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HOW DO COMPOSITE MATERIAL PROPERTIES CHANGE WITH ONE OF THEM UNCHANGED?

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Abstract. A few words about the history and importance of composite materials, dispersed systems with multicomponent dispersion medium and dispersed phase, in the progress of civilization are in the beginning of the paper. This and the methodology of the fields of material properties in the coordinates of composition and process factors, described by experimental-statistical (ES) models, underlie the research presented in this paper. One of the main tools of the methodology is random scanning of "composition-process" fields of material properties. The aim of the work is to show how this tool allows to evaluate the change in properties if one of them should be unchanged, using the examples of solving two tasks in the study of lightweight gypsum concrete, with cenospheres and perlite as fine aggregates. Microsphere size distribution with average about 0.1 mm and average size of perlite grains about 0.3-0.5 mm could suggest rather compact piling and forming relatively steady skeleton.

ES-models of the dependences of density and compressive and flexural strength on the content of aggregates and dosages of two chemical additives have been used, built on the results of the designed natural experiment, in which property levels were determined for 18 compositions.

In computational experiments the compositions (of filler at fixed average values of admixtures dosages) are generated, and the estimates of their properties by the models allow isoparametric analysis to be performed. In the first example, compositions in which the concrete density level goes beyond the specified boundaries of the isoparametric corridor are excluded from the analysis. Changes in strength are estimated under condition of an approximately constant required density. The strongest compositions under this condition can be assessed. In the second case, the compressive strength must be the required constant. Changes in density and flexural strength under this condition are evaluated based on their levels in compositions remaining in the isoparametric corridor of compressive strength. In this case, the lightest compositions of a given strength can be determined. Isoparametric analysis has proven to be quite useful in materials science.

Keywords: experimental-statistical model, isoparametric analysis, lightweight gypsum concrete, cenospheres, perlite, strength, density.

Introduction. Composite materials with natural matrices and reinforcements of local origin have been used since ancient times. The authors of [1] compare the importance of this fact with the discovery of fire and the invention of the wheel. Nowadays, the composites, with a variety of dispersion media and dispersed phases, present the special class of High-Performance Materials (HPM), those that best serve exactly what they are designed for [2-4]. HPM is called one of top achievements of modern civilization.

Building composite materials are complex multicomponent dispersed systems. Nested multicomponentity is characteristic (complex chemical additives, a mixture of three mineral fillers with three grain sizes each). When studying and developing building composites the methodology of composition-process fields has proved to be effective [5, 6]. It allows the fields of material properties Y (structural, technological, and performance characteristics, criteria of utilization and ecology, any other criteria, including cost) in the coordinates of composition and process factors (CP-factors), vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_i, \ldots, x_k)$, to be described. Experimental-Statistical models [5], built on the results of designed natural experiment [7, 8], are used as the functions $Y(\boldsymbol{x})$. They make it possible to extract directly inaccessible information hidden in the data with the help of computational experiments, carrying out the random scanning of the property fields [5, 9, 10]. The individual and combined influence of the factors on Y can be evaluated, the acceptable, optimal and compromise CP-solutions can be estimated. Among the problems that could be solved is the one indicated in this paper title. It is necessary to estimate the changes in $Y(\boldsymbol{x})$ when the level of one Y must be kept constant. The way to solve the problem is shown below on the base of building material science specific study.

So, **the aim of the study** presented in this paper has been, firstly, to promote the way to solve the problems of keeping one property of material unchanged and of evaluating the variations of others under this condition.

Secondly, to see the changes in the properties of lightweight gypsum concrete, when specified level of one of the properties must be maintained constant.

To solve the problems of this kind V.A. Voznesensky put forward and developed [11] isoparametric analysis (IPA). The procedure was quite complicated. Nowadays, IPA is carried out using computational materials science methods [5, 12]. Many problems have already been solved with the help of IPA. This paper presents another one.

