EXPERIMENTAL-STATISTICAL MODELING IN COMPUTATIONAL MATERIALS SCIENCE

Tatiana V. Lyashenko and Vitaly A. Voznesensky
Odessa Academy of Civil Engineering, PO Box 376, Odessa 270000, Ukraine

Abstract

Experimental-Statistical Modeling (ESM), presenting efficient means for multi-criterion search for rational solutions in specific industrial conditions, proves to be important component of computational materials science. By ESM is meant the complex of methods and actions that encompasses justified choice of experimental conditions, optimal design of experiment, building a set of regression models, solving the typical and special engineering problems. Pointed out in the paper are the cases where ESM may be most efficient, particularly, at research and development stages and to ensure quality of productions. The use of ESM when investigating two composite materials is demonstrated.

To minimize the content of polyester in composite on its base by optimization of mineral and grain compositions of the filler used have been the models of new kind "Mixtures, Technology - Properties", the concept of "material property field" and its generalizing indices. When developing cement composite for structures without redundancy studied has been the influence of ratio between contents of two additives on mean and minimal possible levels of quality indices. By results of modeling the probabilistic indices the compositions of high ensured level of material strength have been chosen.

Introduction

Computational materials science and traditional materials science are concerned with the same problems of studying the relations between material composition, structure, and properties as well as their changes under technological and operational effects. One of engineering purposes therewith is to find optimal compositions and processing parameters providing specified properties of materials.

To solve such problems computer assisted materials science, however, may use various theoretical and phenomenological models, of different levels (atomic-molecular, structure flaws, heterophase, matrix - filler, material - construction) and languages, in combination [4]. One of the most important components of computational materials science is constituted of complexes of Experimental-Statistical Models (ES-models), that are indispensable to searching for rational engineering solutions in particular industrial conditions and may be included in expert systems (as convolutions of empirical information).

By Experimental-Statistical Modeling (ESM) is meant [6] the set of methods and actions aimed at drawing as much as possible scientific and industrial information from experimental results [5, 6]. This set (some of its elements corresponding to known in USA "response surface methods") integrates following main interrelated blocks:

1. Justified choice of experimental conditions, with selection of factors, limits of varying them, and quality criteria, taking into account physico-chemical, industrial, and other apriori knowledge.

2. Optimal design of experiment, with regard to chosen conditions, including rational (for this particular problem) form of polynomial model (as a rule, of higher-than-first degree) and possible existence of preset experimental points and "forbidden areas" in factor region.

3. Building regression models that, with all insignificant estimates eliminated, are accepted as adequate to object behavior. In some situations, to have two above conditions fulfilled, used is special algorithm of "generated experimental error" for preset risk levels of hypotheses testing.

4. Solving industrial problems by ES-model for separate quality criterion and by complex of them. More than 20 problems may be considered to be typical for users of ESM (optimization of response level, minimization of resources consumption, evaluation of factors' roles, estimating the size of a region of acceptable solutions and confidence limits for engineering recommendations, etc.).

The Conditions of Experimental-Statistical Modeling Being Efficiently Used

The results of realizing the ESM for analysis and optimization of structure, properties, and ✓ technology of Denise and porous composites with silicate and polymer matrices over 25 years [2 - 9] proved its high efficiency (especially in research works) when:

1. Creating new materials with physico-chemical foundation for choosing appropriate limits of composition and technology insufficiently developed, i.e., when rapid "break" into new area of production is needed.

2. Designing the technology based on new physical and physico-chemical actions on traditional material structure formation processes, developing new methods of composite quality control.

3. Partial or total change-over from source materials with a stable quality level to production wastes; if need be, reducing the consumption of hard-to-get or expensive component (polymer in particular), without deterioration of material below preassigned quality level, through introduction of more widespread or low-cost analogue or at expense of intensification of technological processes (mixing, heat exchange, etc.).

4. Controlling the quality and saving the resources at the expense of complicating a composition by introducing modifiers - multi-fraction fillers and chemical additives.

5. Widening the range of requirements to conventional materials (increasing the number of quality criteria) that necessitates compromise solutions because of objective distinctions in mechanisms of structure formation and distruction, in mechanisms of transfer and so on (e.g., low viscosity of technological mix + high strength of composite).

6. It is necessary to control the composition and technology not according means but probabilistic quality and reliability indices (guaranteed with preassigned risk quality level, risk of product failure under specified action, etc.); this is important when materials are used for objects without redundancy (pipelines, reservoirs, shields, etc.).

Complex of ES-models on its own or in combination with other models of computational materials science makes it possible to carry out computational experiment changing the strategy of searching for engineering solutions and allowing new knowledge about materials to be derived from the models.

The Search of Polymer-Saving Compositions of Multi-fraction Filler for Composite Material

Description of industrial problem. Multi-fraction fillers provide wide range of possibilities to control the properties of polymer compositions. The cost of special preparation of such fillers is offset by savings in polymer, the most energy-intensive ingredient.

