Influence of temperature conditions on wood polymer-sand composite

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Abstract. The subject of this research is new wood polymer-sand composite and the study of its frost resistance using computer experiment. Industrial waste in the form of sawdust, chips, lumpy waste and polyethylene terephthalate are used as the filler. A computer program has been developed for modelling the structure and physical properties of building blocks from wood polymer-sand composite. The program enables to set (in the windows of the interface form in the program code) geometric and physical parameters of building blocks and material components, as well as test conditions for cyclic heating and cooling to the maximum temperature during operation. It explores the effect of parameters on internal and surface destruction of building blocks. The program is applicable for a wide range of composite component concentrations, building blocks’ geometric parameters, variety of mechanical and thermal cycling tests. The influence of wood polymer-sand composite formulation on the structure has been studied during thermocyclic testing. The dependences of broken bonds on wood concentration, cartograms of bond breaking of wood polymer-sand composite with a wood concentration from 20 to 80% have been obtained. Recommendations for optimizing the formulation of wood polymer-sand composite blocks are given to minimize bond breaking during thermal cycling.

1. Introduction
Currently, creation of wood-polymer composites (WPC) is a very promising area of research. The fillers of this composite are waste of woodworking and logging industries. Such materials are distinguished not only by high performance properties, which enable to use them in a humid environment (where timber products cannot be used). They are also cheap. These composites are environmentally friendly and enable more efficient use of harvested wood. Composite materials with wood filler can be used for the manufacture of decking, finishing and roofing materials, garden and park furniture, noise screens, piers, doors, windows, etc. That is, the scope of products from WPC is extremely wide, and improving their properties is a promising research area.

A review of articles on wood-based polymer composites (the availability of compatibles on the market having comparable technical and operational characteristics) showed the following. There are products made of composite on the market in which polyethylene [1] and polypropylene [2], polyvinyl chloride [3] or others [1, 4] are used as a binder. Wood waste [5], mainly wood flour, is used as fillers [6]. The main distinguishing feature of wood-sand composites is the use of polyethylene terephthalate (PET) [7, 8] and modifier in the form of glyoxal. Such composition was not found in foreign sources.
The advantage of this solution, in comparison with analogues, is that the initial raw material is a plastic bottle, which only needs to be washed, crushed and dried. This fact greatly affects the price of finished products. This material relates to the field of compositions and technology of highly filled composite materials and products based on dispersed wood-plant fillers and thermoplastic polymer binders. It can be used in construction, engineering, furniture and other industries. The scientific novelty of the work lies in the theoretical justification and development of resource-saving technology for creating a new type of a composite. It is based on wood waste and polymer binder from which it is possible to manufacture products for industrial and civil construction. Rational and full use of sawmill and woodworking waste has acquired critical importance, and stays relevant to this day. This development enables to utilize a huge amount of forest industry waste. In addition, the use of wood waste as a building material will make it possible to replace wood in some areas. In its turn, it will reduce logging and increase woodworking efficiency. All this undoubtedly leads to an improvement of environmental situation.

Thus, after analyzing WPC products on the market, the formulation of the composite, called wood polymer-sand composite (WPSC) has been proposed. This material has absorbed all the best properties of the well-known WPC (water resistance, moisture resistance, high bending strength). Moreover it has also acquired new advantages that analogs do not have (the possibility of using any wood waste, higher strength due to the content of sand, cheapening production due to the fact that most of the constituent materials are household (PET flakes, obtained by recycling containers made of polyethylene terephthalate) and wood (woodworking and forestry waste: chips, sawdust, wood chips, lumpy waste) waste, as well as sand, which is available and inexpensive material [9].

The purpose of the work is to solve the problem of rational and full use of sawmill and woodworking waste as secondary technological raw materials.

2. Materials and methods

In order to widen the geography of building material, it must be resistant to temperature fluctuations. Testing of building materials according to 10060.0-95 State Standard were carried out as follows.

The determination of the frost resistance of a stone was carried out on cubic shape samples with an edge of 40-50 mm or cylinders with a diameter and height of 40-50 mm. Initially, the samples were kept in water at 20°C for 48 hours, then placed in a freezing chamber, bringing the temperature to minus 17-25°C (holding time is 4 hours). After that, the frozen samples were placed in water with a temperature of 20°C and kept at this temperature until complete thawing, but not less than 2 hours. Then the cycle repeated. 5 samples were tested for compression after 15, 25 and 50 cycles of freezing and thawing.

Currently, accurate data can be obtained not only with the help of a physical experiment, but also with the help of a computer experiment. So, mathematical model of the structure and properties of the material was created for WPSC study. Computer programs were created on its basis, with the help of which it is possible to investigate the behavior of material of different formulation in various conditions.

The particle dynamics method was used to model the structure and mechanical properties of WPSC. It was increasingly used in various branches of science and technology in the recent decades [10-12]. The simulated wood polymer-sand composite (WPSC) was divided into a large number (1 000–20 000) of elements in order the model had a high spatial resolution (figure 1).