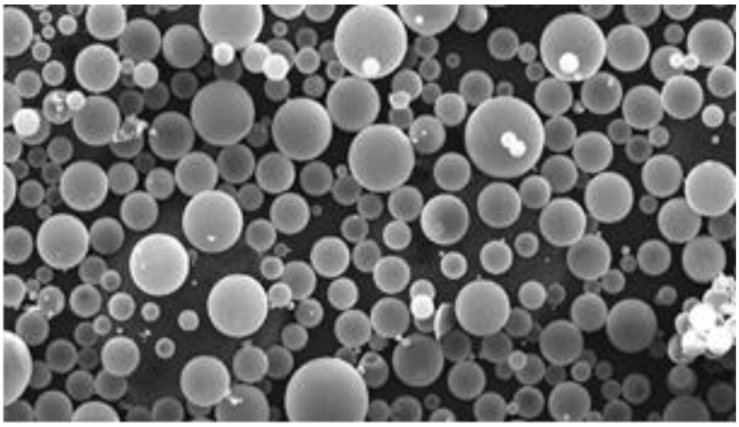

Fig.1 Cenospheres

When developing the lightened gypsum concrete on the base of β-hemihydrate [13] it was suggested that alumina-silica microspheres (cenospheres, Fig. 1) formed as a part of fly ash [14, 15] could replace (totally or partially) water absorbing aggregates, perlite in particular, and reduce the quantity of mixing water and the decrease in strength. The cenospheres have low density and heat conductivity, spherical form, chemical inertness, high hardness and melting temperature [15, 16].

The methods. Two groups of composition factors varied in the designed experiment are shown in Table 1, corresponding to their values being the levels of normalised factors, $|x_i| \leq 1$ (1).

Table 1 –Values of composition factors in the experiment

i	Factor X_i		Levels		
			$x_i = -1$	$x_i = 0$	$x_i = +1$
1	Aggregate factors – quantities (gypsum volume %) of:	cenospheres (CS)	30	50	70
2		perlite (P)	0	15	30
3	Matrix factors − dosages (% of gypsum mass) of:	superplasticiser (SP)	0.3	0. 5	0.7
4		air-entraining admixture (AE)	0.2	0.5	0.8

$$x_i = \frac{X_i - X_{0i}}{\Delta X_i}, \quad X_i = x_i \cdot \Delta X_i + X_{0i} \ , \qquad (1)$$

where x_i – is normalised value of the i^{th} factor, X_i – natural value, X_{0i} – center of variation range, ΔX – half range (variation interval).

Microsphere size distribution with average about 0.1 mm and average size of perlite grains about 0.3-0.5 mm could suggest rather compact piling and forming relatively steady skeleton.

The factor ranges have been chosen basing on preceding trials. In particular, the lower limit of CS is conditioned by revealed growth of strength when introducing up to 20-30% of cenospheres. The required amount of water for each β-hemihydrate based composition provided mix spread of 18 cm (at glass table).

Material property levels measured according to Ukrainian standards were determined for 18 compositions, corresponding to the points of the synthesized 4-factor D-optimal design of the 2^{nd} order [7, 17, 18]. Density ρ (kg/m^3), compression and bending strength f_{cm} and $f_{c.tf}$ (MPa), and heat conductivity λ (W/m/K) were among the properties.

The data obtained have made it possible the fields of material properties in four composition coordinates (of vector $\boldsymbol{x}$) to be described by non-linier 4-factor experimental-statistical models like (2) and (3) written in structured form. Block (a) contains effects of the aggregates, block (b) includes effects of the admixtures, block (c) presents synergetic effects of the aggregates and admixtures. The models are adequate to experimental data at the errors of 1% for ρ and 6% for f_{cm}, with significant coefficients at 10% risk.

$$\rho = 945.2 \begin{array}{|l|}\hline -39.5x_1 \pm 0\ x_1^2 + 6.5x_1x_2 \\ -73.3x_2 \pm 0\ x_2^2 \quad \text{(a)} \\ \hline -5.5x_3 + 10.9x_3^2 + 7.5x_3x_4 \\ -9.8x_4 + 11.8x_4^2 \quad \text{(b)} \\ \hline \end{array} \begin{array}{|l|}\hline \pm 0\ x_1x_3 \\ \pm 0\ x_1x_4 \\ +5.6x_2x_3 \\ -8.7x_2x_4 \ \text{(c)} \\ \hline \end{array} \qquad (2)$$

$$f_{cm} = 5.46 \begin{array}{|l|}\hline -0.75x_1 \pm 0\ x_1^2 \pm 0\ x_1x_2 \\ -1.14x_2 \pm 0\ x_2^2 \quad \text{(a)} \\ \hline -0.36x_3 + 0.40x_3^2 \pm 0\ x_3x_4 \\ -0.55x_4 + 11.8x_4^2 \quad \text{(b)} \\ \hline \end{array} \begin{array}{|l|}\hline +0.19x_1x_3 \\ \pm 0\ x_1x_4 \\ +0.22x_2x_3 \\ \pm 0\ x_2x_4 \ \text{(c)} \\ \hline \end{array} \qquad (3)$$

The uniformly distributed aggregate compositions were generated, 1000 points (x_1, x_2), for which the levels of the properties were determined by ES-models at constant values of admixtures contents (centers of their ranges). The reasonable number of points is conditioned by the size of factor domain under consideration (2^k, [5]). The vertices of k-dimensional factor cube, 4 vertices (±1) of the square {x_1, x_2} in our case, are added to generated random points to take part in computational experiment (since they could not theoretically be generated [5]).

