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Compromise optimisation of heat insulating and mechanical properties of high performance autoclaved aerated concrete

Methods of computational building materials science enable quite complicated problems to be solved, specifically, the multifactor technological solutions, which would provide the compromise optimum by large number of material quality criteria, to be found. To find the compromise values of composition-process (CP) parameters, in particular, for fibrous polymer-cement dry mixes /1/, slag alkaline binders /2/, modified epoxy mortars /3/, iterative random scanning of material property fields in CP-coordinates has been used. The search has been carried out with the help of computational experiments (and Monte Carlo method) on the fields of properties described by experimental-statistical (ES) models built on the data obtained in the designed natural experiments.

In this particular work to find compromise solutions for autoclaved aerated concrete technology new version of the search /4/ is tried: generated in computational experiments are only those levels of CP-factors (normalised between -1 and $+1$, distributed by discrete uniform law), that could be fixed within real technology.

Conditions of experiment and modelling

The influence of nine CP-factors on structure and properties of autoclaved aerated concrete was studied /5/ in collaboration with “NIPISilicatobeton”. The concrete blocks were produced there, at industrial conditions, in keeping with technology regulations of 56 different composition-process variants, according to specially synthesised design of experiment. The design has “replaced” two- and three-level full factor experiments 2^k and 3^k , with 512 and 19683 trials for number of factors $k = 9$.

Physical-mechanical properties of the material were determined at specialised laboratory. The parameters of porous space and thermo-physical characteristics of 56 autoclaved aerated concretes were determined with method of laser porosimetry. The data obtained allowed the complex of non-linear nine-factor ES-models for complex of material properties to be built and analysed.

The composition-process factors X with ranges of varying them in the experiment, $X_0 \pm \Delta X$, are presented in Table 1. Also indicated for each factor is regulation step h assigned (basing on specific technology and engineering logic) for generating the levels of factors in computational experiment. Then the number of possible values of factor X_i equals $m_i = 1 + 2 \cdot \Delta X_i / h_i$, with probability of each value being $p_i = 1/m_i$.

Thus the total number of competitive CP-variants of autoclaved aerated concrete that could be produced (in accordance with Table 1) equals $17 \times 13 \times \dots \times 11 = 14.5 \times 10^9$ at the

Table 1. Nine composition-process factors (X) with their levels in experiment and conditions of regulation for computational experiment

Index (i)	Factor	Natural experiment		Computational experiment
		Central value $X_{0,i}$	Semi-interval ΔX_i	Step h_i
1	Flowability of mixture by Suttard viscosimeter, D (sm)	27	4	0.5
2	Moisture of sand (when grinded together with lime), $w_s\%$	5	3	0.5
3	Specific surface of the sand S_s (m^2/kg)	250	100	20
4	Time of isothermal heating in autoclave, τ (hour)	8	4	0.5
5	Operating pressure of steam, p (MPa)	1	0.2	0.05
6	Dosage of aluminum powder A% (by mass of dry components)	0.07	0.03	0.005
7	Mix activity (content of CaO in lime-sand mixture) $a_{CaO}\%$	17	3	0.5
8	Temperature of mixing water, t_w °C	35	10	2
9	Quantity of cement C% (of mix mass)	10	10	1

beginning of the search. In the course of the search, the number of such variants decreases steeply due to elimination of factor levels that would be of no use for approaching the compromise.

The specimens of autoclaved aerated concrete were cut from the blocks made according to 56 variants of technology regulations. Determined experimentally were, in particular, the density of concrete γ (kg/m^3), coefficient of heat conductivity λ ($mW/m/K$), compression strength R_c (MPa), strength R_b (MPa) and ultimate deformability ϵ (mm/m) under bending.

These data allowed the quadratic nine-factor ES-models (with variables conventionally normalised to $|x_i| \leq 1$) to be built for material properties (insignificant estimates being eliminated from the set of 55 coefficients of each model by sequential regression analysis). Such model for bending strength (1), with 42 significant coefficients, describes the field of R_b in nine CP-coordinates, with maximal level $R_{b,max} = 3.2$ and minimum $R_{b,min} = 0.2$ MPa.

