DESIGN OF REPAIR COMPOSITIONS FOR CONCRETE BY WORKABILITY AND DURABILITY CRITERIA WITH METHODS OF COMPUTATIONAL MATERIALS SCIENCE

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Abstract

To find the compositions for repair and protection of concrete that would guarantee the required mix workability and material strength, maximal resistance to water and petroleum at minimal content of epoxy resin computational experiments on property fields have been carried out using experimental-statistical models and Monte Carlo method.

Key words

Overlay, epoxy composite, compromise optimisation, Monte Carlo method.

1 INTRODUCTION

Polymer composites present effective means to repair concrete surfaces and to protect them from negative effects. When designing specially purposed composites two interrelated problems sharpen – a number of criteria increases as well as number of factors to control them. It is in such cases that computational materials science methods, combining physical and computational experiments, are called for. The elements of this methodology based on the concept of material property fields [1-4] described by experimental-statistical (ES) models were used when developing and studying epoxy compositions for repair of concrete surfaces and for protection against adsorption active liquids (water, petroleum, and so on).

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2 EXPERIMENT AND MODELS

Four composition factors separated into two groups, «Modifiers» and «Mineral framework», were varied in experiment [5], according to non-symmetric 18-point design. Dosages of organic modifier (furfural), $X_1 = X_{1\cdot 0} \pm \Delta X_1 = 5 \pm 5$, and fine grained mineral modifier (zeolite), $X_2 = 8 \pm 8$ м.р. (for 100 mass parts of epoxy resin «Macro» at 18 м.р. of hardener), comprised the 1st group. Quantities of quartz sand, $X_3 = 175 \pm 125$, and diabase powder, $X_4 = 70 \pm 20$ м.р., formed the 2nd group. Workability of 18 mixes was estimated by effective viscosity, determined with rotational viscometer. Strength and durability indices were determined on 2×2×8 см specimens. On experimental values of the properties of the mixes and hardened composites ES-models were built (with normalised variables $x_i = (X_i - X_{0\cdot i})/\Delta X_i$, $|x_i| \le 1$), evaluating the influence of composition on the properties (Y), in particular, the criteria involved in the search for rational compositions.

The levels of three criteria have been specified. Effective viscosity (at shear rate $\gamma' = 1\ s^{-1}$) has "corridor" restrictions, $150 \le \eta \le 500$ Pa·s. The requirements for compression strength and bending strength are $R_c \ge 90$, $R_b \ge 50$ MPa.

Coefficients of water and petroleum resistance after 6 month of exposure (K_w and K_p), as durability indices, should be maximized.

Structured ES-models built for all the criteria, such as model (1) for petroleum resistance (with ± 0 indicating insignificant terms at risk 0.1), describe the full fields of material properties $Y(\mathbf{x})$, in coordinates of all composition factors under study, $\mathbf{x} = (x_1, x_2, x_3, x_4)$.

$$K_p = 1.05 \begin{array}{c} \boxed{\begin{array}{l} +0.01x_1 - 0.03x_1^2 \pm 0\ x_1x_2 \\ \pm\ 0\ x_2 \pm\ 0\ x_2^2 \qquad (a) \end{array}} \\ \boxed{\begin{array}{l} \pm\ 0\ x_3 \pm\ 0\ x_3^2 \pm 0\ x_3x_4 \\ +0.01x_4 - 0.07x_4^2 \qquad (b) \end{array}} \end{array} \boxed{\begin{array}{l} +0.02x_1x_3 \\ +0.02x_1x_4 \\ +0.02x_2x_3 \\ \pm\ 0\ x_2x_4 \\ \quad (c) \end{array}} \qquad (1)$$

Block "a" of such model evaluates the influence of modifiers on the property at medium content of mineral framework components ($x_3=x_4=0$). Block "b" characterises the effects of the filler and sand at medium dosages of furfural and zeolite ($x_1=x_2=0$). Block "c" expresses the synergism between two factor subsystems.