The simulation was performed in a two-dimensional space XZ, while the elements had the same circular shape with the same diameter $d_E$. Elements according to their physical properties were divided into three types (wood, polymer, and sand). Elements had the ability to move in the process of mechanical testing of the sample according to the laws of classical mechanics. It led to a change in the shape and condition of the entire sample [13-14].

In this case, a program designed to simulate the destruction of building blocks structure made of wood polymer-sand composite as a result of changes in the temperature of blocks was used.

The program enabled to set the main geometric and physical parameters of the building block and material components in the windows of the interface form and in the program code, as well as test
conditions for cyclic heating and cooling to the maximum possible temperature during operation. It also studied the effect of parameters on the internal and surface destruction of the building block.

![Figure 1](image)

**Figure 1.** Representation of WPSC in the model as a combination of a large number of elements of three types (highlighted with dark - wood, gray - is sand, white - is a polymer). The outer rectangle limits the movement of WPSC fragments.

During the work of the program, both the appearance of the block structure (figure 2a) and broken bonds between the elements (shades of gray in figure 2b) were displayed on the screen. The first cycle of temperature change: heating of the model block from 273 to 360 K and cooling to 220 K led to the appearance of about 1.5 thousand broken bonds (figure 2).

The study of the concentration effect of WPSC components was carried out in two stages. At the first stage, the effect of wood concentration was studied at a ratio of polymer and sand concentrations of 2:1 [9, 15]. At the second stage, a two-factor study was carried out in which both the wood concentration and the sand concentration were changed (the polymer concentration was a dependent variable on the two main factors).

The program is applicable for a wide range of concentrations of the composite components, the geometric parameters of the building block, a variety of thermal cycling tests.

For definiteness, wood fragments were represented as chips (fragments extended in one direction) oriented along the long side of the block. Five cycles of heating to 360 K and cooling to 220 K were carried out for each studied wood concentration. In this series of computer experiments, the wood concentration \( C_w \) was changed from 20 to 80%, while the concentrations of the remaining components were maintained in the ratio \( C_{Pl} : C_{Sa} = 2 : 1 \).

3. Results and discussion

It was found that with an increase in the concentration of wood, the number of bonds broken by the time of termination of thermal cyclic tests decreases. So, at a wood concentration of 20%, the number of broken bonds is approximately twice as high as at a concentration of 50%. Apparently, wood has a reinforcing function and strengthens the internal structure of the material. Also, the adhesion between the polymer matrix and wood is better than the adhesion between the polymer matrix and sand, therefore increasing the concentration of wood increases the thermal cyclic resistance of the WPSC.

Thus, it is advisable to increase the concentration of wood in the material composition in order to increase the resistance of WPSC blocks to temperature fluctuations, since wood has high adhesion to the polymer matrix and performs reinforcing function.

More complete recommendations on the optimal WPSC composition by the criterion of resistance to temperature fluctuations can be given on the basis of a two-factor study. To ensure the comparability of optimization results for a number of other properties, a series of computer
Figure 2. The image displayed on the screen during the program operation: (a) - the structure of the composite material; (b) - cartogram of the distribution of internal irreversible deformations in the building block during thermal cycling.

Experiments were carried out (according to the same plan as in the study of resistance to compression) that is, the concentration of wood $c_W$ and at the same time the concentration of sand $C_{Sa}$ was changed from 10 to 50% in steps of 10%. The polymer concentration was calculated as $C_{Pl} = 100\% - C_W - C_{Sa}$. The structure turned out to be unstable in the 25 possible combinations of $C_W$ and $C_{Sa}$ parameters in four cases. We conducted separate computer experiments for the 21 point of the composition diagram on thermal cyclic testing of a model WPSC block (figure 3) determining the number of broken bonds $N_b$ and recalculating them into the specific area of cracks $S_b$ (table 1, figure 4).
Table 1. Specific crack area $S_t$ at various concentrations of wood $C_W$ and sand $C_{Sa}$.

| $C_{Sa}$, % | 10  | 20  | 20  | 40  | 50  |
|-------------|-----|-----|-----|-----|-----|
| 10          | 36.74 | 31.69 | 23.02 | 21.90 | 11.06 |
| 20          | 33.79 | 29.17 | 25.12 | 17.88 | 14.09 |
| 30          | 34.57 | 27.99 | 19.85 | 20.07 | 11.12 |
| 40          | 32.05 | 22.46 | 18.66 | 12.55 | – |
| 50          | 29.13 | 23.65 | –   | –   | – |

The following formula was obtained for calculating the number of broken bonds as a result of approximation of computer experiments:

$$S_t(C_{Sa}, C_W) = -2.930 \cdot 10^{-3} C_{Sa}^2 + 1.287 \cdot 10^{-3} k_2 C_W^2 - 2.446 \cdot 10^{-4} C_{Sa} C_W - 0.0210 C_{Sa} - 0.635 k_3 C_W + 43.264,$$

where $C_{Sa}$ and $C_W$ are expressed as percentages, $S_t$ – with respect to the area of cracks in square meters in one cubic meter of material volume.