This and similar models for γ , R_c , ϵ , and λ are used to solve the compromise optimisation problem for autoclaved aerated concrete of mark D800 (density γ between 740 and 840) and class 7.5 (strength R_c between 9.6 and 12.9).

$$\begin{aligned}
R_b = & 1.92 \\
& +0.06x_1 + 0 x_1^2 + 0 x_1x_2 + 0 x_1x_3 -0.10x_1x_4 -0.08x_1x_5 -0.03x_1x_6 + 0 x_1x_7 + 0 x_1x_8 +0.03x_1x_9 \\
& +0.12x_2 -0.33x_2^2 + 0 x_2x_3 -0.03x_2x_4 +0.03x_2x_5 +0.03x_2x_6 -0.04x_2x_7 + 0 x_2x_8 -0.03x_2x_9 \\
& +0.13x_3 + 0 x_3^2 -0.08x_3x_4 -0.02x_3x_5 +0.09x_3x_6 + 0 x_3x_7 +0.02x_3x_8 +0.03x_3x_9 \\
& +0.07x_4 +0.13x_4^2 -0.15x_4x_5 -0.04x_4x_6 +0.15x_4x_7 +0.02x_4x_8 +0.04x_4x_9 \\
& +0.05x_5 -0.10x_5^2 -0.05x_5x_6 +0.09x_5x_7 + 0 x_5x_8 +0.04x_5x_9 \\
& -0.50x_6 + 0 x_6^2 + 0 x_6x_7 +0.05x_6x_8 -0.10x_6x_9 \\
& +0.03x_7 +0.26x_7^2 -0.06x_7x_8 -0.13x_7x_9 \\
& -0.07x_8 +0.13x_8^2 +0.01x_8x_9 \\
& +0.22x_9 + 0 x_9^2
\end{aligned} \tag{1}$$

The index of toughness $H = R_b \cdot \varepsilon$ defining crack resistance should be maximised. Minimised are heat conductivity λ and the levels of two energy consuming factors of autoclave technology, heating time τ and steam pressure p (factors x_4 and x_5).

Main elements of compromise optimisation algorithm

At initial (zeroth) stage of the first iteration (stage "1/0") N_g random numbers distributed by discreet uniform law in the full range ($-1 \leq x_i \leq +1$) of each factor are generated. The random points thus obtained simulate N_g variants of autoclaved aerated concrete technology within the whole region of CP-parameters under study (k -dimensional cube, $k=9$). Added to them are 2^k vertices of the cube ($x_i = \pm 1$). In this particular case $2^9=512$ points have been added to $N_g=10000$, i.e., $N_{1/0} = 10512$ variants are in competition at stage "1/0" (more than 6 orders less than number of lattice points by Table 1). For $N_{1/0}$ composition-process variants the levels of 6 property fields (of γ , R_c , λ , and H , that should be scanned, R_b and ε under control) are determined by ES-models. Thus the matrix of the results of computational experiment is formed (matrix size being 10512×6).

At the next stage "1/1" the rows, which do not satisfy the requirements, firstly, of the mark ($740 \leq \gamma \leq 840$), then of the class ($9.6 \leq R_c \leq 12.9$), are deleted from the matrix. The CP-variants (115 in this case) complying with requirements of specifications (for γ and R_c) belong to the region of admissible solutions (RAS) remaining for the search. The levels of two optimality criteria (λ , H) for admissible variants turn out to be restricted in their ranges of possible values (RPV). In particular, $RPV\{\lambda\} = 221-147 = 74 \text{ mW}/(\text{m}\cdot\text{K})$ (Fig. 1); succeeding in advancing half the RPV will decrease the upper value of heat conductivity coefficient by near 20%. RAS defines the ranges of admissible levels for each of CP-factors (Fig. 2). In this particular case, 8 from 9 factors hold their levels between -1 and $+1$ at stage "1/1". Only the range of the dosage of gas-former (x_6) has contracted by half.

At final stage of the 1st iteration ("1/2") the improvement of each optimality criterion within its RPV is carried out, from the worst level ($\lambda = 177$, $H = 2.52$, Fig. 1) towards the best one ($\lambda = 161$, $H = 3.63$).

