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Original Empirical Research

Forecasting the Properties of Multicomponent Mineral Polymer Composite Materials

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Abstract
Introduction. Advances in the construction industry are causing new composite materials to emerge. This is preceded by experimental studies, particularly analytical techniques for predicting the properties of new materials. Polymer composite materials (PCMs) which have proved to be efficient in other industries are commonly utilized in construction as well. PCMs have a number of features that should be taken into consideration while developing analytical techniques. PCM is considered under the condition of isotropy of the final material and compliance with the mixture rule during its manufacture. The objective of the study is to analytically determine the predicted strength limits of multicomponent composite materials with mineral fillers.
Materials and methods. There are diverse methods for identifying the characteristics of polymer composites. An integral method for determining the modulus of elasticity and the Poisson's ratio of a binary polymer composite material is set forth, based on the assumption that there is a relationship between the elastic potentials of the composite components. The transition of analytical forecasting of characteristics from binary to multicomponent polymer composite material is also shown.
Results. The major characteristic of building polymer composites is their strength. A formula has been obtained for the analytical determination of the predicted tensile strength of a binary polymer composite material, and the predicted tensile strength for some multicomponent polymer composite materials has been obtained based on these formulas as well.
Discussion and Conclusion. The results enable us to conclude that while forming the composition of a multicomponent polymer composite material, it is recommended that fillers with similar characteristics, in particular, elasticity modules are combined.

Keywords: multicomponent polymer composite, binary polymer composite, polymer matrix, powder filler, mixture rule, modulus of elasticity, Poisson's ratio, modulus of deformation, shear modulus, volume fraction, tensile strength

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Оригинальное эмпирическое исследование

Прогнозирование свойств многокомпонентных минерально-полимерных композитных материалов

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Аннотация
Введение. Прогресс строительной индустрии приводит к возникновению новых композитных материалов. Этому предшествуют экспериментальные исследования, в частности, аналитические приемы прогнозирования свойств

новых материалов. В строительстве широкое распространение получили полимерные композитные материалы (ПКМ), которые хорошо зарекомендовали себя и в других отраслях промышленности. ПКМ имеют ряд особенностей, которые следует принимать во внимание в процессе разработки аналитических методик. Рассмотрение ПКМ происходит при условии изотропии конечного материала и подчинения правилу смеси при его изготовлении. Целью настоящего исследования является аналитическое определение прогнозируемых пределов прочности многокомпонентных композитных материалов с минеральными наполнителями.

Материалы и методы. Существуют различные методики определения характеристик полимерных композитов. Предложена интегральная методика определения модуля упругости и коэффициента Пуассона бинарного полимерного композитного материала, основанная на предположении, что между упругими потенциалами составных частей композита существует связь. Также показан переход аналитического прогнозирования характеристик от бинарного к многокомпонентному полимерному композитному материалу.

Результаты исследования. Важнейшей характеристикой строительных полимерных композитов является их прочность. Получена формула для аналитического определения прогнозируемого предела прочности бинарного полимерного композитного материала, также на основе данных формул получен прогнозируемый предел прочности для некоторых многокомпонентных полимерных композитных материалов.

Обсуждение и заключение. Полученные результаты позволяют сделать вывод о том, что при формировании состава многокомпонентного полимерного композитного материала целесообразно сочетать наполнители с близкими по величине характеристиками, в частности, модулями упругости.

Ключевые слова: многокомпонентный полимерный композит, бинарный полимерный композит, полимерная матрица, порошковый наполнитель, правило смеси, модуль упругости, коэффициент Пуассона, модуль деформации, модуль сдвига, объемная доля, предел прочности

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Introduction. The development of the construction industry is causing more and more new materials, commonly composites, to emerge. This happens prior to a stage of experimental research where a rational composition is selected, as well as experimental samples are tested. Research can be time-consuming and costly, thus analytical techniques for predicting the properties of new materials are of interest. Polymer matrix composite materials (PCMs) are commonly used in various fields, including construction. Further on materials with a polymer matrix and one or more powder fillers formed by simply mixing these components without any chemical reactions between them will be considered. In this case, the PCMs obey the mixture rule [1]. Let us also assume that the composite as a whole and its individual components are isotropic and obey Hooke's law. For these materials, it is essential to obtain analytical expressions enabling the strength limits of the composite to be identified depending on the strength of its components.

