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DOES ABRASION RESISTANCE CORRELATE TO STRENGTH?

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Abstract. The tasks of building materials science in solving which the analysis of correlation between material properties is necessary or could be useful are named. Attention is drawn to the fact that estimates of correlation coefficient or other characteristics of properties relation can be invalid, if experimental data from which they are calculated present the wide range of compositions and process parameters. The algorithm of computational experiment on the local composition-process fields is outlined, which enables the dependences of correlation measures on composition-process conditions to be described. With the help of such computational experiment the answer to the question in the title has been obtained for carbamide binder filled with mixture of silicon carbide fine grains and fine and coarse grains of andesite, about correlation of abrasion resistance to strength in dependence on degree of filling.

Keywords: correlation of properties, composition-process field, experimental-statistical model, computational experiment, filled carbamide binder, abrasion resistance, strength.

ЧИ КОРЕЛЮЄ ЗНОСОСТІЙКІСТЬ З МІЦНІСТЮ?

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Анотація. Названо задачі будівельного матеріалознавства, при вирішенні яких необхідний або корисний аналіз кореляції властивостей матеріалу. Звертається увага на те, що оцінки коефіцієнту кореляції та інших характеристик зв’язку властивостей можуть виявитися невірними, якщо дані натурного експерименту, за якими вони розраховані, представляють широкий діапазон складів і режимів обробки. Коротко викладено алгоритм обчислювального експерименту на локальних рецептурно-технологічних полях, що дозволяє описати залежності мір кореляції від рецептурно-технологічних умов. Для наповненого карбамідного сполучного за допомогою обчислювального експерименту отримано відповідь на питання про кореляцію зносостійкості з міцністю, залежно від ступеня наповнення.

Ключові слова: кореляція властивостей, рецептурно-технологічне поле, експериментально-статистична модель, обчислювальний експеримент, наповнене карбамідне сполучне, зносостійкість, міцність.

КОРРЕЛИРУЕТ ЛИ ИЗНОСОСТОЙКОСТЬ С ПРОЧНОСТЬЮ?

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Аннотация. Названы задачи строительного материаловедения, при решении которых необходим или полезен анализ корреляции свойств материала. Обращается внимание на то, что оценки коэффициента корреляции и других характеристик связи свойств могут оказаться неверными, если данные натурного эксперимента, по которым они рассчитаны, представляют широкий диапазон составов и режимов обработки. Кратко изложен алгоритм вычислительного эксперимента на локальных рецептурно-технологических полях, позволяющий описать зависимости мер корреляции от рецептурно-технологических условий. Для наполненного карбамидного связующего с помощью вычислительного эксперимента получен ответ на вопрос о корреляции износостойкости с прочностью, в зависимости от степени наполнения.

Ключевые слова: корреляция свойств, рецептурно-технологическое поле, экспериментально-статистическая модель, вычислительный эксперимент, наполненное карбамидное связующее, износостойкость, прочность.

Introduction. The need to analyse correlation between structural, technological, and operational properties (criteria *Y*) of composite materials could arise during research and development, in manufacturing process, and throughout their service life. As it was already noted [1-2], there exist at least three reasons.

Firstly, quantitative descriptions of interrelations between criteria *Y* are indispensable when arranging express-control of material quality, in particular, on the base of non-destructive tests [3-4], when sufficiently precise and reliable calibration curves are required.

Secondly, they are useful when designing the composites – searching for and setting the composition and process (CP) parameters, values of CP-factors (*X*) that would provide the specified or the best possible levels of the properties. It could be important to know how strongly the properties are interrelated, is it doable to reduce the number of criteria, by which material should be designed and optimised, or to change the levels of properties independently. Specifically, can elasticity modulus be lowered without loss in strength when developing the composite for the layers, which would damp dynamic loads of equipment?

Thirdly, the analysis of correlation can help in revealing CP-conditions under which the mechanisms of structure formation or destruction change. The substantial variations of correlation measures with CP-factors might point to such conditions.

It is these possible changes in properties relations from zone to zone of the factor region that are essential in all three situations. However, the measures of the relation between some Y_i and Y_j , coefficient of correlation $r\{Y_iY_j\}$, in particular, are usually estimated on the data obtained in multifactor natural experiment, with a minimum of trials. These data are insufficient to establish the facts, that responses *Y* to various values of *X* over the whole region under study could present the samples from different populations (properties of compositions of essentially different structures), and to reveal, with reliable numerical estimates, the existence or the absence of correlation and distinctions in relations between material properties in various CP-zones. It is practically impossible to derive the dependences of the changes in relations of properties on composition and process parameters directly from the data of real experiments [1].