To reduce the content of polyester, when designing composite on its base, optimal mineral and grain compositions of the filler were being searched [2, 6]. Mineral composition was varied by loading various quantities of quartz, marble, and clinker grains measured in parts v_i of i-mineral in taken as unity total mass of filler ($0 \leqslant v_i \leqslant 1$). Grain composition was defined and varied by portions of grains of different size evaluated by their specific surface S (m^2/kg). "Small" grains had S=310-350, medium-size fraction - 90-100, "large" grains - 45-50 m^2/kg, the sum of portions of each size w_i ($0 \leqslant w_i \leqslant 1$) being equal to 1. Thus, considered as mono-fillers and in their mixes were nine powders (their portions $v_i w_i$ ranging from 0 to 1):

quartz grains, small ($v_1 w_1$), medium ($v_1 w_2$), large ($v_1 w_3$),
marble grains, small ($v_2 w_1$), medium ($v_2 w_2$), large ($v_2 w_3$),
clinker grains, small ($v_3 w_1$), medium ($v_3 w_2$), large ($v_3 w_3$).

The influence of other structure-formative factors on composite properties had to be also analyzed. The most important of them was filler to polymer mass ratio, the degree of filling (F/P = X), varied from 1.5 to 2.5 (normalized factor $x = (X-2)/0.5$, $|x| < 1$). Its level had to be maximized to minimize polymer content, with complex of requirements to composite quality being fulfilled. Among quality criteria there were effective viscosity η of technological mix (at deformation speed of 1 s^{-1}) and compression strength (R) of hardened composite, the requirements for one of products being $30 < \eta \leqslant 90$ Pa.s, $R \geqslant 150$ MPa.

To estimate optimal levels of factors v and w ES-models with linearly linked elements and methods of building and analyzing them were necessary.

Models with mixture variables. The composition of material consisting of q components is represented traditionally by parts v_i of these components, linked by linear condition $v_1 + v_2 + \dots + v_q = 1$. Such representation is referred to as "Mixture" (M). Design of experiments in (q-1)-dimensional simplexes is successfully employed when examining the influence of M on its properties (quality Q). The description of the system "Mixture - properties" (MQ), by ES-models, in particular, is most conveniently mapped in series of ternary mixture diagrams, triangles with isolines of properties, criteria presenting Q.

Technical properties of materials (of composites specifically) are determined not only by mixture but by conditions of processing it into a product and by operating conditions. Corresponding to these conditions vector x of p mutually independent factors (some composition factors among them) presents factor subsystem named "Technology" (T). Design of experiment for MTQ-system in factor space that combines (q-1)-dimensional simplex and p-dimensional cube is considered in fundamental work [1] and some others [3, 6]. The models of these systems may be represented by ternary diagrams transformed under effects of technological factors.

The special type of systems presents those with two groups of mixture variables (vectors **v** and **w**), subsystems M_1 and M_2. Therewith each mixture may characterize essentially different feature of an object. This is indeed the case described above, with M_1 and M_2 corresponding to mineral and grain compositions of the filler. To describe the influence of this multi-fraction filler on properties of polymer composition at fixed level of filler-polymer ratio (x = const) the models for properties Y of M_1M_2Q-system in a form (1) of structured reduced polynomial (with 15 coefficients) [6] have been used.

$$Y = \boxed{A_{12}v_1v_2 + A_{13}v_1v_3 + A_{23}v_2v_3 \quad (a)}\ \boxed{+ B_{12}w_1w_2 + B_{13}w_1w_3 + B_{23}w_2w_3 \quad (b)}$$

$$\boxed{\begin{array}{l} + C_{11}v_1w_1 + C_{12}v_1w_2 + C_{13}v_1w_3 \\ + C_{21}v_2w_1 + C_{22}v_2w_2 + C_{23}v_2w_3 \\ + C_{31}v_3w_1 + C_{32}v_3w_2 + C_{33}v_3w_3 \quad (c) \end{array}} \qquad (1)$$

Block (a) in Eq. (1) describes the influence of mixing different mineral grains on property Y (synergism of minerals) independently of their dispersity. Block (b) presents the effects of mixing the grains of different size no matter of what minerals. Coefficients C_{ij} in block (c) correspond to property level when there is only component i in Mixture 1 and only component j in Mixture 2, i.e., to property of composite on "pure" filler.

To describe more complex systems, M_1M_2TQ, used may be special reduced polynomials [6] or the products of reduced polynomial of type (1) and usual polynomial of independent factors. In this way the factor from Technology-group, the degree of filling, has been included into (1) by replacement of numerical coefficients with parabolic functions $A_{ij}(x)$, $B_{ij}(x)$, and $C_{ij}(x)$. This gives the form of model with 45 terms.

