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COMPUTATIONAL EXPERIMENTS WHEN STUDYING MATERIALS PROPERTIES INFLUENCED BY "MIXTURE" FACTORS

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Abstract. Short information on computational materials science is given, with the methodology of material properties fields, in composition and process coordinates, as the part of it and as the background of the study presented in this paper. One of the main means of the methodology is random scanning the whole and local fields. These tools were developed and used to solve many problems in materials science related to the properties defined by mutually independent factors. The purpose of the study presented in this paper has been to develop the tool for random scanning the fields of properties effected by "mixtures" of *q* components, linearly related portions of components in rangers from 0 to 1, with their sum equal to 1. In these cases, the factors domain (or subregion of it) presents the simplex. The special designs of experiments to get reduced polynomials describing the fields in simplex coordinates are used. Two procedures for generating any number of uniformly distributed points on the simplex have been developed. These points define the virtual mixtures simulated in computational experiments. The procedures were tested by scanning the fields of two rheological characteristics of lime suspension filled with "short", “medium", and "long" cellulose fibers. Experimental-statistical models in the form of reduced polynomials for effective viscosity at shear rate equal to1 s^{-1} and for the rate of destruction of liquid structure (parameters of power-law model of flow, $K = \eta_1$ and m) obtained in previous study are used to determine the levels of these characteristic for each of simulated mixture. Computational experiments were carried out, in which the fields of η_1 and m in whole simplex domain and in some of its zones were scanned, allowing the generalizing indices of the fields and different correlations between η_1 and m in different zones of mixture triangle to be estimated.

The developed tools, the procedures of generating random points, which would define the simulated compositions of the "mixtures", make significant contribution to the progress of the methodology of recipe-technological fields of properties and to computational materials science.

Keywords: design of experiment, simplex domain, experimental-statistical model, effective viscosity, rate of destruction, lime suspension, cellulose fiber.

Introduction. In 1992 the first issue of the international journal "Computational Materials Science" (CMS) was published [1]. That year has been proposed (Voznesensky V.A., 1993) to be considered the year of the birth of this direction of science. The aim of CMS and the journal declared at the title page of the first issue has been "to enhance the communication between experimental materials research and computational work on both existing and new, advanced materials and their applications". Since then the scope of the journal expanded quite a lot [2].

Analysis of recent research and publications. The methodology of composition-process fields (recipe-technological fields, [3, 4]) was put forward as the component of computational materials science. The field $Y(\boldsymbol{x})$ of material property (any characteristic of material structure, any criterion of its quality, even its cost) presents the values of Y in coordinates of material composition and parameters of production and exploitation processes, vector of CP-factors $\boldsymbol{x} = (x_1, x_2, \ldots, x_i, \ldots, x_k)$.

Random scanning the fields has become one of the main instruments of the methodology [3, 4, etc.]. It was developed for domain of normalised factors (1):

$$-1 \leq x_i \leq 1. \quad (1)$$

Random scanning the whole or local fields means: generating uniformly distributed points in factor domain or its subregions (compositions and process factors values corresponding to the points); calculating the levels of $Y(\boldsymbol{x})$ by its model. In most cases multifactor polynomial experimental-statistical models (ES-models, [5]) are used.

When studying multicomponent disperse systems, the building composites among them, the system of factors under study or some of them (factor subsystem) can present the "mixture". This is when the portions (from 0 to 1) of the components forming the mixture (1 in a sum) should be considered as the factors. It can be the mixture of fractions of the grains of several size or different minerals, or the portions of the components in complex chemical admixtures, etc.

"Mixture" (***M***) is the system (subsystem) of linearly related factors v_i, the portions of the components forming the mixture (2). M_q is the mixture of q components.

$$0 \leq v_i \leq 1, \ \Sigma v_i = 1, \boldsymbol{v} = (v_1, v_2, \ldots, v_i, \ldots, v_q) \in \Omega_v. \quad (2)$$

The domain Ω_v of factor space is (q-1)-dimensional simplex (segment, triangle, tetrahedron ...). In these cases of linearly related factors the special kinds of polynomials are used as the models of the fields $Y(\boldsymbol{x})$, basing on corresponding experiment designs [6-12].

To carry out the scanning of property fields in such domains one should have the means to get uniformly distributed points in them.

So **the aim of the study** presented in this paper has been to develop the procedure of generating the random points on the simplex and to test it solving some specific material science problem.