This can be achieved due to virtual, computational experiments. The necessary information can be "mined" with statistical trials on *Composition-Process Fields* of material properties described by *Experimental-Statistical* models [1-2, 5-7]. The paired samples of any size (for any number of generated CP-conditions) needed for such analysis and for building possible prediction equations are simulated. The method, though already used in the studies of various composites [1-2, 5-10], was either just mentioned or expounded as a part of composition-process fields methodology.

In this paper the essence of the method, that would allow the transformations in relations of the properties to be evaluated, is presented applied to answering the question in the title.

Results of the natural experiment. The relation between abrasion resistance and strength of the filled carbamide composites is analysed. Used are the data obtained when developing the compositions for industrial floors [11]. Varied in experiment were 3 formulation factors X_i (i = 1…3) normalised to $|x_i| \le 1$ (Table 1). Abrasion resistance *A* (h/g) and compression strength *R* (MPa), among other properties, were determined for 15 compositions (according to design of experiment, 15 vectors $\boldsymbol{x}$ in cubic factor region). These data are shown in Fig. 1 (coefficients of determination for linear trend and 3rd degree polynomial being 0.50 and 0.61 respectively).

Table 1 – Values of varied dosages of the components

i	Factor X_i	Values		
		$x_i = -1$	$x_i = 0$	$x_i = +1$
1	Filler-polymer mass ratio (degree of filling F) considered as both structure formative and economical factor that should be maximised to reduce polymer content	2	2.25	2.5
2	Mass part of silicon carbide (abrasive production waste, specific surface 320±10 m^2/kg) in fine fraction of the filler (SC%)	0	30	60
3	Mass part of andesite coarse grains (specific surface 70±5 m^2/kg) in total amount of the filler (CA%).	20	40	60

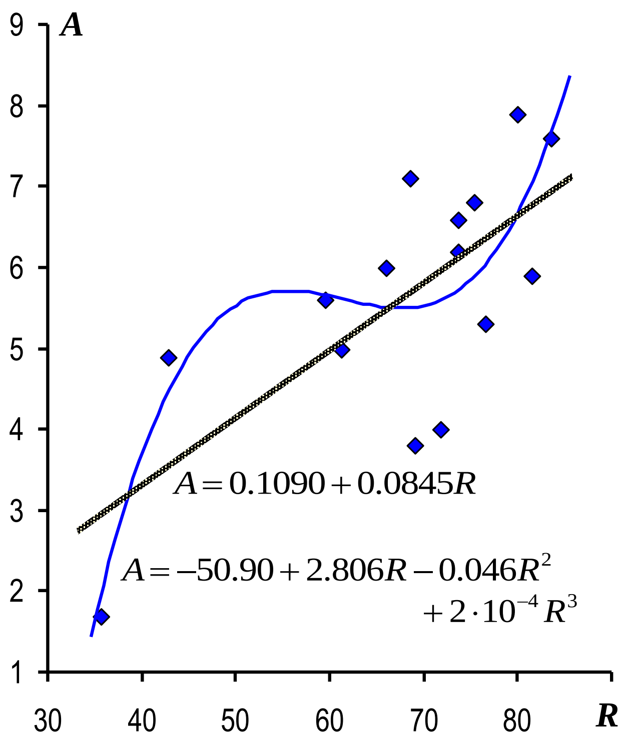

Fig. 1. Scatter diagram of the results of natural experiment and trend lines

Though $r\{AR\}$ = 0.71 (estimated by 15 pairs of experimental values of A and R for compositions from the whole cubic factor region under study) formally implies the significant positive linear relation between 2 properties (at risk less than 1%), such conclusion could be incorrect, since this paired sample of values could present quite differently formed structures.

The experimental data allowed ES-models (1-2) to be built (at 10%-risk, experimental errors s_e equal to 1.3 and 0.41 respectively), describing the whole composition fields $R(\boldsymbol{x})$ and $A(\boldsymbol{x})$, in whole region of all k = 3 varied factors.