Each field can be represented by its generalising indices [1, 4]. Important in this particular problem are maximal levels of $K_w(\mathbf{x})$ and $K_p(\mathbf{x})$ and their absolute increases over the field: $K_{w\cdot max} = 1.12$ at $x_1=x_2= +1$, $x_3= -1$, $x_4= -0.44$; $K_{p\cdot max} = 1.08$ at $x_1= +0.71$, $x_2= +1$, $x_3= +1$, $x_4= +0.18$; $\Delta K_w = 0.21$ and $\Delta K_p = 0.19$.

The sixth criterion is the quantity of epoxy resin in composition, E (kg/t). It should be minimized, by 4-factor hyperbolic deterministic relationship (2).

$$E = 10^5 / (5x_1 + 8x_2 + 125x_3 + 20x_4 + 376) \qquad (2)$$

The minimal level of field $E(\mathbf{x})$ is $E_{min} = 187$ kg/t, when there are no modifiers in composition with lowest content of mineral phase ($x_1=x_2=x_3=x_4= -1$).

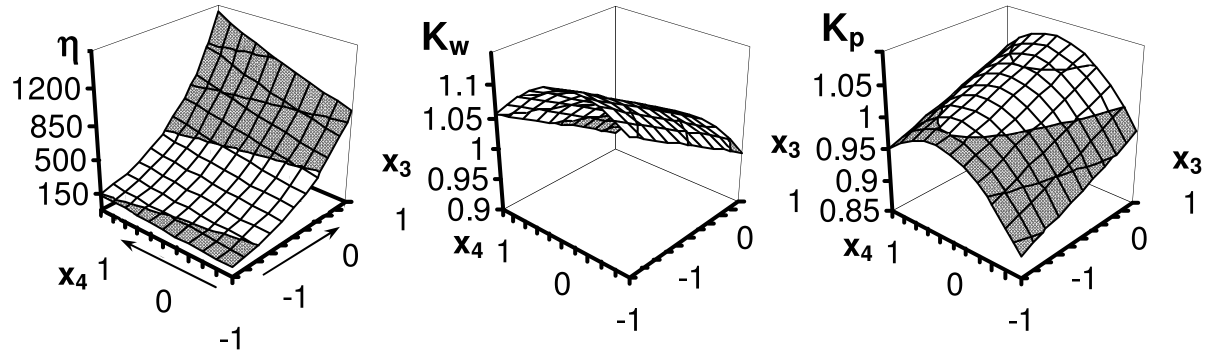

Figure 1 The fields of mix viscosity and resistance coefficients in coordinates of filler and sand contents (at maximal dosages of furfural and zeolite)

The impossibility to have the composite of highest resistance with minimal expenditure of polymer becomes clear when comparing the coordinates of $K_{w\cdot max}$, $K_{p\cdot max}$ and E_{min}. Representations of the local fields $\eta(x_3, x_4)$, $K_w(x_3, x_4)$, and $K_p(x_3, x_4)$ at $x_1=x_2=+1$ (fig. 1) shows that the best compositions by individual optimality criteria (K_w, K_p) do not coincide and could not satisfy the specified requirements (η). Consequently, a compromise solution should be found.

3 COMPUTATIONAL EXPERIMENT

Firstly, in computational experiment on the property fields using Monte Carlo method isoparametric analysis [6] was carried out to study the changes in material properties under condition of mix viscosity being constant [5]. At this constraint the region of mixes was found to exist which would provide increased durability indices and specified strength. This gave grounds for multi-criterion search for compositions that would guarantee the required mix viscosity and composite strength and improve durability indices with as small quantity of epoxy resin as possible. To find compromise solutions the version of algorithm [6] has been used in which the region of admissible compositions is determined by guaranteeing (at given risk α) levels of restriction criteria (R_c, R_b, and η). Such stringent requirements are defined by inclusion of confidence intervals (ΔY) in the limiting levels.