The random compositions have been got with the help of Excel analysis package. All calculations are carried out in Excel.

After sorting these data by the level of the property Y_{IS}, which should remain specified constant C_{IS}, those of compositions (the points $\boldsymbol{x}_{is}$) are left for participation in the analysis, the values of Y_{IS} at which, according to the model $Y_{IS}(\boldsymbol{x})$, fall within the isoparametric corridor $C_{is} \pm \Delta Y_{is}(\boldsymbol{x}_{is})$. The width of the corridor ΔY_{is} can be assigned based on the technical conditions of a specific task and, obviously, should cover the confidence interval [18] for Y_{IS} estimates (by the ES-model).

The levels of other Y under consideration are calculated by corresponding model at each $\boldsymbol{x}_{is}$, showing their changes in isoparametric corridor, that is, at approximately the same level of Y_{IS}. The best, for this or that Y, values of $\boldsymbol{x}_{is}$ can be estimated.

The results of the research. The following results have been obtained when solving two tasks of IPA.

In the first case approximately constant level of ρ should be provided. This could be conditioned by specification for the material to be used in certain constructions, wall partitions or even floor coverings, for example. In the second case f_{cm} should be "almost constant" for similar reasons.

The level assigned for ρ as Y_{IS} was ρ_{is} = 950 ± 10 kg/m^3. The results of scanning the field of ρ_{is} in acceptable region is shown in Fig. 2.

Shown in Fig. 3 are the results of scanning the fields of f_{cm} and $f_{c.tf}$ at $\rho \approx 950$ kg/m^3. The following maximal levels of these properties and the contents of the aggregates providing them under this condition are $f_{cm\ max} \cong 6.1$ at x_1 = -0.86, x_2 = 0.25 (CS = 32.8, P = 18.8) and $f_{c.tf\ max} \cong 2.2$ at x_1 = -0.93, x_2 = 0.34 (CS = 31.4, P = 20.1).

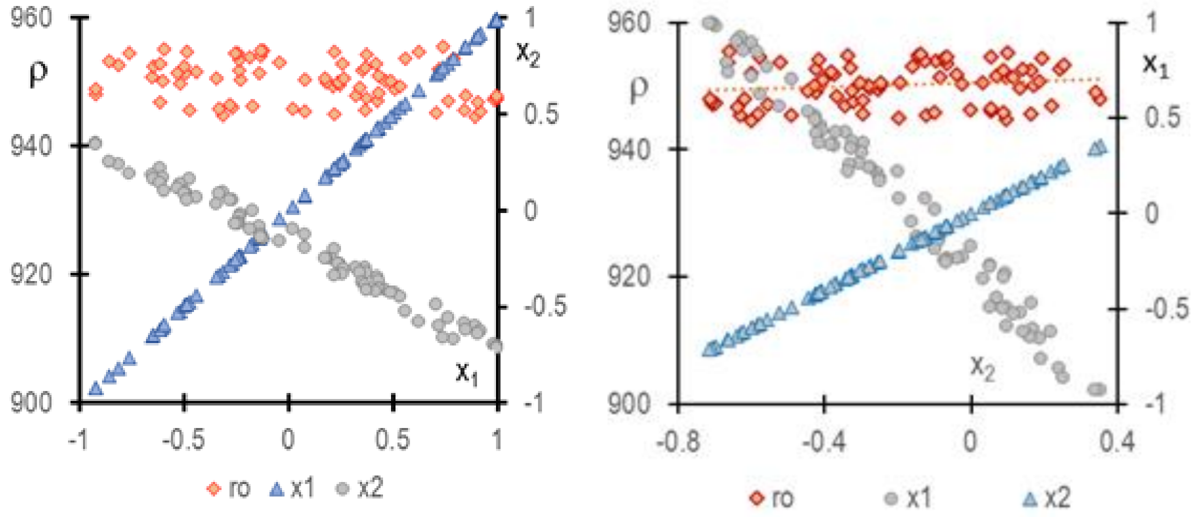

Fig. 2. Approximately constant density of about 9.5 (kg/m^3)
provided by variation of content of aggregates CS and P (x_1, x_2)

In the second case the level assigned for f_{cm} as Y_{IS} was $f_{cm\ is}$ = 5.0 ± 0.2 MPa.

