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Optimization of the Material Structure and Composition of Cement Based Composites

A. M. Brandt* & M. Marks

Institute of Fund. Techn. Research, Polish Academy of Sciences, 00-049 Warszawa, Swietokrzyska 21, Poland

Abstract

The materials considered in the paper are called concrete-like composites or materials with cement based matrices. These are not only ordinary and high performance concretes, but also materials with different admixtures, dispersed fibre reinforcement, polymers, etc. The matrix may be improved by several procedures and in this continuous phase different inclusions are randomly dispersed. The concretes, when treated as composite materials, may be studied and designed using modern methods developed for advanced high strength composites and mathematical optimization. In the paper a few important objective functions (criteria), constraints and variables are examined from the viewpoint of material design. The fracture energy is considered as an important feature of the material resistance against cracking. The amount of the fracture energy required for a given mode of rupture may be calculated using more or less approximate formulae, based on simplified assumptions. The main aim of the paper is to demonstrate through simple examples how the optimization approach may be used in practical situations of the design of high performance concretes. © 1996 Elsevier Science Limited.

INTRODUCTION

Optimization approach to any activity in technology, economy or other fields is aimed at methods of determination of the best solutions in an objective way. In particular, optimization of composite materials deals with problems of selection of values of several variables which determine the composition and internal structure. Also, other variables like methods of production and curing may be included.

In the paper the optimization approach is limited to materials with cement based matrices, like ordinary plain concretes, polymer concretes, fibre reinforced concretes, etc. These materials are used in building and civil engineering. Their properties are related in a very complicated way to their internal structure and composition. Usually, these materials are designed in an iterative process, starting with given objectives and limits. The design procedures are based on previous experience with extensive use of the trial and error approach. These methods are often qualified as vague and non-direct and results depend considerably on talent and experience of the designer.

The optimization methods are aimed at certain input of rational indications for design. It is considered as useful, and in many cases even necessary, to support the traditional design methods by that objective approach. This seems particularly helpful in design of composite materials where, due to a large number of design criteria and variables, any intuitive approach to design is difficult.

The optimization of structures was studied already by Galileo in 1634 and since that a few thousands of valuable papers have been published in this field. The optimization of materials was started not so long ago and the results obtained are not numerous. Short list of papers on optimization of composite materials is given and commented on in Refs 1 and 2. A review of papers published in the USSR was given by Teters *et al.*[3] Mullin and Mazzio in Ref. 4 have shown the importance of optimization of composite materials taking into account the fracture processes.

*Author to whom all correspondence should be addressed.

Interesting remarks on optimization of concretes are published by Popovics (in Refs 5 and 6) who attracted attention on the applicability of relatively simple methods and procedures. Valuable developments concerning useful and realistic objective functions related to strength and to fracture energy for fibre reinforced composites were also given in Kelly and MacMillan,[7] Li *et al.*[8] and Mallej *et al.*[9] Brandt has shown[1,2,10] that the determination of maximum fracture energy of fibre reinforced cement based composites as a function of direction of fibres is not a trivial problem. The results of calculations were developed later in Refs 11 and 12, where experimental verifications were presented. The problem of optimal orientation of fibres was also studied by Marks.[13,14] The cement based materials fulfil all definitions of composite materials and the application of the well developed mechanics of composites seems to be fruitful. The methods, concepts and solutions obtained for high strength composites applied for construction of vehicles, aircrafts and rockets may be least partly used for cement based composites.

In the paper an attempt is presented of how to design and optimize brittle matrix cement based composites using methods and solutions taken from two well advanced field: mechanics of composites and mathematical optimization.

OPTIMIZATION OF MATERIALS

The problem of optimization of a material may be formulated as analogue to structural optimization, cf. Refs 15 and 16. An optimal material is described by a set of decisive variables x_i ($i=1,2,..,n$) which minimize or maximize an optimization criterion.

Variables x_i are considered as independent and together with arbitrary selected parameters they determine completely the object of optimization: a structure or a material. These are material variables.

In the problems of structural optimization the variables are determining the shape of the structure, distribution in space of its elements, shape and dimensions of cross-sections, etc. Also the physical properties of the constructional materials may be considered as variables.