The minimal and maximal levels of the fields are:

R_{min} = 35.6 MPa (at $x_1 = x_2 = -1$, $x_3 = +1$),

R_{max} = 84.1 (at $x_1 = -0.93$, $x_2 = +0.62$, $x_3 = -1$),

A_{min} = 2.05 h/g (at $x_1 = x_2 = -1$, $x_3 = +1$),

A_{max} = 8.21 (at $x_1 = -0.47$, $x_2 = +1$, $x_3 = -0.22$),

the increase with composition being 2.4 and 4.0 times respectively.

The values of factors providing the maxima do not coincide, thus suggesting again that degree of correlation might differ from one subregion of compositions to another. The models enable to find this out, since they define not only the whole fields, $R(x_1, x_2, x_3)$ and $A(x_1, x_2, x_3)$, but infinite variety of the local ones, for any factors subsystem at any factors subregion.

$$\begin{aligned} R = 75.3 &\pm 0\,x_1 - 1.7x_1^2 - 1.1x_1x_2 + 2.4x_1x_3 \\ &+ 9.4x_2 - 4.7x_2^2 + 4.6x_2x_3 \\ &- 11.0x_3 - 4.8x_3^2 \end{aligned} \quad (1)$$

$$\begin{aligned} A = 6.69 &+ 0.22x_1 - 0.47x_1^2 - 0.52x_1x_2 + 0.85x_1x_3 \\ &+ 1.45x_2 \pm 0\,x_2^2 \pm 0\,x_2x_3 \\ &\pm 0\,x_3 - 1.12x_3^2 \end{aligned} \quad (2)$$

Computational experiment. To examine the possible changes of properties correlation the following algorithm is used.

0. At this step the computational experiment is designed. One or more (less than k) factors are chosen to be fixed at several values. These are "changing" factors (x_{ch}). From value to value they change the local fields of the properties Y in coordinates of remaining, "gradient" factors (x_{gr}), forming the field. Substitution of certain x_{ch}-values into whole ES-model gives the models of corresponding local fields.

In particular, equations (3-4), with $x_1 = +1$ substituted in (1-2), describe the fields of strength and abrasion resistance in coordinates of filler composition at upper degree of filling (Fig. 2a, c).

$$R(x_2, x_3 / x_1 = +1) = 73.6 + 8.3x_2 - 4.7x_2^2 + 4.6x_2x_3 - 8.6x_3 - 4.8x_3^2 \quad (3)$$

$$A(x_2, x_3 / x_1 = +1) = 6.44 + 0.92x_2 \pm 0 \quad x_2^2 \pm 0 \ x_2x_3 + 0.85x_3 - 1.12x_3^2 \quad (4)$$