The methods include the following.

The generating of random numbers is carried out with the help of Excel analysis package. In Excel all calculations are carried out. Other means (including specially designed) can be also used.

To test the procedure in practice the results of previous research [13] are applied, in particular, the models for two parameters of Ostwald-de-Waele rheological equation [14], power law model written here in logarithmic form (3). The coefficient K in (3) is equal to the effective viscosity η_1 (Pa·s) at shear rate $\gamma' = 1$ s^{-1}, and the exponent $m < 0$ characterizes the rate of destruction of fluid structure during shear deformations – the higher |m|, the less stable is the fluid structure during flow.

$$\ln\eta\,(\boldsymbol{x}) = \ln K(\boldsymbol{x}) + m(\boldsymbol{x}) \cdot \ln\gamma'. \quad (3)$$

Among the dozens of the models of non-Newtonian fluid flow [15] the power law model, the good one for engineering applications in certain ranges of shear rate, is commonly used.

It should be underlined that the parameters in (3) are not the constants, of specific non-Newtonian fluid, of certain composition, as they are commonly considered, but the functions of composition factors. Effective viscosity can be estimated by such model for any composition at any shear rate in the ranges under study, as it was done, in particular, in [3, 16, 17]. The model (3) illustrates the possibility and usefulness of combining the models of different levels [3], for instance, ES- model and structural simulation models [18, 19].

Viscosity curves and models of type (3) in the range of γ' between 0.066 and 8.41 c^{-1} were obtained (adequate with error not more than 5%) when studying [13] lime suspension filled with Technocel® cellulose fibers of three lengths. The rotational rheometer "Polimer" RPE-1M was used to get the curves.

The portions of fibers of three lengths were varied in the experiment: v_1 – mass fraction of "short" fibers, with nominal length of 200 μm; v_2 – fraction of "medium" length fibers, 1000 μm; v_3 – fraction of "long" fibers, 2500 μm. They present the mixture (4) of 3 fractions (q = 3).

$$0 \leq v_i \leq 1, \ \Sigma v_i = 1, \boldsymbol{v} = (v_1, v_2, v_3). \quad (4)$$

The amount of fibers introduced into the suspension remained constant – 0.9 parts by mass per 100 parts of lime, at water-lime ratio equal to 1.

The experiment was carried out according to simplex-lattice design of incomplete 3rd degree [7], the points being the same as in non-saturated simplex-centroid design of the 2nd order [8]. The points of the design are given in Table 1.

Table 1 – Compositions of 7 mixtures according experiment design

Points	1	2	3	4	5	6	7
v_1	1	0	0	0.5	0	0.5	0.333
v_2	0	1	0	0.5	0.5	0	0.333
v_3	0	0	1	0	0.5	0.5	0.333

The data obtained in the designed natural experiment have allowed the models (5) and (6) of the kind (7) to be got, for $\ln\eta_1$ and $|m|$ (the effects insignificant at 10% risk have been eliminated). The isolines of these two rheological parameters are shown in Fig. 1.

$$\begin{aligned}\ln K = \ln\eta_1 = \ & 2.978v_1 - 0.533v_1v_2 - 1.489v_1v_3 \pm 0\, v_1v_2v_3 \\ & + 2.593v_2 - 0.223v_2v_3 \\ & + 2.761v_3\end{aligned} \tag{5}$$

$$\begin{aligned}|m| = \ & 0.951v_1 \pm 0\, v_1v_2 + 0.158v_1v_3 + 0.867\, v_1v_2v_3 \\ & + 1.025v_2 - 0.158v_2v_3 \\ & + 0.892v_3\end{aligned} \tag{6}$$

$$\begin{aligned}Y = \ & A_1v_1 + A_{12}\, v_1v_2 + A_{13}v_1v_3 + A_{123}\, v_1v_2v_3 \\ & + A_2v_2 - A_{23}v_2v_3 \\ & + A_3v_3\end{aligned} \tag{7}$$

These are the models used in computational experiments, to illustrate statistical trials on simplex with application of procedures presented below.