Shown in Fig. 4 are the results of scanning the fields of ρ and $f_{c.tf}$ at $f_{cm} \approx 5.0$ kg/m^3. The following minimal level of ρ and maximal $f_{c.tf}$ with the contents of the aggregates providing them under this condition are: $\rho_{min} \cong 854.7$ kg/m^3 at x_1 = 0.63, x_2 = 0.34 (CS = 31.4, P = 20.1) and $f_{c.tf\ max}$ = 2.2 at x_1 = 0.76, x_2 = -0.95 (CS = 65.2 , P = 0.0).

The estimates of properties levels in Figs. 2-4 are the results of one realization of statistical trials. However, the estimates obtained after numerous realizations of compositions imitation converge to estimates quite close to presented results (practically coinciding).

The existence of significate positive correlation between density and strength is considered evident and is known from various studies of materials. It was shown [11] for lightened gypsum concrete under study, in particular. But here we see that the same density can correspond to greater or less strength (Fig. 3). And rather low density could be accompanied by rather high strength (Fig. 4). This fact could not be directly observed from experimental data. This was revealed in computational experiment for isoparametric analysis.

Conclusions. It was managed in the presented study to demonstrate the new capabilities, the special facet of computer isoparametric analysis. It could be especially useful in multicriteria multifactor studies of any high-performance materials.

This conclusion is based on the results of solving two specific tasks in the study of lightweight gypsum concrete filled with cenospheres and perlite particles. In the first one material

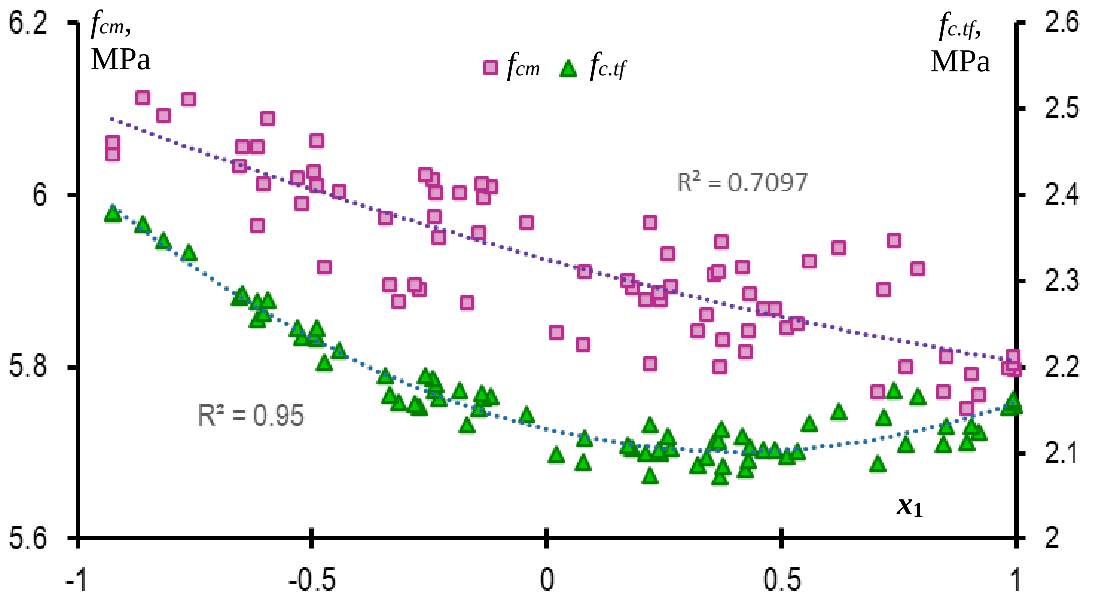

Fig. 3. Changes of strength with "constant" density about 9.5 kg/m^3, provided by varying the content of aggregates CS and P (x_1, x_2)