Design of experiment, models, and diagrams "Triangles on Triangle". It is convenient to represent the M_1M_2Q-models for two three-component mixtures by diagrams "Triangles on Triangle" [2, 6]. In Figure 1a shown are 7 mixture triangles of "grain composition" in vertices, middles of sides, and in the centre of carrying triangle - "mineral composition of filler". The inverse presentation is also possible.

To build models (1) saturated D-optimal design has been synthesized by authors' algorithm [6]. The algorithm allows designs in cubes, simplexes and their products, with possible additional constraints ("forbidden zones") and preset points, to be built. 15 points of design for model (1) are numbered in Figure 1a, point N1 in the centre being a compulsory one. The experimental design for M_1M_2TQ-models (including F/P) has been got by repeating the shown design at three levels of x (-1, 0, +1) with rotating the points on triangles through 120° while passing to next level. Complex of ES-models for technological, structural, and operational properties of composite has been built on the results of the experiment.

In 7 triangles of grain composition (Figure 1a) shown are the isolines of technological mix viscosity η (Pa.s) at F/P=2.5. Its extremal values are indicated, maximal level invariably corresponding to $w_1=1$ (maximal specific surface) and minimal - to mix of grains of all three sizes. Under the influence of mineral composition η_{max} and η_{min} vary as well as w_1:w_2:w_3 and grains specific surface $S\{\eta_{min}\}$ providing minimal viscosity.

Useful for industry results may be obtained with the help of the concept of "property field" [6, 8, 9]. Each small triangle diagram in Figure 1a presents viscosity field $\eta(w_1, w_2, w_3)$ changing when mineral composition **v** is changed. These changes may be analyzed, the fields compared and controlled with the assistance of the complex of field generalizing indices $G_\eta\{w\}$. Among them might be extrema and their co-odinates, increases, gradients, and any other useful for research purposes numerical characteristics. The analysis is carried out on the base of "secondary" ES-models relating estimates of $G_\eta\{w\}$ with factors **v**. The isolines of three generalizing indices are shown in Figure 1:

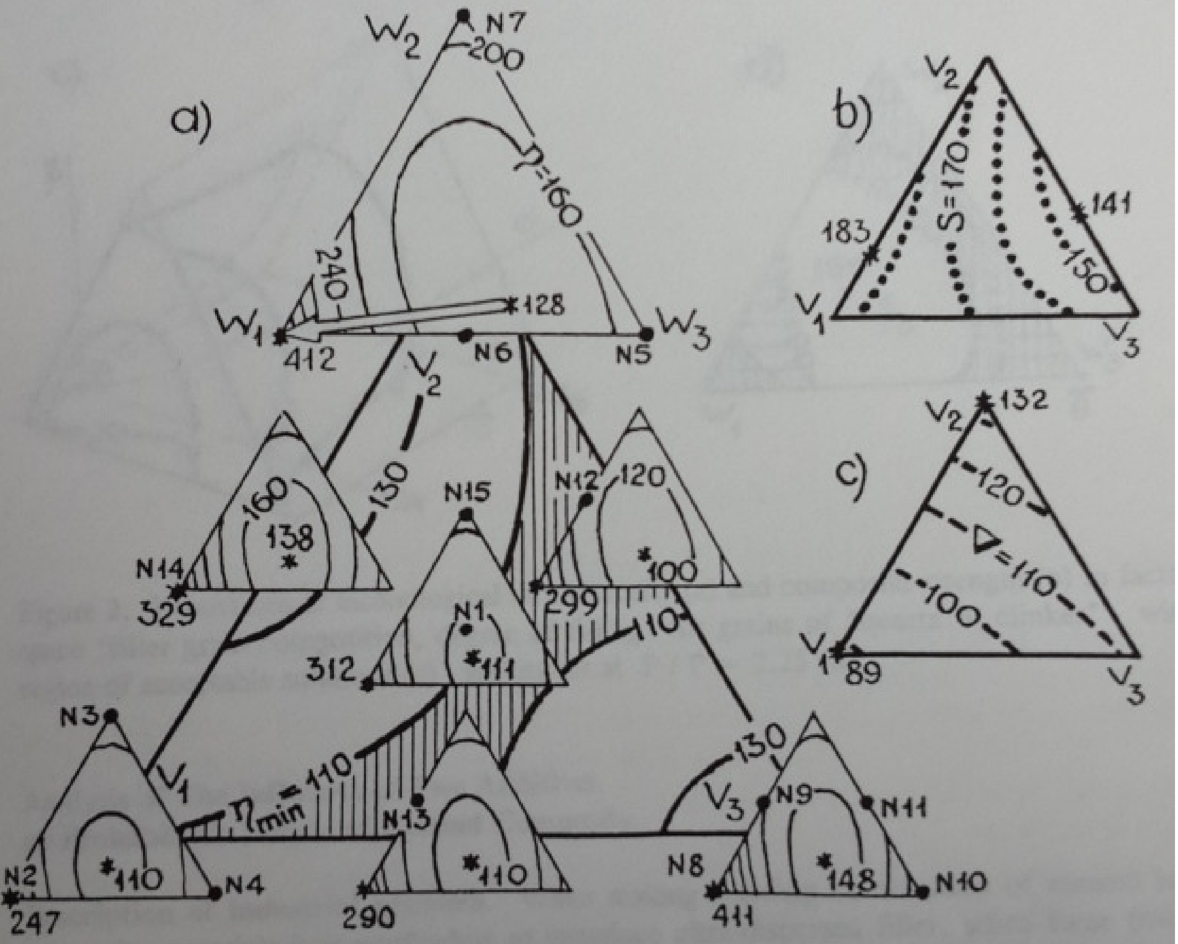

Figure 1. Seven diagrams "grain composition - viscosity" and isolines of minimal viscosity η_{min} on mineral composition triangle (a), variations of specific surface $S\{\eta_{min}\}$ (b), and gradient of viscosity ∇ (c) in dependence of mineral composition

η_{min} defines the conditions to obtain the most technological mix through controlling filler size distribution (Figure 1a, carrying triangle),
$S\{\eta_{min}\}$ describes structure-formative capability of pure and mixed minerals (Figure 1b),
$\nabla = (\eta_{max} - \eta_{min}) / (S\{\eta_{max}\} - S\{\eta_{min}\})$, gradient of viscosity (per 100 m^2/kg of specific surface), characterizing the stability of structure-formative capabilities of mineral mixtures.

The complex of generalizing indices is used to interpret modeling results in material science and chemical engineering terms.

Choosing the optimal composition of multi-fraction filler. M_1M_2TQ-models including filler to polymer mass ratio make it possible to choose fraction composition of filler optimal by polymer loading criterion, with properties of polymer composite being provided.

When influence of F/P, ranging from 1.5 to 2.5, on the properties is analyzed the triangle factor space $\{w_1, w_2, w_3\}$ at various v = const is transformed into prisms $\{w_1, w_2, w_3, x\}$ (Figure 2). In Figure 2a shown inside such prism are isosurfaces of viscosity for mixture of quartz and clinker ($v_1=v_3=0.5$). The isosurfaces of "sail" shape are convex in direction of maximal filling. Consequently, with η = const the content of polymer may be reduced at the expense of optimal grain composition of the filler.

The operational properties of composite may be formed according to different regularities to those of technological properties. In Figure 2b shown are isosurfaces of compression strength for mixture of quartz and clinker. Answering to requirements $30 \leqslant \eta \leqslant 90$ Pa.s, $R \geqslant 150$ MPa is the part of prism in Figure 2c inside the boundaries corresponding to three isosurfaces (shown in Figure 2a,b). Grain composition triangle in Figure 2d presents the cut of prism and isosurfaces $\eta = 90$ and $R = 150$ for F/P = 2.25. Shown inside is the region of acceptable solutions (with η_{min} = 73 Pa.s, R_{max} = 156 MPa) bounded by viscosity isoline from the side of small grains and by strength in areas of middle and large grains. Relative size of this region P = 60% of the area of grain factors space. This characteristic presents important generalizing index of one-criterion and multi-criterion field, evaluating the possibilities to control material quality within specified limits. The most economic in quantity of resin is consisting of small and large grains composition at point α (Figure 2c), where F/P = 2.38. In comparison with composition filled with small grains, at point β, the saving of resin is more than 70 kg per ton of composite.

The admissible region (Figure 2c,d) would shrink with greater number of requirements to composite quality and with restricting surfaces corresponding to ensured levels of properties, taking into account prediction errors of M_1M_2TQ-models.

Conclusions to the problem. 1. 15-20% of resin may be saved with no loss of quality of polyester composite through optimization of grain and mineral compositions of the filler. 2. Structured models of the type "Mixtures, Technology - Properties" with mixtures variables of different origin and independent factors are useful for solving problems of materials science, chemical technology, etc. 3. The concept of property field and its realization through field generalizing indices and secondary models allows non-trivial knowledge about materials to be got. 4. Diagrams "triangles on triangle" and their analogues present efficient tools for representing property fields.