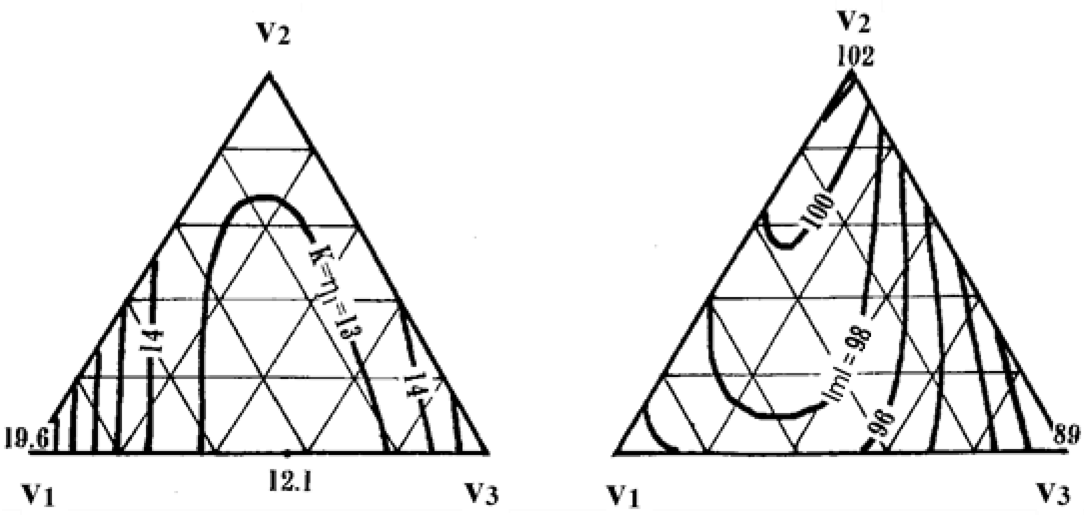

Fig. 1. Isolines of effective viscosity η_1 (Pa·s) and of destruction rate $|m|\cdot 10^2$ on mixture triangles

The **results** include the following.

Firstly, the *procedures of generating random points* (*mixtures*) *in simplex domain* themselves.

Any number of random values ξ_i for q variables (i = 1…q) uniformly distributed inside (0, 1) limits are generated.

The transformations of generated ξ_i to v_i that would provide (2), $\Sigma v_i = 1$, have been put forward.

1. The simplest one (8):

$$v_i = \xi_i / \sum_{i=1}^{q} \xi_i \tag{8}$$

2. Another one (9):

$$v_i = a_i + \xi_i \cdot d_i \cdot d / S, \text{ if } S \geq d, \tag{9}$$

$$v_i = a_i + \xi_i \cdot d_i + (d-S) \cdot d_i \cdot (1-\xi_i) / (\Sigma d_i - S), \text{ if } S < d,$$

where i = 1, … q; a_i, b_i – lower and upper borders of the range of v_i;

$d_i = b_i - a_i$; $d = 1 - \Sigma a_i$; $S = \Sigma \xi_i \cdot d_i$.

One hundred of the points obtained using formular (8) are shown in Fig. 2.

The points at the vertices of the triangle are added since their coordinates cannot be generated principally (as any fixed exact values).

Secondly, *usage of the developed procedures* for scanning the fields of rheological characteristics of the suspension filled with fibers.

Some results of one realization of scanning the field $\eta_1(v_1, v_2, v_3)$ are shown in Fig. 3. The levels of the field at each point shown in Fig. 2 were determined by model (5). The error of the model was not accounted for, but multiple realization of scanning, with multiply generated distribution of points (mixtures), showed the convergence of results to the field determinate by model (5).