Guaranteeing levels for strength are calculated as $R+\Delta R$. This gives (at α=5%) $R_{c.05}$ = 91 and $R_{b.05}$ = 53.3 MPa (with account for experimental errors s_{Rc} = 0.7 and s_{Rb} = 2.4 MPa, averaged value of prediction variance function [7] $\overline{d}$ = 0.70, and quantile t_{05} = 1.645 corresponding to risk α=5%). Similarly, the lower (L) guaranteeing level of viscosity is calculated, $\eta_{L.05}$ = 165.5 Pa·s (Δ=15.5 at $s\{\eta_L\}=\delta\{\eta\}\cdot\eta_L=0.075\cdot150 = 11.2$). When tightening the upper (U) level (at $s\{\eta_U\}=0.075\cdot500 = 37.5$) $\Delta\eta$ = 51.6 is subtracted from the upper standard value thus giving $\eta_{U.05}$ = 448.3 Pa·s.

As initial values for criteria to be optimised median levels of corresponding fields are taken: $K_{w.M} = 0.5(K_{w.max}+ K_{w.min}) = 0.5(1.11+0.93) = 1.02$, $K_{p.M} = 0.5(1.08+0.89) = 0.98$, $E_M = 0.5(459+187) = 323$ кg/t.

The search procedure is based on results of computational experiment on complex of M property fields Y(**x**) described by ES-models with iterative use of Monte Carlo. The procedure includes the dialog with computer and allows guaranteeing composition-process parameters (acceptable, optimal, compromise) to be found.

At the initial stage of 1st iteration (stage "1-0") N random vectors **x** (compositions) are generated, uniformly distributed in the field region (Ω_x). In this particular problem Ω_x is 4-dimension cube, N =1000 plus 16 vertices (±1, ±1, ±1, ±1) added. This is as if multi-dimensional net was thrown on factor region (the average step between knots equals Δx_i / $N^{0.25}$ = [1-(-1)] /$1016^{0.25}$= 0.36). Levels of all M properties in N points (specifically, M=6, N=1016) are calculated by ES-models.

At stage "1-1" the admissible region Ω is formed. To do this, N_Ω points fallen within admissible region by levels of restriction criteria are picked out. The other N – N_Ω points are eliminated. In the particular problem 63 compositions (offering $R_c \geq 91$, $R_b \geq 53.3$, $165.5 \leq \eta \leq 448.3$ and levels of K_w, K_p, and E not worse than median) have remained in Ω (fig. 2a), with 953 unacceptable compositions removed. The region of search has contracted – its volume in relation to initial region is almost an order less (K_Ω in fig. 2b).

At stage "1-2" the approach to individual optima ($K_{w \cdot max}$ = 1.12, $K_{p \cdot max}$ = 1.08, E_{min} = 187) is carried out (fig. 3a). Factor ranges are cut down (fig. 3b). Search region shrinks to the region of compromise Ω_{comp} (K_Ω about 0.001, fig. 2b). The particular results of optimisation at this stage – the values of optimality criteria better than median levels ($K_{w.1-2}$ =1.05 > $K_{w.M}$ =1.02, $K_{p.1-2}$ =1.03 > $K_{p.M}$ =0.98, E_{1-2} =291 < E_M =323, fig. 3a). The further progress to the optima at this iteration is impossible.

The process should be continued at the next iteration, with new 1000 points being generated in extended (accounting for Δx_i) region of compromise (shown in fig. 3b) plus the points obtained at previous iteration (fig. 2a). At the second iteration the primary emphasis has been on the search for compositions providing as high level of petroleum resistance as that of water resistance ($K_p \approx K_w \geq 1.05$). The main concern at the third iteration has been with lowering polymer content without impairing the achieved levels of durability indices.

Stage «3-2» has brought the boundaries of Ω_{comp} much closer together (with factor intervals from 0.14 to 0.38 in units of normalised factor space, fig. 3b). The upper and lower levels of resistance criteria over compromise region have practically closed up (fig. 3a). So the search process has been stopped.