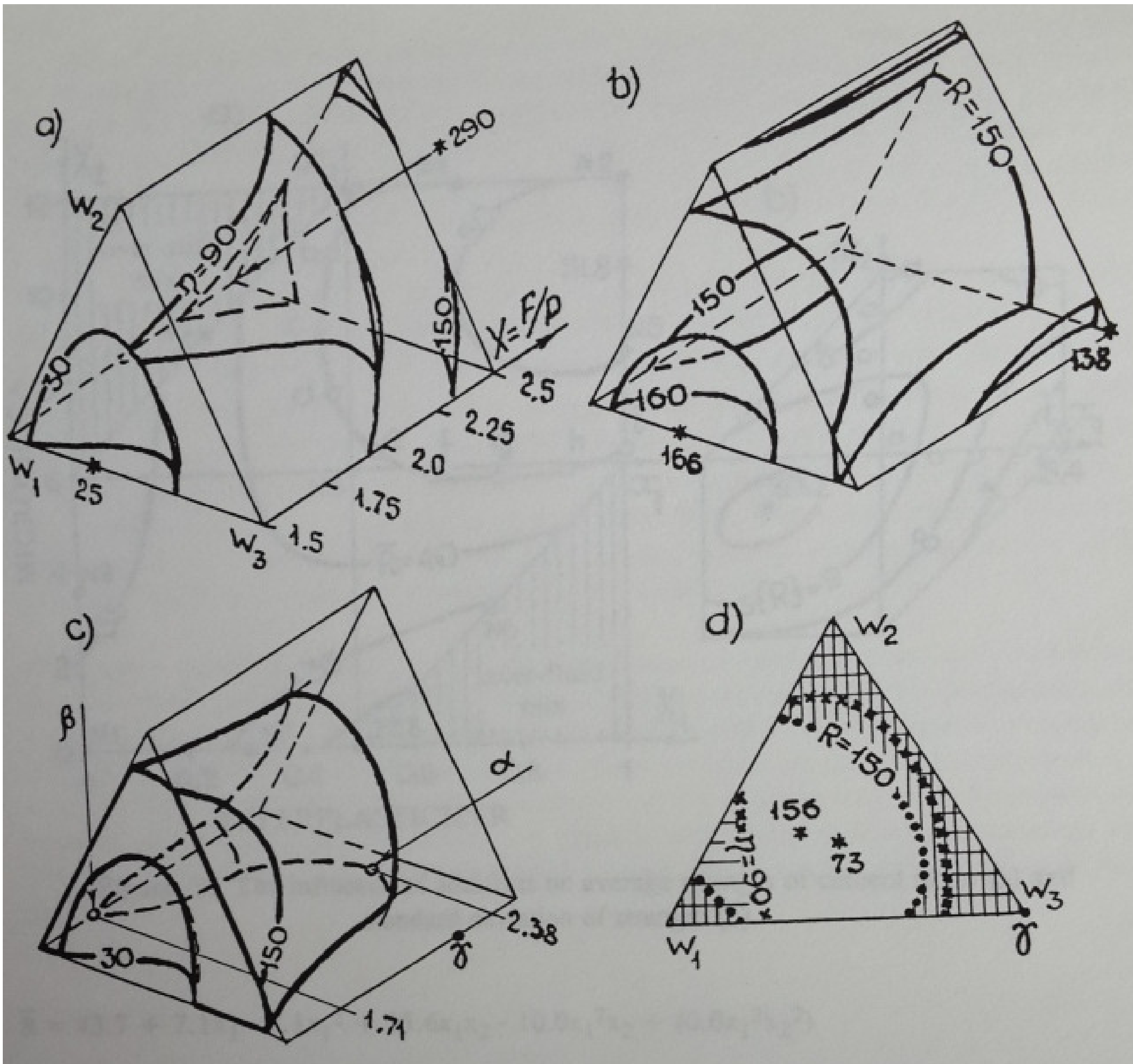

Figure 2. Isosurfaces of technological mix viscosity (a) and composite strength (b) in factor space "filler grain composition, degree of filling" for grains of "quartz + clinker" with region of acceptable solutions (c) and its cut at $F / P = 2.25$ (d)

Analysis of The Influence of Two Additives on Probabilistic Indices of Cement Composite

Description of industrial problem. When making building construction of cement base composite materials it is worthwhile to introduce ultra-dispersed filler, silica fume (micro silica, MS), into binder. Three effects therewith may be obtained: cement specific content reduced, operational properties of composite improved, and certain ecological problems solved, since MS presents the waste of ferro-alloy production.

However, the specific surface of MS-particles is nearly 10 times that of cement grains.

Therefore this filler increases steeply the viscosity of technological mix and might unfit it for making products. That is why introduced with the filler has to be organic agent decreasing mix viscosity, superplasticizer (SP). In doing so it is desirable to introduce MS and SP in the proportion that would provide viscosity variation within narrow limits conditioned by design of forming equipment.