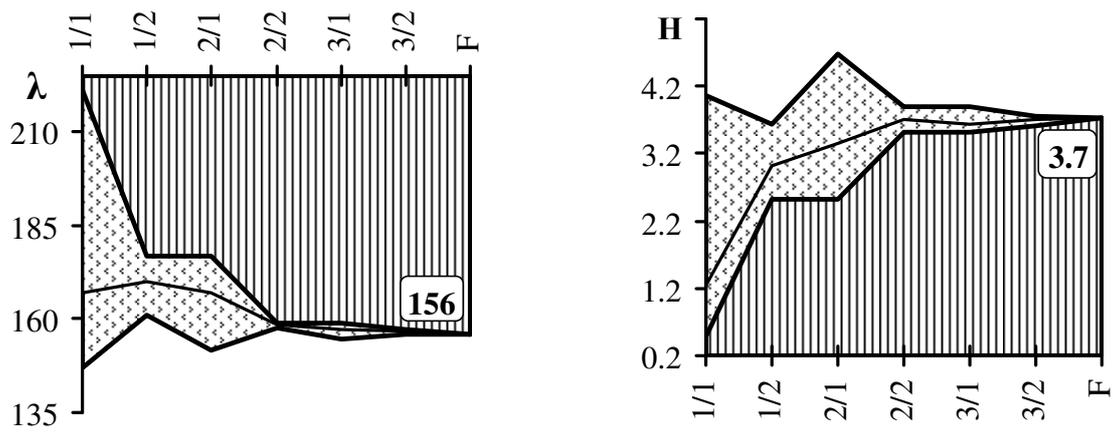


Fig. 1. Changes in ranges of optimality criteria at stages of the search for compromise