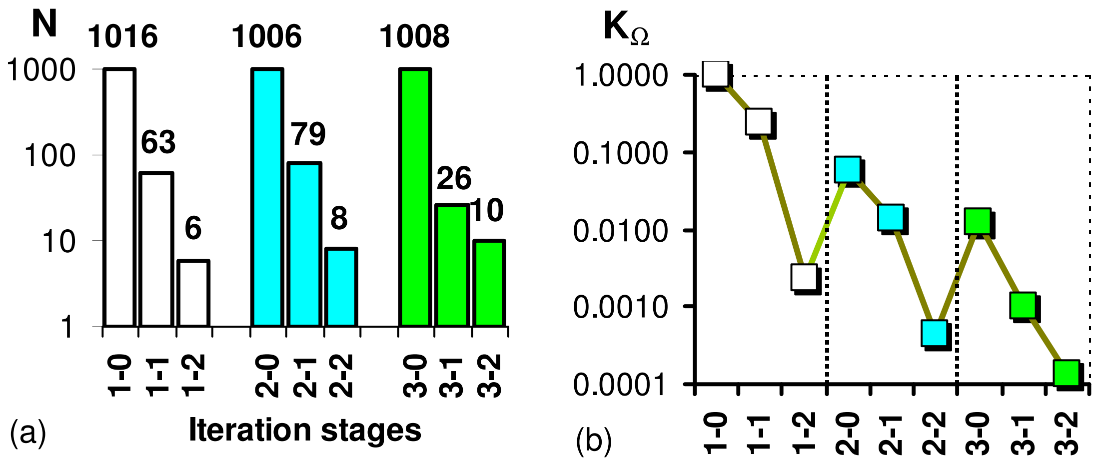

Figure 2 The changes of number of points in search region (a) and of its relative volume (b) during the course of computational experiment