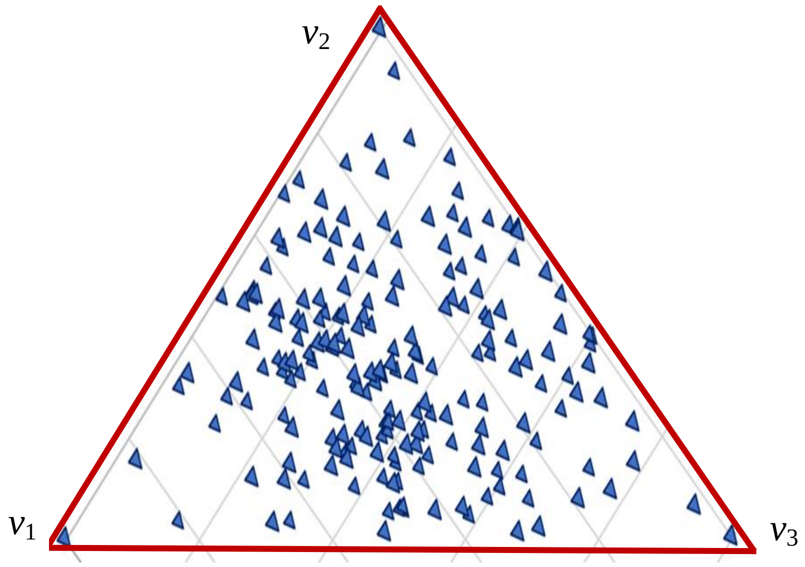

Fig. 2. The hundred random points inside the simplex and 3 fixed points at its vertices

Not only can the main generalizing indices $G\{v_1, v_2, v_3\}$ of the field $\eta_1(v_1, v_2, v_3)$, such as minimal and maximal levels and their coordinates, be determined after sorting the mixtures by the values of Y (η_1 in this case) but the other valuable numerical characteristics too. The important one among them, the "size" of the region of acceptable mixtures, the ratio (**Ω**) of the number of compositions that would comply with specified levels of Y (set by a customer or some standard, or by an idea of researcher) to the quantity of all compositions under consideration [3, 4, 20]. The estimates of this and other G can be seen in Fig. 3.

Analysis of correlation of η_1 with $|m|$ in various subregions of mixture factors domain can be carried out using the developed procedures.

The scatter diagram of the values of two rheological characteristics determined for 7 mixtures in natural experiment shows the absence of correlation, as the diagram presenting the generated sample of 103 paired values also does (Fig. 4).

			Random series				*Normalised*						*Ranked series (by η_1)*					
Coefficients of model	Estimates of coefficients	Mixture number	Number of mixtures								**103**	Mixture number	Number of mixtures				**103**	
			Maximum										Maximum					
			1.00	**1.00**	**1.00**		**1.00**	**1.00**	**1.00**	**1.00**	**2.98**		**1.00**	**0.72**	**1.00**	**2.98**	**19.65**	**max**
			Average										Average					
			0.55	**0.49**	**0.42**		**0.38**	**0.33**	**0.30**	**1.00**	**2.63**		**0.32**	**0.35**	**0.32**	**2.58**	**13.26**	**average**
			Minimum										Minimum					
			0.00	**0.00**	**0.00**		**0.00**	**0.00**	**0.00**	**1.00**	**2.51**		**0.00**	**0.00**	**0.00**	**2.51**	**12.30**	**min**
			ξ1	***ξ2***	***ξ3***	***sum***	***v1***	***v2***	***v3***	***sum***	**lnη1**		***v1***	***v2***	***v3***	**lnη1**	**η1**	
A $_1$	**2.98**	*1*	1	0	0	1	1	0	0	1	2.98	*1*	1	0	0	2.98	19.65	**max**
A $_2$	**2.59**	*2*	0	1	0	1	0	1	0	1	2.59	*3*	0	0	1	2.76	15.82	
A $_3$	**2.76**	*3*	0	0	1	1	0	0	1	1	2.76	*49*	0.7936	0.1157	0.0907	2.76	15.76	**$h_1 > 15$**
A $_{12}$	**-0.53**	*4*	0.6102	0.9847	0.0179	1.6127	0.3784	0.6106	0.0111	1	2.61	*56*	0.6993	0.2366	0.0640	2.72	15.15	**W = 4/103=**
A $_{13}$	**-1.49**	*5*	0.5788	0.0235	0.4803	1.0825	0.5346	0.0217	0.4437	1	2.51	*57*	0.0291	0.3596	0.6113	2.67	14.51	**3.88%**
A $_{23}$	**-0.22**	*6*	0.7168	0.7465	0.259	1.7224	0.4162	0.4334	0.1504	1	2.59	*21*	0.0619	0.2349	0.7032	2.66	14.33	
A $_{123}$	**0.00**	*7*	0.9575	0.5327	0.1597	1.6499	0.5804	0.3228	0.0968	1	2.65	*10*	0.0426	0.4354	0.5220	2.65	14.21	**$13 < h_1 < 15$**
		8	0.6271	0.4622	0.8968	1.9861	0.3157	0.2327	0.4516	1	2.54	*7*	0.5804	0.3228	0.0968	2.65	14.14	**Ω = 55/103=**
		9	0.3171	0.7507	0.2666	1.3344	0.2376	0.5626	0.1998	1	2.58	*37*	0.5046	0.4530	0.0424	2.64	14.02	**53.40%**
		10	0.0693	0.7089	0.8497	1.6279	0.0426	0.4354	0.522	1	2.65	*48*	0.4816	0.4913	0.0271	2.64	13.98	
			•	•	•													
		37	0.9029	0.8105	0.0758	1.7892	0.5046	0.453	0.0424	1	2.64	*17*	0.1608	0.6891	0.1500	2.59	13.26	**average**
		38	0.3573	0.6532	0.7270	1.7374	0.2057	0.3759	0.4184	1	2.57	*12*	0.2177	0.7246	0.0577	2.58	13.25	
		39	0.9749	0.2639	0.4756	1.7143	0.5687	0.1539	0.2774	1	2.58	*65*	0.1808	0.7136	0.1057	2.58	13.24	
			•	•	•													
		102	0.7112	0.2612	0.2370	1.2095	0.5880	0.2160	0.1960	1	2.61	*77*	0.4744	0.0609	0.4648	2.51	12.30	
		103	0.4100	0.1562	0.9249	1.4910	0.2749	0.1048	0.6203	1	2.53	*78*	0.4209	0.0861	0.4930	2.51	12.30	**min**