When composite is used in "without-redundancy" structure (shield, pipeline, etc.) its efficiency is defined not by average level of quality (of property R in particular), $\overline{R}$, but by probabilistic indices, specifically, by minimal possible (with risk α) quality level R_α . Optimization of material composition and technology (vector of factors **x**) by models $\overline{R}(\mathbf{x})$ and $R_\alpha(\mathbf{x})$ may give the same results $\mathbf{x}_{opt}$ only in specific situations when values of R are normally distributed and its standard deviation s, or variation coefficient v, do not depend on **x**. In real problems of materials science these prerequisites are not frequently fulfilled inasmuch as distribution laws of R are transformed under effect of technological and composition factors. Thus $\mathbf{x}_{opt}\{\overline{R}\}$ and $\mathbf{x}_{opt}\{R_\alpha\}$ may differ essentially. This should be kept in mind when designing the composites for non-redundant constructions.

The purpose of one particular stage of investigation has been the optimization of the contents (in cement paste) of superplasticizer, SP = X_1, in the range between 0 and 1% (in mass of cement), and of silica fume, MS = X_2, ranging from 0 to 12%. Taken as optimality criteria have been average strength of hardened cement stone, $\overline{R}$ (MPa), and minimal possible strength (with $\alpha = 0.05$), R_{05} (MPa). The viscosity of mix containing SP and MS has been required to be between 1 and 8 Pa.s, the limits being specified by viscosity of additiveless mix (SP = MS = 0).

Optimal design of experiment and models. There has been little sense in designing two-factor experiment in whole square of normalized factors $x_1 = (X_1-0.5)/0.5$, $x_2 = (X_2-6)/6$, considering that in its two subregions non-producible mixes would be got. With adding great quantity of PS ($x_1 \rightarrow +1$) to cement paste without MS ($x_2 \rightarrow -1$) the mix becomes over-fluid. With adding much silica fume ($x_2 \rightarrow +1$) to paste without SP ($x_1 \rightarrow -1$) the mix becomes over-stiff. So "corner" areas corresponding to high SP and MS concentrations have been cut off, factor region presenting the hexagon shown in Figure 3a.

Experience in modeling has shown, that when describing probabilistic indices it is appropriate to built models in the form of incomplete cubic and biquadratic polynomials. Thus two-factor incomplete biquadratic polynomial with 9 terms has been taken as initial model. To build such models synthesized has been D-optimal design with preset central point N3 (Figure 3a), symmetric about diagonal of the square.

Experimental test has shown the fulfillment of restriction on mix viscosity: 7.5 - 8.0 Pa.s at points N4 and N9, 0.9- 1.2 Pa.s at points N6 and N7. At each point the values of material properties have been determined with testing 50 "twin-specimens". This has allowed both parametric characteristics of properties distributions ($\overline{R}$, s, v, coefficients of non-symmetry and excess) and non-parametric statistics (α-quantiles R_α, their ratios, etc.).

Built has been the complex of adequate models (with only significant coefficients) describing the influence of SP and MS concentrations on mean levels of properties and probabilistic quality indices. Thus, the model (2) for average compression strength (MPa) has been got.