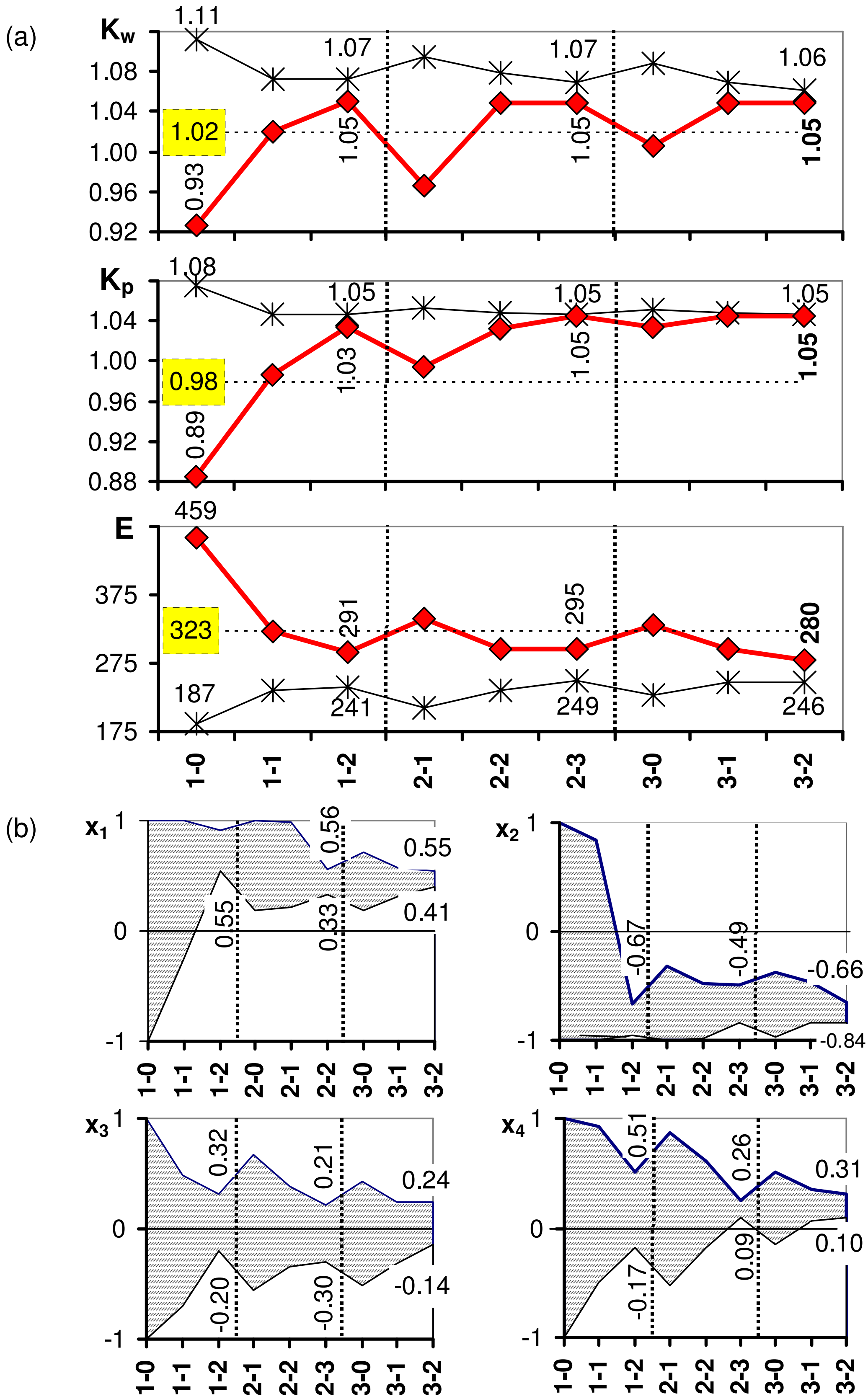

Figure 3 Changes of lower and upper levels of optimality criteria (a) and composition factors (b) at stages of iterations during the search for compromise solution

The composition chosen by results of computational experiments contains 262 kg/t of epoxy resin “Macro”. This is 60 kg less than median level. Mix viscosity is about 300 Pa·s, strength $R_c = 102$, $R_b = 53.5$ MPa. Coefficients of resistance to water and petroleum have near the same values $K_w \approx K_p \approx 1.05$.

4 CONCLUSION

The composite on “Macro” resin has been designed for repair and protection of concrete elements in water-transportation structures. The requirements for mix workability and material strength and resistance have been satisfied. The compromise compositions found have been included in projects of overlays for the channel in circulation water-supply system at one of nuclear power stations in Ukraine and water removal structures at some railway stations in Lithuania.

Methods of computational materials science allows rational engineering solutions to be found when studying and developing special purpose concretes and other multi-component building materials.

LITERATURE

[1] Voznesensky, V.A.; Lyashenko, T.V.: Modelling, analysis and optimization of brittle matrix composites properties fields. In: Brittle Matrix Composites 4. Proc. 4th Int. Symposium. Cambridge, Warsaw : Woodhead Publ. Ltd., 1994. pp. 255-263, ISBN 1-85573-183-X, ISBN 83-902146-0-1.

[2] VOZNESENSKY, V.A.; LYASHENKO, T.V. *Experimental-statistical modelling in computational materials science*. Odessa: Astroprint, 1998. ISBN 966-549-057-5.

[3] LYASHENKO, T.V. *Building materials property fields* (*concept*, *analysis*, *optimisation*). Abstract of Thesis for Doctor of Science Degree (in Ukrainian). Odessa State Building and Architecture Academy, Odessa, 2003.

[4] Lyashenko, T.V.: The concept of property fields – methodical base for extracting information from ES-models in computational materials science (in Russian). In: Bulletin of Odessa State Building and Architecture Academy, no. 12. Odessa, 2003. pp. 171-179.

[5] Lyashenko, T.; Dovgan, A.; Sharshunov, A.: Isoparametric Analysis on Property Fields of Modified Epoxy Composite (in Russian). In: Bulletin of Odessa State Building and Architecture Academy, no. 13. Odessa, 2004. pp. 101-107.

[6] Lyashenko, T.; Voznesensky, V.; Boiko S.; Shtakelberg D.: Analysis of concrete property fields and search for the best compositions using Monte Carlo method. In: Brittle Matrix Composites 7. Proc. 7th Int. Symposium. Cambridge, Warsaw: Woodhead Publ. Ltd., ZTUREK, 2003. pp. 351-358. ISBN 1-85573-769-8, ISBN 83-917926-6-8.

[7] VOZNESENSKY, V.A.; LYASHENKO, T.V.; OGARKOV, B.L.: *Numerical methods of computer-aided solutions of construction and technological problems* (in Russian). Kiev: Higher School, 1989. ISBN 5-11-001439-6.