Fig. 3. Fragment of the table of scanning the field $\eta_1(v_1, v_2, v_3)$ with some generalizing indices of the field

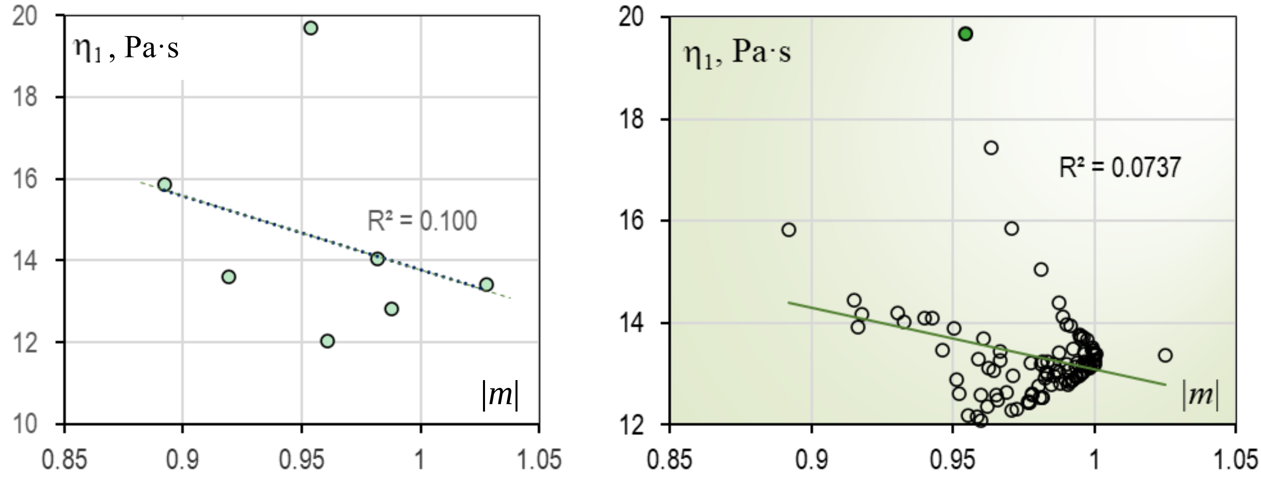

Fig. 4. Scatter diagrams of the values of η_1 and $|m|$ obtained in natural experiment (7 compositions) and in computational experiment (103 compositions) over the whole domain of mixtures under study

It would be reasonable to assume a significant difference in the structures of suspensions with fibers of different lengths and with their mixtures, and, consequently, a different relationship between viscosity and the rate of destruction of the structure.