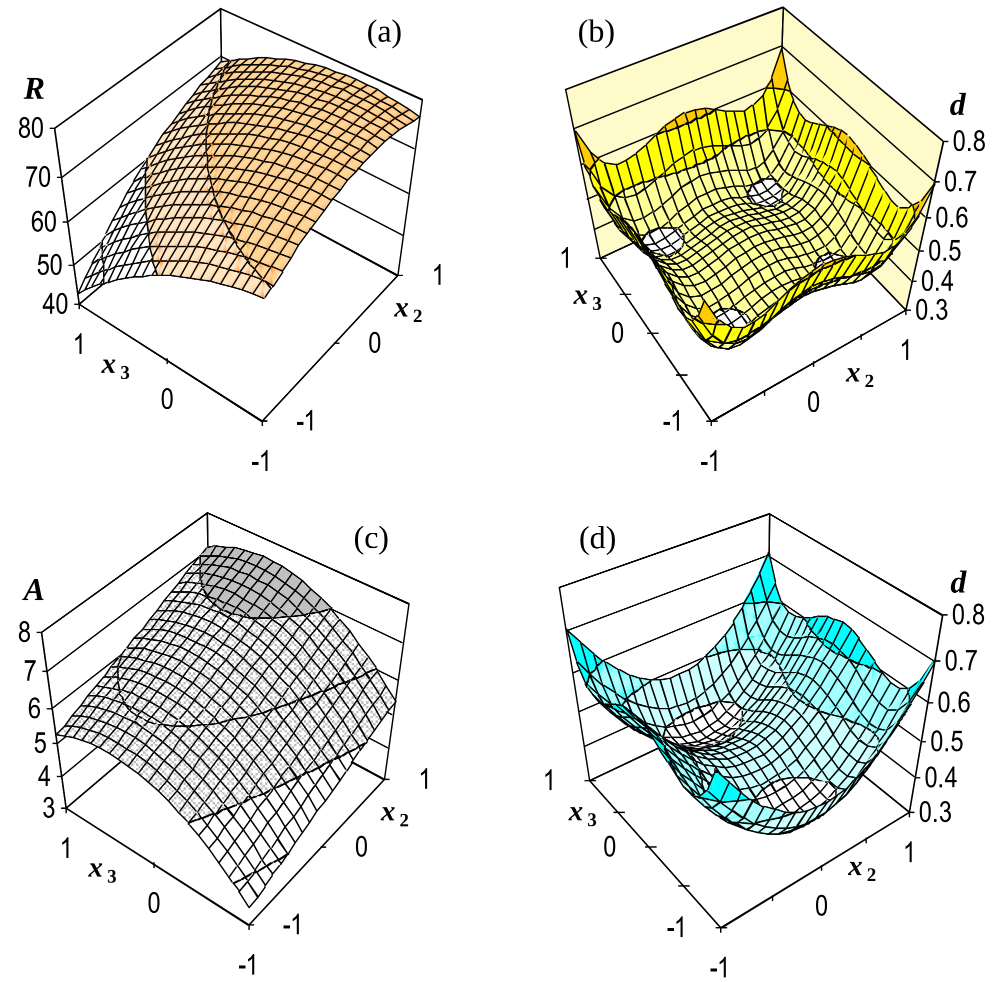

Fig. 2. Local fields and prediction variance functions of strength (a, b) and abrasion resistance (c, d) in coordinates of filler composition, *SC* and *CA* (x_2 and x_3) at upper degree of filling, $F = 2.5$ ($x_1 = 1$)

To account for experimental and approximation errors the prediction variance function [12-14], *d*-function, defined by experiment design and structure of the model (cleaned from insignificant effects), is analogously obtained for each of local models. Shown in Fig. 2b, d are *d*-functions for (3-4) respectively.

1. At each fixed value of $\boldsymbol{x}_{ch}$ generated are N points $\boldsymbol{x}_{gr}$ (CP-parameters) uniformly distributed inside the region of gradient factors (with boundaries $x_{gr.i} = \pm 1$).

2. For each of generated $\boldsymbol{x}_{gr}$ the random errors $\Delta Y(\boldsymbol{x}_{gr})$ and random level $Y(\boldsymbol{x}_{gr}) + \Delta Y(\boldsymbol{x}_{gr})$ for both properties under consideration are calculated (5), with corresponding experimental errors s_e and t distributed by standard normal law. Such values for R and A are shown in Fig. 3a-b, d-e.

$$\Delta Y(\boldsymbol{x}_{gr}) = t \cdot s_e \cdot [d(\boldsymbol{x}_{gr})]^{0.5} \quad (5)$$

The addition of random errors to values of Y at uniformly distributed $\boldsymbol{x}_{gr}$ inside multidimensional domain transforms the model-determinate fields into the "random fields" and makes the results of computational experiment closer to those of potential natural experiment (with Monte Carlo method participating twice – when simulating the point of the field and its level).

One realisation of random field $R(x_2, x_3 / x_1 = +1)$ and that of $A(x_2, x_3 / x_1 = +1)$ are shown in Fig. 3c, f.