In the case of the material optimization, the variables are: nature and quality of components, their distribution in space, their reciprocal relations like adherence, etc. Also methods of production may be considered as discrete variables provided that they determine final or transitory material properties.

The decisive variables belong to a feasible set. It means that their values beyond imposed limits cannot be accepted in the problem for constructional, functional or other reasons. The constraints may have the form of equalities or inequalities

$$g_p(x_i) = 0, p = 1, 2,...,r \quad (1)$$
$$h_s(x_i) \leq 0, s = 1, 2,...,t$$

or simply limit values may be imposed

$$\underline{x}_i \leq x_i < \bar{x}_i, i = 1, 2,...,n,$$

lower and upper bars indicate imposed lower and upper limit values, respectively. For example, the variables which determine the components are limited to available materials and their possible properties. All constraints determine the set of feasible solutions. The variables may be defined as continuous or discontinuous (discrete) ones. As continuous variables the quantities (e.g. volume contents) of particular components may be considered. A few discrete kinds of a component represent discontinuous variables, e.g. different types of Portland cement may be used in the composition.

The properties of the components as well as their effective distribution in a composite material are random variables. Their final values and their nominal values determined by testing are subjected to unavoidable scatter. If in an optimization problem only design and nominal values are considered, then that is a deterministic approach. In an opposite case, when the distribution functions are taken into account, the stochastic problem of optimization may be formulated.

Optimization criteria describe basic properties of materials. They are also called objective functions. In structural optimization we choose: minimum volume or weight, maximum bearing capacity or strength, maximum stiffness, minimum cost, etc. as optimization criteria. In material optimization the objective functions describe selected properties which are considered as important and decisive for the material quality and applicability. The solution consists of determination of these values of design variables which extremize these properties. As material properties all physical, chemical and other properties may be considered. For engineering materials, particularly important are mechanical properties like strength, Young's modulus, specific fracture energy, durability but also specific cost.

Let us consider a set of independent variables x_i, (i = 1, 2,..., n). The optimization criterion is expressed by these variables as function $F(x_i)$ subject to constraints of different kinds and forms, e.g. the limited volume of material may be presented as an integral. If the problem is formulated with one single criterion with constraints (1), then the necessary conditions for a maximum of the objective function are derived from the Kuhn–Tucker theorem (Kuhn and Tucker[17] and Brandt ed.[15]) and have following form:

$$x_i\frac{\partial F^*(x_i)}{\partial x_i}=0;\ \frac{\partial F^*(x_i)}{\partial x_i}\leq 0;\ \frac{\partial F^*(x_i)}{\partial \mu_p}=0;\quad (2)$$

$$\mu_s\frac{\partial F^*(x_i)}{\partial \mu_s}=0;\ \frac{\partial F^*(x_i)}{\partial \mu_s}\leq 0;$$

$x_i \geq 0$, $i=1, 2,..., n$;here $\mu_s \geq 0$, $s=1, 2,..., t$, and μ_p, $p=1, 2,..., r$ are so called Lagrange multipliers, and

$$F^*(x_i)=F(x_i)+\sum_{p=1}^{r} g_p(x_i)+\sum_{s=1}^{t}\mu_s h_s(x_i)\quad (3)$$

In the structural and material optimization problems there are several common features. These problems are correctly formulated when criteria, constraints and variables are defined. Sometimes the design variants are incorrectly called "optimal solutions". Calculation of a few cases and selection of the best one is not an optimization approach. There is no optimal solution without clear determination of the sense and within what feasible region.

It should be also stressed that the optimization problem is solved not on a real structure or material, but on their approximate models. The results of optimization procedure are dependent on assumptions and approximations admitted for these models.

The material optimization does not replace entirely the material design, because it may not cover certain aspects and requirements that determine the material completely. That is justified by necessary simplifications and assumptions accepted in the optimization problem. Contrary to this, in the material design, all requirements should be satisfied. That is why the material optimization, like the structural optimization, does not replace design but is a part, in which some intuitive procedures are replaced by objective calculations.

The sensitivity of the objective function with respect to variables is a separate problem. When the objective function does not depend on the decisive variables, then probably the variables are incorrectly selected.

Verification of separation between constraints and objective functions may be important. It occurs sometimes that small modification of a constraint may influence considerably the objective function. In such a case the resignation of preliminary assumptions concerning constraints may be justified.