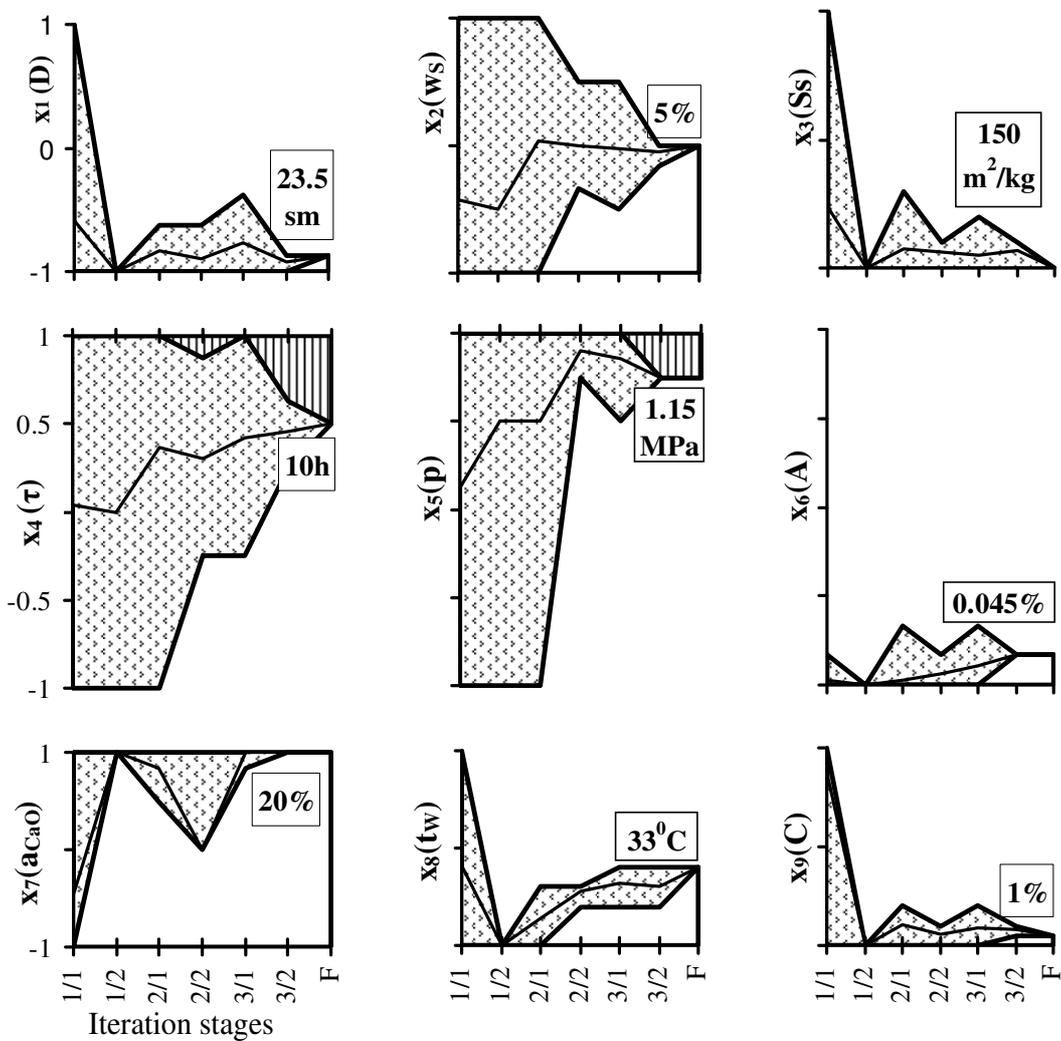


Fig. 2. Changes in ranges of composition-process factors along the search for compromise optimum

Therewith two ranges (of importance for technologist) form: purposefully widened range of the gain in criterion level (RG, vertical shade in fig. 1) and the “pulsing” range of compromise (RC). The steps for each criterion in step-by-step improvement are chosen by technologist in the dialog with a computer. After 1st iteration $N_{1/2} = 4$ variants of the technology fall within $RC\{\lambda\}$ and $RC\{H\}$.

The index of effectiveness when minimising λ equals $E\{\lambda\} = RG\{\lambda\} / RPV\{\lambda\} = (221-177)/74 = 0.59$, the level of $E\{H\}$ being practically the same since no priorities have been assigned to the criteria. The factor ranges have shortened. However near the border of multi-factor region some CP-variants with useful combination of optimality criteria levels and decreased expenditure of resources could be missed in random scanning. So it is reasonable to widen the narrowed ranges at least by one step $h\{x_i\}$ in both directions.

In thus widened CP-region new $N_g = 10000$ random CP-variants are generated at stage 2/0, to which $N_{1/2} = 4$ best variants from the 1st iteration are added. At stage 2/1 excluded are not only the variants inadmissible by specifications (by γ and R_c), but also those which have the levels of optimality criteria worse than achieved at previous iteration.

Then the procedure is repeated. As compromise ranges of all criteria decrease (to 7-10% of RPV) it is reasonable to seize an opportunity to reduce the expenditure of resources, specifically, by energy consuming factors. In this particular case time τ of isothermal heating in autoclave (x_4) and operating pressure of steam p (x_5) have been minimised at stage "3/2", practically without sacrifice of material quality. It has been possible to lower the upper limits of compromise ranges $RC_{3/1}$ (containing 33 variants of technology) by 1.5 h and half an atmosphere respectively. As a result $N_{3/2} = 3$ competing variants have remained in $RC_{3/2}$.

The effectiveness indices of compromise optimisation: by heat conductivity $E\{\lambda\} = 0.86$, by toughness $E\{H\} = 0.87$, the properties under control being also improved – $E\{R_b\} = 0.65$ and $E\{\varepsilon\} = 0.89$. The variants remaining at final stage are of equal value from engineering point of view. The choice of final variant (F) could be subjective or based on new additional criteria.

The best composition-process solution

The chosen variant F of composition and process parameters allows competitive autoclaved aerated concrete of mark D800 ($\gamma = 756 \text{ kg/m}^3$) and class B7.5 ($R_c = 9.9 \text{ MPa}$) to be produced, with optimised levels (Fig. 1) of heat conductivity ($\lambda = 156 \text{ mW/(m}\cdot\text{K)}$) and crack resistance (characterised by index of toughness $H = 3.7 \text{ kJ/m}^3$). These values of the quality criteria are provided by CP-variant of reduced energy consumption (Fig. 2): flow of the mixture $D = 23.5 \text{ sm}$, moisture of sand $w_s = 5\%$, specific surface $S_s = 150 \text{ m}^2/\text{kg}$, time of isothermal heating $\tau = 10 \text{ h}$, pressure of steam $p = 1.15 \text{ MPa}$, dosage of aluminium powder $A = 0.045\%$, mix activity $a_{\text{CaO}} = 20\%$, temperature of mixing water $t_w = 33^\circ\text{C}$, quantity of cement $C = 1\%$.

Conclusion

The algorithm of compromise optimisation at discrete levels of CP-variables is well suited and comfortable for adapting the search parameters, in dialog with a computer, to flexible conditions of the problem. The algorithm can be recommended to search for multi-parametric admissible, optimal, and compromise solutions for mix-proportions and parameters of production process, especially when purposeful minimisation of energy consuming factors is required.

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