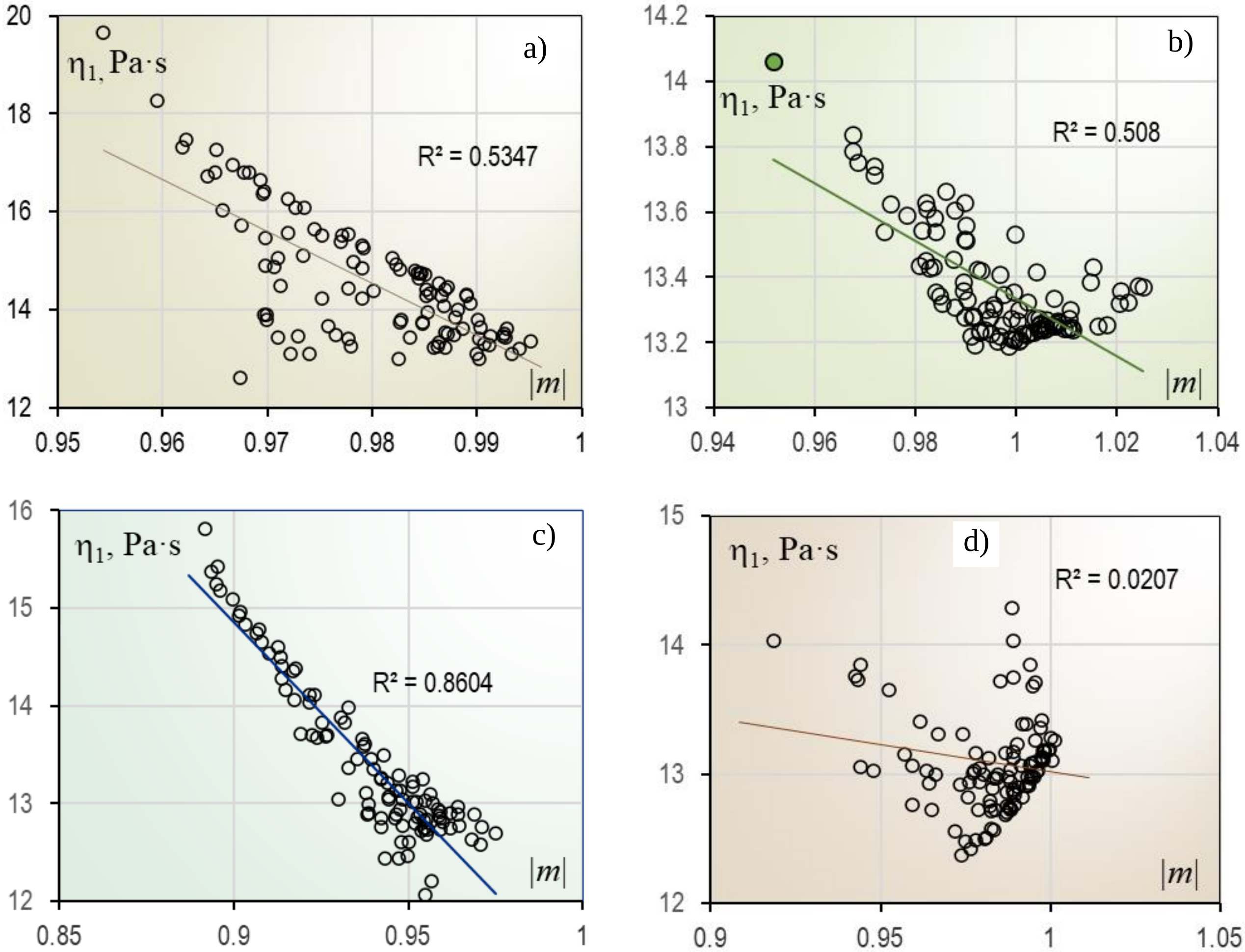

Fig. 5. Scatter diagrams obtained in computational experiments:
a – in zone of mostly "short" fibre; b – in zone of mostly "medium" fibre;
c – in zone close to vertex v_3 (of "long" fibre); d – inside the triangle

The computational experiments in various zones of mixture triangle have been carried out to estimate the correlation of η_1 with $|m|$, both developed procedures (8, 9) of generating linearly related mixture factors being tried. Some results are presented in Fig. 5.

The levels of $|m|$ and η_1 were estimated, in particular, at the following limits of factors values:

- $0.6 \le v_1 \le 1$, $0 \le v_2 \le 0.4$, $0 \le v_3 \le 0.4$ (Fig. 5, a);
- $0 \le v_1 \le 0.3$, $0.7 \le v_2 \le 1$, $0 \le v_3 \le 0.3$ (Fig. 5, b);
- $0 \le v_1 \le 0.4$, $0 \le v_2 \le 0.4$, $0.6 \le v_3 \le 1$ (Fig. 5, c);
- $0.1 \le v_1 \le 0.8$, $0.1 \le v_2 \le 0.8$, $0.1 \le v_3 \le 0.8$ (Fig. 5, d).