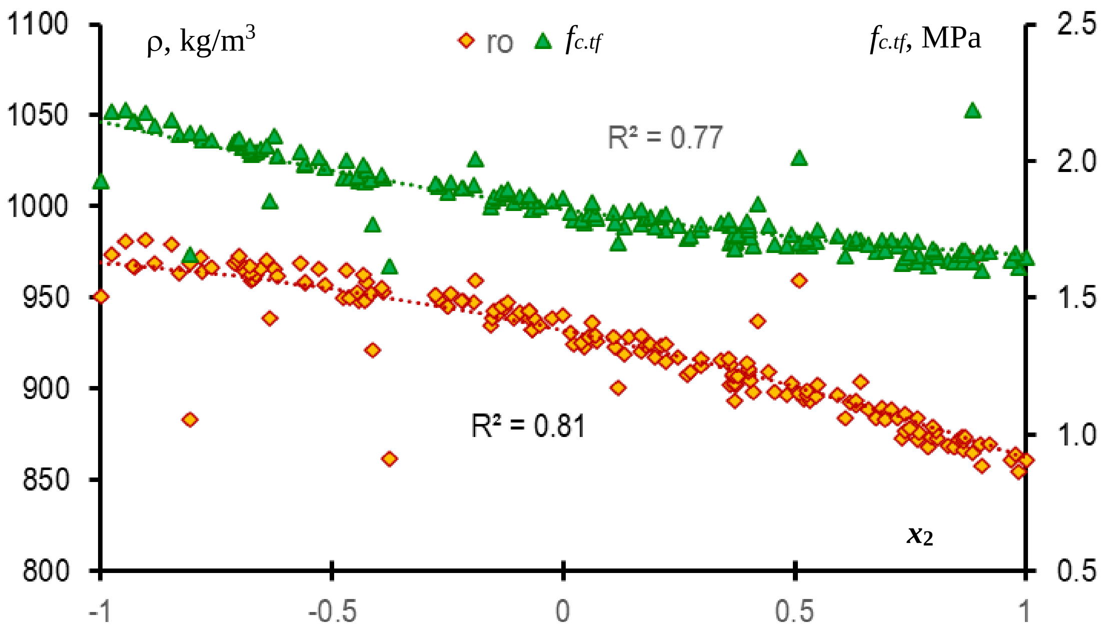

Fig. 4. Changes of density and bending strength under condition of f_{cm} ≈ 5.0 kg/m^3, provided by varied content of aggregates P and CS (x_2, x_1)

density was to be kept approximately constant and variation of compression and bending strength under this condition should be considered. In the second task the compression strength had to be about the specified constant and changes in the density and bending strength under this condition were shown. It had turned out that the materials of the same density could be of significantly different strength, and relatively low density could be accompanied by rather high strength.

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ЯК ЗМІНЮЮТЬСЯ ВЛАСТИВОСТІ КОМПОЗИЦІЙНОГО МАТЕРІАЛУ, ЯКЩО ОДНА З НИХ НЕЗМІННА?

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Анотація. Статтю відкривають кілька слів про історію та важливість у розвитку цивілізації композиційних матеріалів, дисперсних систем з багатокомпонентними дисперсійним середовищем та дисперсною фазою. Це та методологія полів властивостей матеріалів в координатах рецептурно-технологічних факторів, які описуються експериментально-статистичними (ЕС) моделями – передумови дослідження, представленого у цій статті. Одним із основних засобів методології є випадкове сканування рецептурно-технологічних полів. Цілі роботи – показати, як цей інструмент дозволяє оцінити зміну властивостей, якщо одна з них має бути незмінною, на прикладі вирішення двох завдань у дослідженні полегшеного гіпсобетону, з ценосферами та перлітом як заповнювачами. Розподіл розміру мікросфер із середнім близько 0.1 мм та середній розмір частинок перліту 0.3-0.5 мм можуть припустити досить компактне їхнє пакування та формування відносно стабільного каркасу. Використовуються ЕС-моделі залежностей щільності та міцностей на стиск та вигині від вмісту заповнювачів та дозувань двох хімічних добавок, побудовані за даними спланованого натурного експерименту. В обчислювальних експериментах генеруються склади (заповнювача при фіксованих середніх значеннях дозування добавок), оцінки для них властивостей по моделям дозволяють виконати ізопараметричний аналіз. У першому прикладі з аналізу виключаються склади, при яких рівень щільності бетону виходить за задані межі ізопараметричного коридору. Оцінюються зміни міцностей за умови приблизно постійної необхідної щільності. Можуть бути визначені найбільш міцні за цієї умови. У другому прикладі необхідною постійною має бути забезпечена міцність на стиск. Оцінюються зміни щільності та міцності на вигин за цієї умови, за їх рівнями у складах, що залишилися в ізопараметричному коридорі для міцності на стиск. У цьому випадку можуть бути визначені найлегші композиції заданої міцності. Електронна мікроскопія може бути рекомендована для візуалізації та розуміння механізмів явищ у міжфазних шарах «матриця-інертні заповнювачі». Ізопараметричний аналіз виявився дуже корисним у матеріалознавстві.

Ключові слова: експериментально-статистична модель, ізопараметричний аналіз, полегшений гіпсобетон, ценосфера, перліт, міцність, щільність.

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