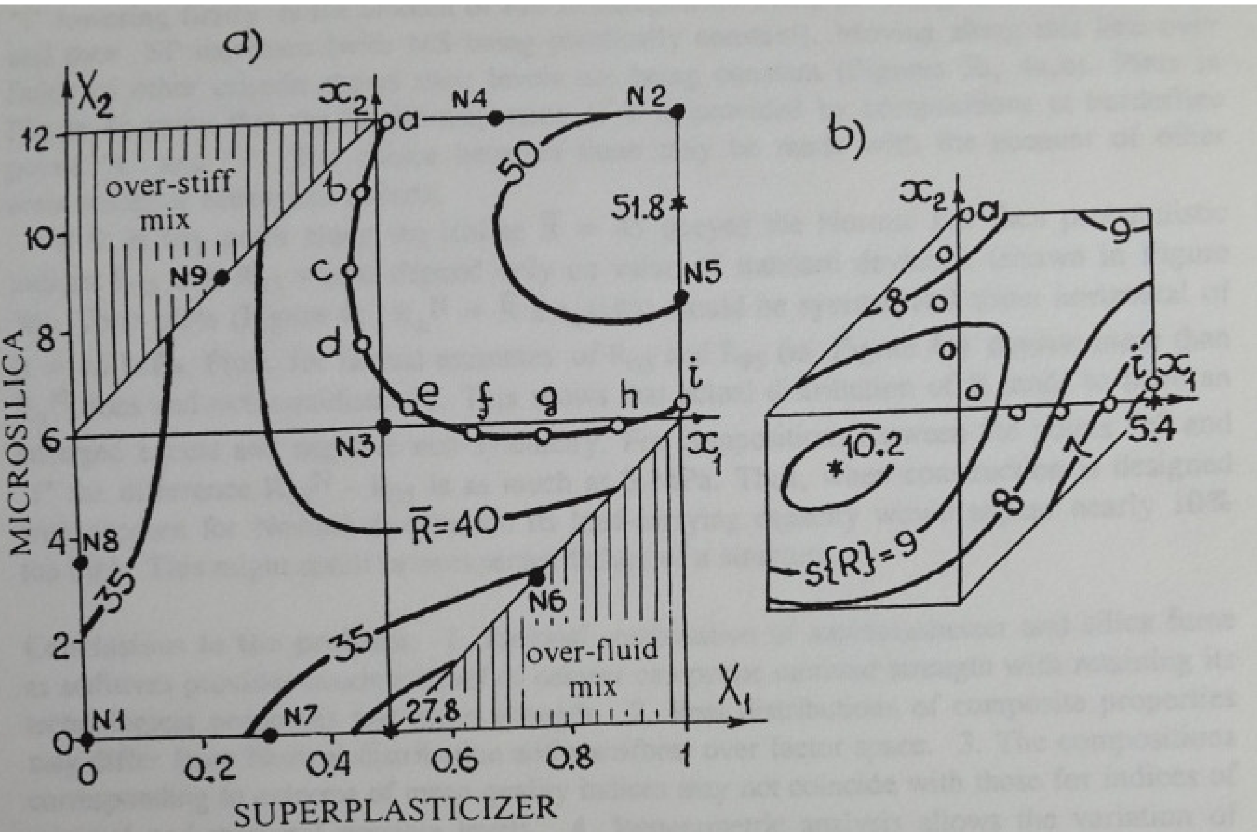

Figure 3. The influence of additives on average strength of cement stone (a) and standard deviation of strength (b)

$$\overline{R} = 43.7 + 7.1x_1 - 7.1x_1^2 + 15.6x_1x_2 - 10.0x_1^2x_2 + (0.0x_1^2x_2^2) + 8.3x_2 - 7.6x_2^2 + (0.0x_1x_2^2) \qquad (2)$$

Diagrams of composite quality indices. $\overline{R}$-isolines, built by model (2) are shown in Figure 3a. Some generalizing indices of this criterion field are: the greatest average strength $\overline{R}_{max}$=51.8 MPa at SP=1% and MS=10%, minimal strength $\overline{R}_{min}$=27.8 MPa, absolute variation $\Delta\overline{R}$=24 MPa, relative variation $\delta\overline{R}$=180%.

Displayed in Figure 3.b are the isolines of sample standard deviation s{R}.The hypothesis that its maximal and minimal values (s_{max}=10.2, s_{min}=5.4 MPa) are statistically equal has been rejected by Fisher's criterion at risk less then 0.005. Then it might be anticipated that extrema co-ordinates for $\overline{R}$ (Figure 3a) will not coincide with those for probabilistic indices. At most of experimental points the hypothesis of R being normally distributed has been rejected (mainly in connection with significant coefficient of non-symmetry). This is why probabilistic indices R_α have been determined as non-parametric estimates - α-quantiles in series of 50 measurements. The level of errors of these estimates is higher than that for $\overline{R}$, however allows useful engineering results to be get.

Isolines of lower probabilistic index of strength, R_{05} (α=0.05) are shown in Figure 4a. The greatest value, $R_{05.max}$ = 34.9 MPa, is achieved at SP=1% and concentration of MS nearly half as much as that in Figure 3a. Extremum $R_{05.min}$ corresponds to essentially different composition than that for minimal $\overline{R}$. Composite sensitivity to controlling its composition by this criterion has also changed (ΔR_{05} = 19.8 MPa, δR_{05} = 230%). Isolines of upper strength probabilistic index, R_{95} (α = 0.95) are displayed in Figure 4b. This response surface is close in shape to the surface of $\overline{R}$ (in Figure 3a) and yet its peak is moved to less concentrations of SP.

For optimal composition in Figure 3a (x_1 = +1, x_2 = 0.68) R_{05} = 32.4 , i.e., 2.5 MPa less then $R_{05.max}$. The hypothesis that there is no strength loss has been rejected by t-criterion at risk about 0.1 . Since distribution of R deviates from Normal law the risk should be estimated with caution, the choice of composition optimal by R_{05} is preferable (x_1 = +1, x_2 = 0, Figure 4a).

Isoparametric Analysis of composite quality indices. The investigation of a system under conditions of its criterion Y being constant has been named by authors as Isoparametric Analysis. Computational experiment with the complex of ES-models makes it possible to do away with labour-consuming experimental works to provide Y = const while varying composition and technology.