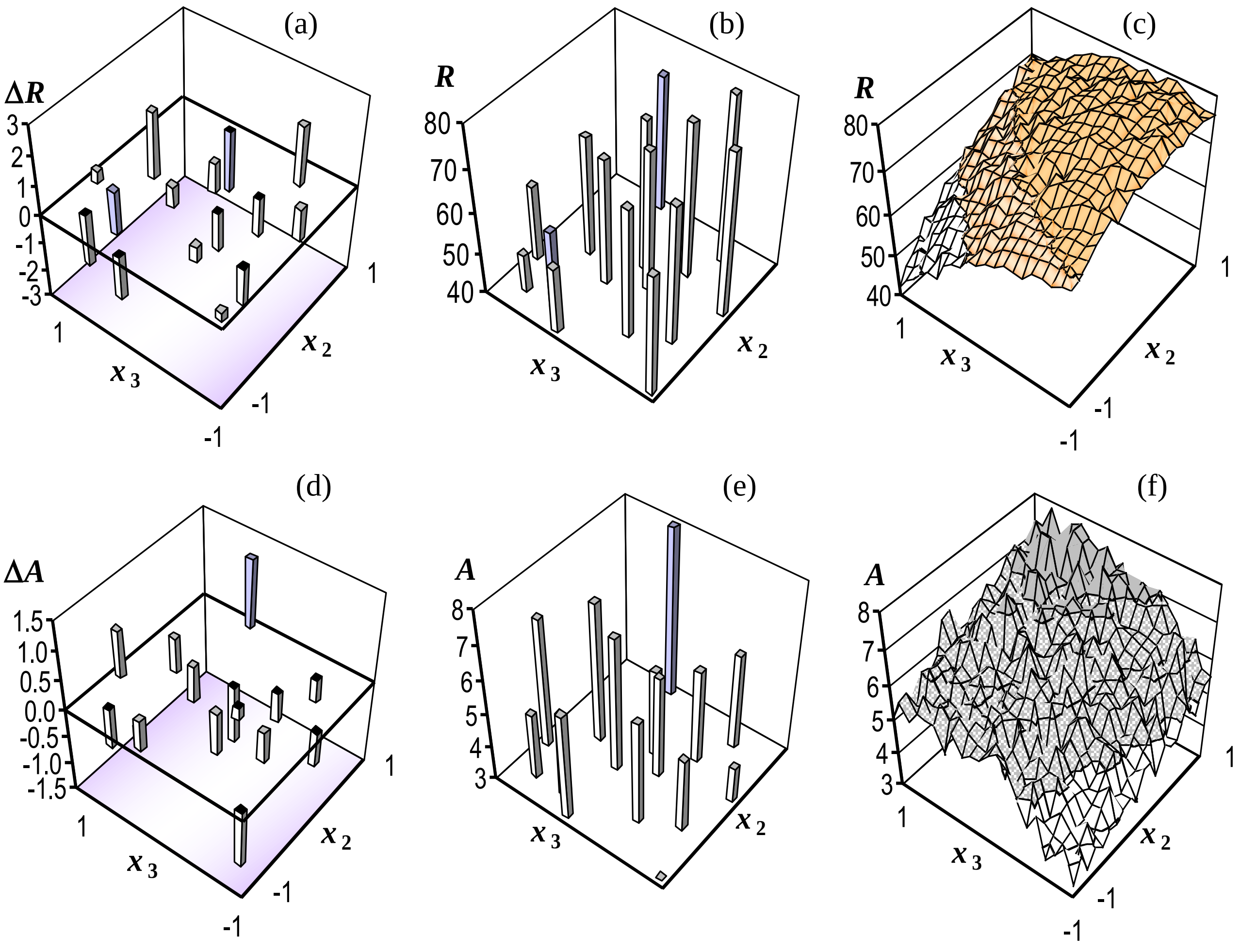

Fig. 3. Generated random errors and property levels for a number of generated compositions and one realisation of random field for compression strength (a-c) and abrasion resistance (d-f)

3. By N pairs of thus obtained random values (Y_i, Y_j) one sample estimate of correlation coefficient $r\{Y_i Y_j\}$ is calculated (or of other measures of relation between two properties, specifically, the slope of regression line).

Scatter diagrams in Fig. 4 display the results of simulating the levels of R and A for generated compositions of the filler at its lower and upper content. The strong positive correlation of A with R at $F = 2$ disappears at $F = 2.5$, evidently because of substantially different structures of the matrix, filler skeleton, and of the composite.