The resulting dependency $S_t(C_{Sa}, C_W)$ is close to linear, so the plot of dependence is close to a plane (figure 4). The threshold level of the maximum specific crack area is 20 m$^2$/m$^3$. Firstly, the effect of the cycle number $N_c$ of temperature variation from 220 to 360 K on the structure of the model WPSC block with a typical concentration of components, size and shape of wood fragments was studied. The index $N_b$ is used to estimate the thermal cyclic destruction of the structure. It is the absolute number of broken bonds in a rectangular model block with a specified number of elements. $N_b$ can be recalculated into a relative indicator for comparison with experimental data (for example, the ratio of the crack area to a volume unit of material).

A visual analysis of the broken bond cartograms made it possible to establish that broken bonds do not arise uniformly in structure, but are grouped into clusters, near the initial adverse fluctuations of the composition (in terms of mechanical coupling) (figure 4).
The second heating-cooling cycle leads to the appearance of additional (about 500) broken bonds, but their number is about three times less than in the first cycle. Subsequent cycles practically do not lead to the appearance of new bonds. If 100 bonds still approximately appear during the third and fourth cycles, then, to subsequent cycles, the structure is stabilized. It is already destroyed in those places where thermal cyclic destructions can occur.

The concentration of WPSC components can significantly affect the stability of building blocks to temperature fluctuations, since it determines the internal coherence of the material. Figure 5 shows the effect of WPSC composition on the structure. The number of broken bonds increases with temperature increase, i.e. after 2-4 cycles of temperature change, WPSC block comes to a stable state. Figure 6 shows that the dependence of the number of broken bonds $N_b$ decreases with increasing wood concentration. It depends on the composition, production conditions, size and shape of wood fragments. It can remain strong or can be destroyed. The program was designed to simulate structure and physical properties of building blocks made of wood-polymer-sand composite.

The program is designed to simulate the structure and physical properties of the building blocks of wood polymer-sand composite. A nomogram for selecting the optimal composition (figure 7), sand and wood concentration (at a polymer concentration: $S_{pl} : S_{Sa} = 2:1$).
condition for minimizing the specific area of cracks $S_t$ after three thermal cycles. The optimum compositional area is darkened ($N_b \leq 2000$).

Analyzing the nomogram $S_t(C_{Sa}, C_W)$ and setting the threshold level for the maximum specific area of cracks of $20 \text{ m}^2/\text{m}^3$ (figure 4, table 1), it can be concluded that the optimum wood concentration is 40-55% with a low sand concentration of 10%. It decreases to 25-30 at a high sand concentration of 50% (figure 7). The resulting optimal area (shaded in figure 7) will be used below to determine the generalized optimal concentration area for several physical properties. The area of impossible compositions and compositions, under which the block spontaneously collapses, is hatched. The number of broken bonds increases with the length of the wood fragment. Thus, the influence of the size of wood fragments on WPSC structure in thermal cyclic tests was determined.

Recommendations to optimize the WPSC composition blocks to minimize bond breaking during thermal cycling (figure 7) were given in [16].

Consider the influence of the wood fragment sizes on the WPSC structure in thermal cyclic testing. The shape and sizes of wood fragments can have a significant effect on the stability of WPSC blocks to temperature fluctuations. A series of six computer experiments was carried out to study this effect. The length of fragments $L_f$ was changed at 5, 15, 25, 35, 50, 65 mm levels with the width of the wood fragment $W_f$ equal to 0.25 $L_f$ (figure 8). The concentration of wood was 50%, polymer - 33%, sand - 17% [9, 16].

It was found that the number of broken bonds $N_b$ remains virtually unchanged in the range $L_f$ from 5 to 35 mm with an increase in the size of the wood fragments. After this it increases noticeably (figure 8). Apparently, at small sizes of wood fragments (up to 25-35 mm) they are uniformly located in the structure and uniformly reinforce it. They also increase the adhesive connectivity of the structure. At large sizes of wood fragments (over 35 mm), the structure is substantially non-uniform. Extended polymer-sand areas are formed between large fragments of wood. A significant amount of broken bonds are formed in such polymer-sand areas due to poor adhesion.

4. Conclusion

Thus, from the standpoint of increasing the stability of WPSC blocks to temperature fluctuations, the size of wood fragments should not be more than 25-35 mm. The influence of WPSC composition on the structure of the material in thermal cyclic tests has been defined, i.e. the number of broken bonds
decreases with increasing wood concentration. The dependence of the number of broken bonds from the length of wood fragments again confirms the conclusion about the influence of wood sizes on the strength properties of WPSC blocks. The concentration of WPSC components can significantly affect the stability of building blocks to temperature fluctuations, since it determines the internal coherence of the material.

Acknowledgement
We are grateful for the financial support of the grantor: Federal State Budget Institution "Foundation for Assistance to the Development of Small Forms of Enterprises in the Scientific and Technical Sphere", "U.M.N.I.K." grant competition.

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