The results could be more impressive in case of wider ranges of the properties under study. Nevertheless, the revealed differences in correlation indicate to the changes in mechanisms of structure formation with changes in specific disperse phase. The changes in mechanisms should be, probably analysed from physical-chemical mechanics point of view [21].

Other tasks and problems of materials science when the mixtures (2) are involved could be solved now, with the help of the developed procedures, as the problems had been solved [3, 20, 22-24], using random scanning the fields in normalized coordinates (1). The "involved mixtures" means that it could be the system of both mutually independent and linearly related factors, and even with two mixtures [3, 12].

The search for the best solution by some criteria of optimality, at any number of specified restrictions and the problems of multicriterial compromise optimization [3, 20, 23, 24], computational experiments for isoparametric analysis [3, 22] and for analysis of the changing generalizing indices of properties fields [3, 12], other tasks that need random scanning the fields of properties can be also fulfilled when whole factor domain or part of it presents q-component simplex.

Conclusions. The new tools have been developed that makes significant contribution to the development of the methodology of recipe-technological fields of properties and to computational materials science. These are the procedures of generating uniformly distributed random points in simplex domain, which define the simulated compositions of the "mixtures".

The procedures have been applied in study of rheological characteristics of lime suspension filled with the mixture of cellulose fibre of three lengths. The way to estimate the generalizing indices of the fields of material properties has been shown. The computational experiments have been carried out in different subregions of mixture triangle to evaluate the correlation of effective viscosity of the suspension with the rate of its structure destruction under certain shear rate. The differing correlation from zone to zone has been revealed.

The developed tools open up new opportunities for studying the variety of the "mixtures, technologies" systems with means of computational materials science.

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ОБЧИСЛЮВАЛЬНІ ЕКСПЕРИМЕНТИ ПРИ ВИВЧЕННІ ВЛАСТИВОСТЕЙ МАТЕРІАЛІВ ПІД ВПЛИВОМ ФАКТОРІВ «СУМІШІ»

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Анотація. Наводиться коротка інформація про комп'ютерне матеріалознавство та про методологію рецептурно-технологічних полів властивостей як його складової. Це передумови дослідження, представленого у цій статті. Один із основних засобів методології полів властивостей – випадкове сканування повних і локальних полів. Цей інструментарій було розроблено та використано під час вирішення багатьох завдань матеріалознавства, коли властивості визначалися дією взаємо-незалежних чинників. Мета представленого дослідження – розробити інструмент для випадкового сканування полів властивостей, що визначаються «сумішами» компонентів q, лінійно пов'язаними їх частками в діапазонах від 0 до 1; сума q часткою дорівнює 1. У цих випадках факторна область (або її підобласть) є симплексом. Використовуються спеціальні плани експериментів, щоб отримати спеціальні наведені поліноми, що описують поля у симплексних координатах. Розроблено дві процедури для генерування будь-якого числа рівномірно розподілених точок на симплексі. Їм відповідають «суміші» у обчислювальних експериментах. Процедури були випробувані при скануванні полів двох реологічних характеристик вапняної суспензії, наповненої короткими, середніми і довгими целюлозними волокнами. Експериментально-статистичні моделі, у вигляді наведених поліномів, для ефективної в'язкості при швидкості зсуву 1 с$^{-1}$ та темпу руйнування структури рідини (параметрів степеневої моделі течії, $K = \eta_1$ та m), отримані в попередньому дослідженні, дозволяють визначити рівні цих характеристик для кожної симульованої суміші. Виконані обчислювальні експерименти, в яких проскановані поля η_1 та m у всій симплексній області та в деяких її зонах, дозволяючи оцінити узагальнюючі показники полів та різну кореляцію η_1 та m у різних зонах сумішевого трикутника.

Розроблені засоби, процедури генерації випадкових точок, які симулюють склади «сумішей», роблять значний внесок у розвиток методології рецептурно-технологічних полів властивостей та в комп'ютерне матеріалознавство.

Ключові слова: план експерименту, симплексна область, експериментально-статистична модель, ефективна в'язкість, швидкість деструкції, вапняна суспензія, целюлозне волокно.

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