In certain problems it is admissible to limit the optimization problem to one single criterion, e.g. a structure of minimum cost or a material of maximum strength may be considered as an appropriate solution. In general, such a formulation has a somewhat academic character and may be used as a simplified example for preliminary explanation of the problem. In most cases the existence and necessity of several criteria is obvious. The multiobjective or multicriteria optimization is the next step, presented below.

MULTICRITERIA OPTIMIZATION

Let us consider n-dimensional space of variables x_i in which objective functions F_j (x_i), j = 1, 2,..., k, are determined, here k is the number of objective functions or functionals. It means that a solution of the problem should satisfy k objective functions and the problem may be formulated as follows: 'determine n-dimensional vector in the space of decisive functions which satisfies all constraints and ensures that the functions F_j have their extrema'.

The decisive functions are the components of the vector X^N in the n-dimensional space. Every point of that space indicates a material, defined by n decisive variables. The feasible region Q is a part of the n-dimensional space and is defined by the constraints (1).

The space of the objective functions R^k has k dimensions. Every point of that space corresponds to one vector of the objective function

F_k (x_i). In that space the feasible region Q is represented by a region $F(Q)$. Without entering into mathematical formulations which may be found in Refs 18–20, it may be proved that the points of feasible region Q are represented by the points in the region $F(Q)$. An example of regions Q and $F(Q)$ are shown in Fig. 1 in the case of $k = 2$ and two-dimensional region.

The optimization problem formulated in this way may have several solutions and the solution appropriate for given conditions should be selected using other arguments. To present that procedure a few definitions are necessary.

The *ideal solution* is an extremum for all objective functions. Because a characteristic feature in multiobjective optimization is that the criteria are in conflict, then the ideal solution is outside the feasible region. That is indicated by point A in Fig. 1(b), in which both objective functions F_1 and F_2 have their maximal values but outside region $F(Q)$.

The solutions of the problem are situated on section BC of the boundary of the feasible region. These are called *nondominated* (*Pareto ideal*) *solutions* or the *compromise set*, it means that no one objective function can be increased without causing simultaneous decrease of at least one other function. In effect, the difficulty is that there is a great number of Pareto solutions. It is therefore necessary to apply other procedure for selection of one solution, called the *preferable solution*.

The compromise set may be determined from the Kuhn–Tucker theorem (2) in which function F from eqn (3) is expressed by

$$F = \sum_{j=1}^{k} \lambda_j F_j, \text{ where } \sum_{j=1}^{k} \lambda_j = 1, \lambda_j \geq 0. \quad (4)$$

For different λ_j, particular points belonging to the compromise set may be found out from eqn (2). It may be in many cases very difficult or even practically impossible to determine the compromise set from eqn (2) considering also eqns (3)and (4). Then the numerical methods should be applied to find out the maximum of function F^*.

The preferable solution may be selected using different assumptions and methods. For example, arbitrary weights may be proposed for each objective function, meaning that some functions are considered as more important than the others. Another method is based on selection of a point on the curve of Pareto solutions which is closest to the ideal solution. For explanation of various methods the reader is referred to manuals on mathematical optimization, for instance Refs 18, 19 and 20.

MULTICRITERIA OPTIMIZATION OF CEMENT COMPOSITES

The application of the optimization approach to cement based composite materials requires selection of appropriate decisive functions and objective functions. Effective solutions of such problems are possible only when the relations between these functions may be presented in an analytical form. These relations should be based either on verified materials models or on experimental results, presented in the form of approximate functions.

The decisive functions (variables) and objective functions (criteria) may be presented in the form of a table (Table 1). Table 1 is shown here as a general indication how the problems may be formulated: what are the possible cri-