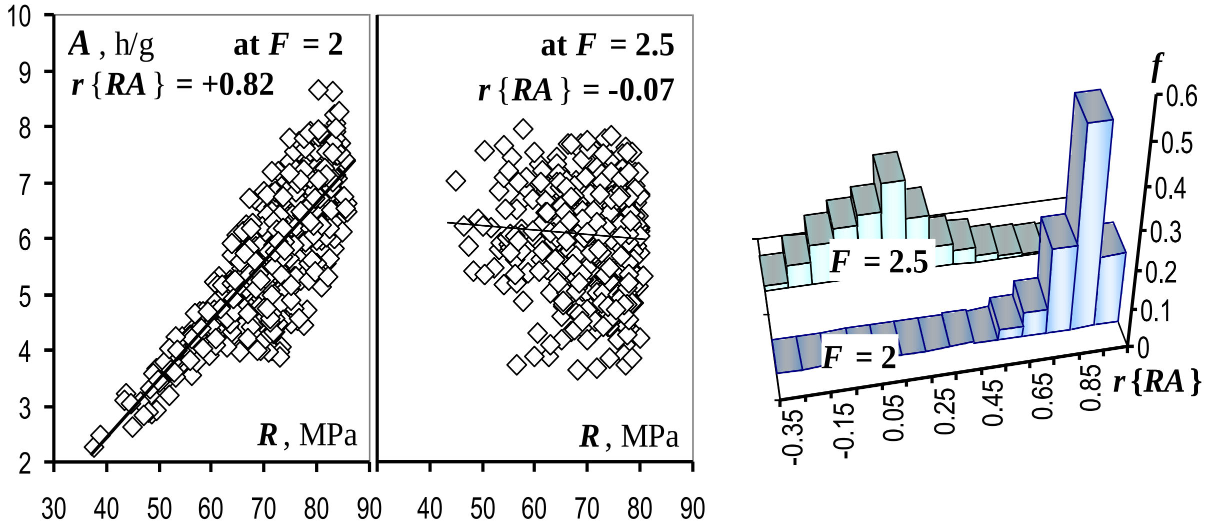

Fig. 4. Strength and abrasion resistance for generated *SC* and *CA* and distributions of coefficient of correlation between 2 properties at lower and upper degree of filling

4. Multiple realization of the procedure enables frequency distribution of correlation measure to be obtained.

Each distribution in Fig. 4 is obtained on 500 estimates of $r_{23}\{RA\}$, each estimate calculated on new paired sample for anew random set of N = 15 vectors (x_2, x_3), the number being equal to number of trials in natural experiment, in whole factor region.

5. The distributions of correlation measure obtained at each fixed value of $\boldsymbol{x}_{ch}$ allow the secondary ES-models (with respect to primary model, by natural data) to be built for this measure.

Such is equation (6) for median value of coefficient of correlation between abrasion resistance and strength (when varied is filler composition) versus degree of filling.

$$r_{23}\{AR\}(x_1) = 0.614 - 0.372x_1 - 0.142x_1^2 \quad (6)$$

Shown with this dependence in Fig. 5 are the ones for quantiles q_{05} and q_{95} estimating the lowest and the highest levels of correlation coefficient (at conventional risk of 0.05).

Conclusions. Strong positive correlation of abrasion resistance with compression strength of the filled carbamide binder does exist at the lowest degree of filling (with ample content of resin forming intergranular layers); credible estimates of *A* by values of *R* can be got with linear calibration equation. These properties do not correlate in the highly filled compositions.

The potential of correlation analysis for materials science would increase if experimental data were enriched with information mined in computational experiments. ES-models make it possible to extract the information latent in experimental data, which are convoluted in the models. Computational experiments on the fields of properties in composition coordinates allow the variety of formulations under study to be stratified, with subregions of compositions educed, for which operational regression equations (reliably predicting the level of some property by the level of the other) could be built.

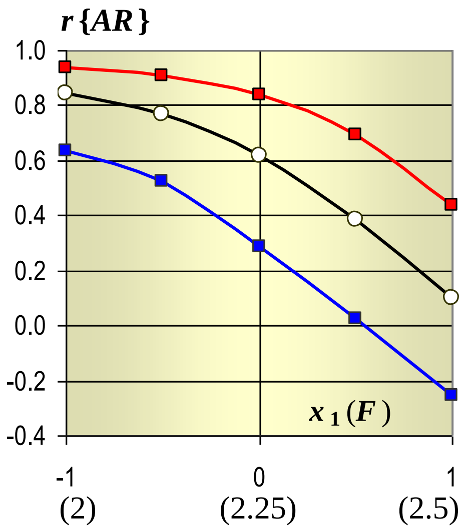

Fig. 5. Coefficient of correlation between abrasion resistance and strength of carbamide binder with varying filler in dependence on filler-polymer ratio

The transformations of the character of relations between the properties of composites when going from one subregion of compositions to another could indicate the change of dominating mechanisms of structure formation.

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