Materials and Methods. There are diverse methods for identifying the characteristics of polymer composites, which assume that all of the material parts are subjected to the same deformations [2] or equal stresses [3], so developers of new materials make use of both approaches yileding an interval property assessment which is subsequently narrowed by means of the Hashin–Strikman [4] or Mori–Tanaka [5] methods. In [6], an integral method for identifying the modulus of elasticity and the Poisson's ratio of a binary material with a polymer matrix and a powder filler was set forth based on the assumption that there is a relationship between the elastic potentials of the composite components (1).

$$s\sigma_1\varepsilon_1 = \sigma_2\varepsilon_2, \tag{1}$$

where the indices “1” and “2” refer to the matrix and filler, respectively, and the parameter s is the ratio of the elastic modulus of the components $s = E_1/E_2$.

In [6], formulas were obtained for identifying the elastic modulus and Poisson's ratio of a binary composite (2) expressed in terms of volumetric deformation and shear modulus:

$$E_\Sigma = \frac{9K_\Sigma G_\Sigma}{3K_\Sigma + G_\Sigma}, \nu_\Sigma = \frac{3K_\Sigma - 2G_\Sigma}{2(3K_\Sigma + G_\Sigma)}. \quad (2)$$

The values included in the right-hand sides of expressions (2) are given by equalities (3) and (4):

$$K_\Sigma = (K_1 K_2)^{\frac{1}{2}} \cdot \frac{m_1 K_1^{\frac{1}{2}} + m_2 K_2^{\frac{1}{2}} s^{\frac{1}{2}}}{m_1 K_2^{\frac{1}{2}} + m_2 K_1^{\frac{1}{2}} s^{\frac{1}{2}}}, \quad (3)$$

$$G_\Sigma = (G_1 G_2)^{\frac{1}{2}} \cdot \frac{m_1 G_1^{\frac{1}{2}} + m_2 G_2^{\frac{1}{2}} s^{\frac{1}{2}}}{m_1 G_2^{\frac{1}{2}} + m_2 G_1^{\frac{1}{2}} s^{\frac{1}{2}}}. \quad (4)$$

In the latter expressions the index "Σ" refers to the composite as a whole, and m_1 and m_2 are the volume fractions of the matrix and filler, respectively, with $m_1 + m_2 = 1$. The examples of binary composites with a polypropylene matrix and various fillers provided in [6] are in good agreement with the theoretical results and the experimental values in [7], i.e., the discrepancy does not exceed 10%. PCM formulations are becoming increasingly complex, and materials with two or more fillers have emerged [8] for which it is also desirable to have similar methods for predicting their characteristics. [9] shows how dependencies (2) can be extended to composites of a more complex composition. For a PCM consisting of n components, expressions (2) must be applied (n – 1) times, sequentially adding new components to the binary composite. At each step, the sum of the volume fractions of the binary material is taken as one.

Research Results. In [9], as an example, the modulus of elasticity and the Poisson's ratio were identified for a three-component PCM with a polypropylene matrix (40%) and fillers made of wood flour (50%) and chalk (10%). At the same time, two variants of the "initial material" — a binary composite - were considered in order to assess the dependence of the final results on the accounting procedure for the fillers (Table 1). All the values in the table, except the dimensionless values, are provided in MPa.

Table 1

Modules of volumetric deformation of composites with a polypropylene matrix

Composite	Matrix			Filler			K_Σ	G_Σ	s	E_Σ	ν_Σ
	m_1	K_1	G_1	m_2	K_2	G_2					
"Initial material" — polypropylene (PP) and wood flour (WF)											
PP + WF	0.44	2917	493	0.56	8333	3846	4091	974	0.14	2707	0.39
Total	0.9	4091	974	0.1	7500	3462	4237	1052	0.3	**2914**	**0.385**
"Initial material" — polypropylene (PP) and chalk (C)											
PP+ C	0.8	2917	493	0.2	7500	3462	3182	599	0.16	1692	0.41
Total	0.5	3182	599	0.5	8333	3846	4226	1053	0.17	**2917**	**0.385**

As can be seen from Table 1, the selected total desired values do not depend on the accounting procedure for fillers. Fillers for building composites with a polymer matrix can be a wide variety of materials. Wood flour, a wood polymer composite (WPC), is typically used. There have been attempts to make use of chalk, talc, marble flour, and other powdery materials such as mineral polymer composites (MPCs) as fillers [7, 10, 11]. The factors restricting the wide use of these composites in construction are the complex technology of manufacturing products using complex extrusion equipment and the high cost of the final products. Nevertheless, it is possible to set up inexpensive mass production, e.g., of composite wall blocks, if extrusion is switched to injection molding technology currently used for producing paving slabs, and employ cement dust and fine gravel as a filler, which have now become readily available due to the consequences of hostilities in the populated areas of the eastern part of Ukraine. Unfortunately, lots of buildings and structures in the liberated territories cannot be restored and are being demolished resulting in a large amount of waste to be potentially reused. It is also possible to utilize dust generated in the factories of the construction industry and mostly easily recycled. Let us look at several materials whose cost and properties from open sources are given in Table 2.