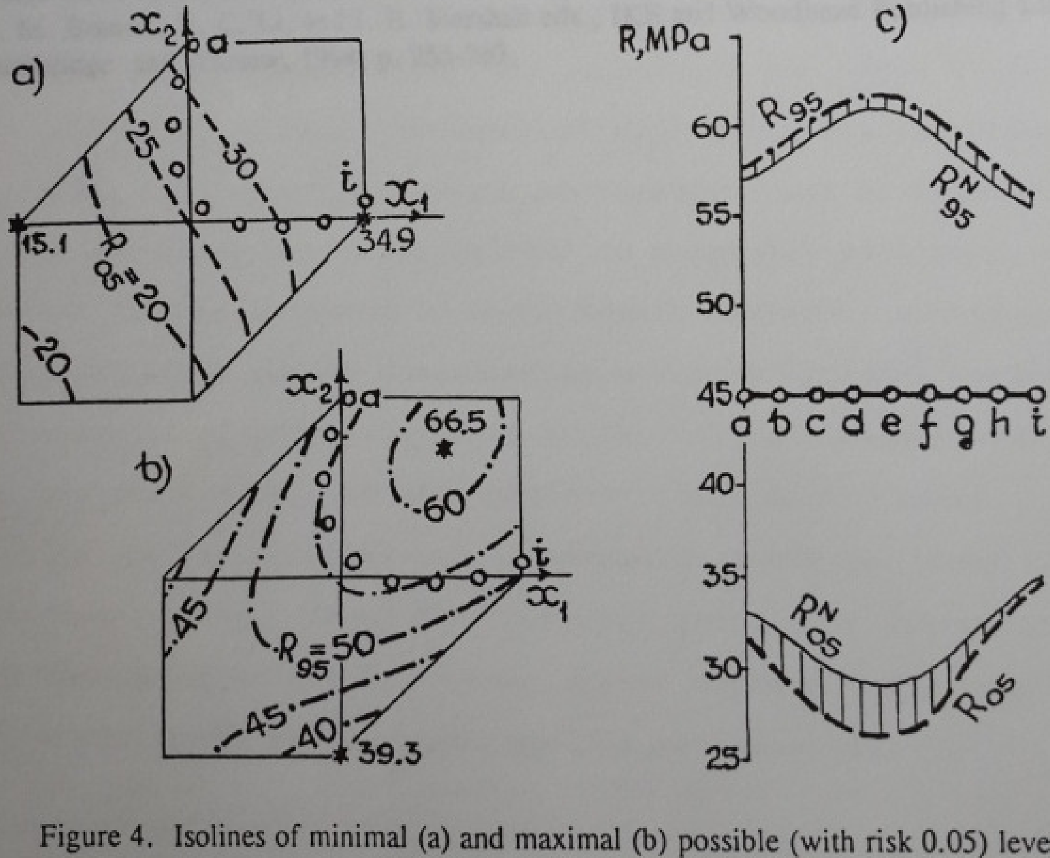

Figure 4. Isolines of minimal (a) and maximal (b) possible (with risk 0.05) levels of strength and isoparametric analysis (c) of probabilistic indices at $\overline{R}$ = 45 MPa

When "moving" along the isoline $Y = \overline{R} = 45$ MPa (Figure 3a) from point "a" to point "i" lowering firstly is the amount of MS in composition (with SP being relatively constant) and then SP increases (with MS being practically constant). Moving along this line over fields of other criteria shows their levels not being constant (Figures 3b, 4a,b). Plots in Figure 4c show that the lowest dispersion of R is provided by compositions at borderline points "a" and "i". The choice between them may be made with the account of other economical or ecological criteria.

If R in any point along the isoline $\overline{R} = 45$ obeyed the Normal law then probabilistic indices R_{05} and R_{95} would depend only on value of standard deviation (shown in Figure 3b). Their plots (Figure 4c, $R_\alpha^N = \overline{R} \pm t_\alpha s\{R\}$) would be symmetrical about horizontal of R = 45 MPa. Plots for factual estimates of R_{05} and R_{95} (in Figure 4c) deviate more than R_α^N does and non-equidistantly. This shows that actual distribution of R tends to have an enlarged excess and negative non-symmetry. For compositions between the points "c" and "f" the difference $R_{05}^N - R_{05}$ is as much as 3 MPa. Thus, when construction is designed with account for Normal distribution its load-carrying capacity would appear nearly 10% too high. This might result in unexpected failure of a structure.

Conclusions to the problem. 1. Rational combination of superplasticizer and silica fume as additives provides maximal level of cement composite minimal strength with retaining its technological properties and mean strength. 2. Real distributions of composite properties may differ from Normal distribution and transform over factor space. 3. The compositions corresponding to extrema of mean quality indices may not coincide with those for indices of minimal and maximal possible levels. 4. Isoparametric analysis allows the variation of property probabilistic indices to be followed in condition of constant average level of the property.

Conclusion

Experimental-statistical modeling as the component of computational materials science is aimed at deriving as much as possible information from experimental results. Complex of models allows the computational experiment to be realized, with results useful for engineering practice and the progress of materials science. Special types of models accounting for specific features of the object under study, the concept of property field, the models for generalizing indices, analysis of probabilistic quality indices, and other means will aid in designing materials and obtaining new knowledge about them.

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