekhnicheskie svoistva polimernykh kompozitsionnykh materialov na osnove PTFE, optimizatsiia ikh sostava i tekhnologii. Vestnik SibADI, 4 (18), 17–21.