Table 2

Characteristics of possible PCM fillers

Filler	Average price per tonn, roubles	Elasticity modulus, MPa	Poisson's ratio	Density ρ, kg/m^3	$K_э$
wood flour	11000	10000	0.3	450	**0.909**
aerosil	9900	6500	0.15	2450	0.657
barite	11750	6000	0.28	4480	0.511
plaster	20000	1400	0.16	2300	0.070
kaolin	5500	5000	0.25	2600	0.909
quartz	5750	7400	0.11	2600	1.287
chalk	2050	8500	0.29	1800	4.146
marble	2000	30000	0.15	2650	15.000
muscovite (mica)	22500	250	0.3	2700	0.011
talcum powder	3050	3500	0.25	2800	1.148
cement dust	950	19000	0.14	1400	20.000
fine crushed stone	550	20000	0.18	2600	36.364

Note that the value of the Poisson's ratio for wood flour is shown in Table 2 differs from the known one for wood. The difference is accounted for by the fact that small particles of wood flour become isotropic, as with such particle sizes the influence of the structural features of the starting material on the coefficient disappears. The relative high cost of composite products can be cut down by using cheaper fillers, therefore, in the last column of the table is the ratio of the elasticity modulus of the filler to its cost, i.e., the coefficient of efficiency of the filler. Obviously, the higher the K_e value, the cheaper the composite. If wood flour is taken as the base material, fillers with a K_e of at least 0.909 will be of interest. These materials are shown in Table 2. The most essential characteristic of building polymer composites is their strength. In [6], a formula was obtained for determining the predicted tensile strength of a binary PCM analytically:

$$\sigma_{com\Sigma} = \frac{3K_i - 2G_i}{3K_i t_i - 2G_i r_i}\sigma_i. \quad (5)$$

with

$$t_1 = \frac{G_1^{1/2}}{m_1 G_1^{1/2} + s^{1/2} m_2 G_2^{1/2}}, t_2 = \frac{s^{1/2} G_2^{1/2}}{m_1 G_1^{1/2} + s^{1/2} m_2 G_2^{1/2}}, \quad (6)$$

$$r_1 = \frac{K_1^{1/2}}{m_1 K_1^{1/2} + s^{1/2} m_2 K_2^{1/2}}, t_2 = \frac{s^{1/2} K_2^{1/2}}{m_1 K_1^{1/2} + s^{1/2} m_2 K_2^{1/2}}. \quad (7)$$

The ultimate strength of the composite is assumed to be the minimum of the two calculations for i, equal to 1 and 2.

(5) can also be used in order to predict the properties of multicomponent materials, which is proved by the results in Table 3 where the combination of fillers chalk and wood flour is also looked at (Table 1).

Table 3

Compressive strength of composite, MPa

Composite	Matrix			Filler			K_Σ	G_Σ	s	σ_{com1}	σ_{com2}
	m_1	K_1	G_1	m_2	K_2	G_2					
"Initial material" — polypropylene (PP) and wood flour (WF)											
PP + WF	0.44	2917	493	0.56	8333	3846	4091	974	0.14	31.1	26.8
Total	0.9	4091	974	0.1	7500	3462	4237	1052	0.3	**27.0**	**17.4**
"Initial material" — polypropylene (PP) and chalk (C)											
PP + C	0.8	2917	493	0.2	7500	3462	3182	599	0.16	29.9	16.8
Total	0.5	3182	599	0.5	8333	3846	4226	1053	0.17	**17.7**	**26.8**

Discussion and Conclusion. Analytical formulas have been thus obtained in order to predict the strength of multicomponent composite materials with a polymer matrix and mineral fillers considerably reducing the time spent on developing new materials by cutting down the number of physical experiments. The numerical results shown in Table 3 enable us to conclude that while forming the composition of a multicomponent PCM, it is advisable that fillers with similar modulus of elasticity are combined. Among the materials in Table 2, marble, cement dust, and fine crushed stone are preferrable. These fillers can be obtained as a result of recycling demolished buildings and structures, including in military zones. The strength of the multicomponent PCMs examined in the paper proves to be sufficient for manufacturing wall blocks which can be produced directly in construction areas and utilized as a construction material for walls and partitions of buildings for various purposes.

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