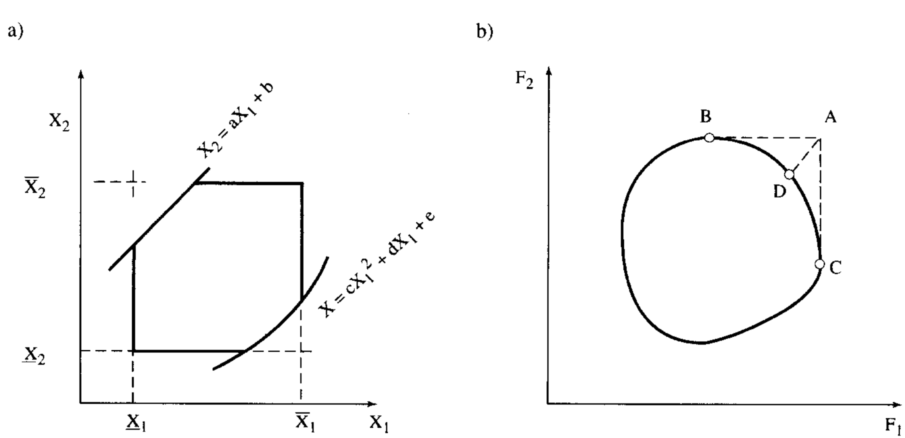

Fig. 1. Feasible regions (a) in variables space and (b) in objective functions space.

Table 1. Examples of criteria (objective functions) and design variables in optimization of concrete-like composites

Criteria Objective functions	*Design variables* — *Basic components*				*Dispersed reinforcement (fibres)*				*Admixtures*				*Other*
	Cement	*Water*	*Sand*	*Aggregate*	*Steel*	*Glass*	*Polymeric*	*Other*	*Plastic.*	*Air entr.*	*Polymers*	*Other*	
Strength compressive tensile elastic modulus other													
Energy tough. Index 15 tough. Index 10 impact fracture energy other													
Economy specific cost exec. cost energy other													
Other													

teria (objective functions) and variables (decisive functions). Their representation in Table 1 is not exhaustive — many others may be selected according to particular conditions of a problem under consideration, meaning the material to be designed. It is not possible to present all of them, and even this does not seem necessary; only a few criteria and variables are shown. It is possible also to imagine a three-dimensional set of optimization problems when different constraints would be considered as a third dimension of such a table. A few numerical examples of problems with one and two criteria have been published.[21] The problem with three criteria of optimisation is presented and solved below.

OPTIMIZATION OF THE REINFORCEMENT OF AN ELEMENT SUBJECTED TO TENSION

Let us consider a simple case of a composite element subjected to direct tension. The element is reinforced by parallel fibres (1D) and angle θ determines their direction (Fig. 2). A similar problem has been solved in previous papers[10,11] but only one criterion and one design variable were considered. Here two criteria describe mechanical properties of the composite materials: the first is related to the absorbed energy at the limit state and the second to the tensile strength. The third criterion concerns the cost of such an element.

There are two independent design variables: angle θ and volume fraction of fibre reinforcement β.

It is assumed that in the considered element only one form of fracture may appear under uniaxial tension and it is a crack perpendicular

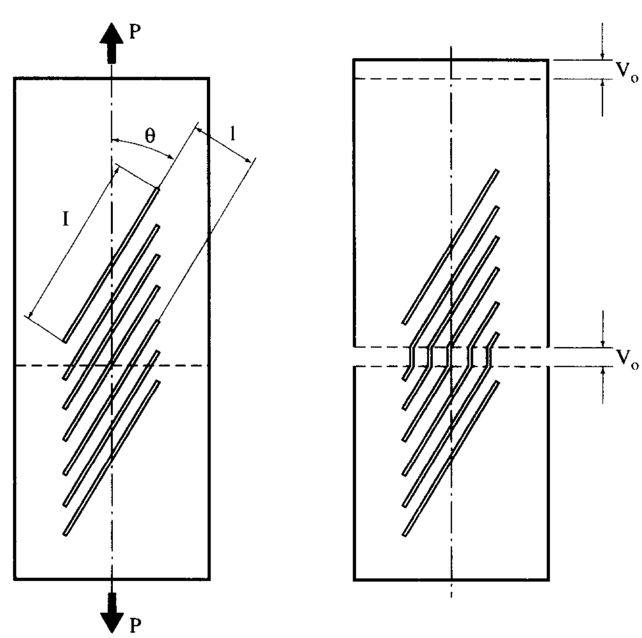

Fig. 2. Fibre reinforced (1D) concrete element subjected to axial tension before and after the crack opening, after Ref. 7.

to the load direction (Fig. 2). The limit state in which the energy is calculated is the crack width equal to v_o. Total energy is calculated as a sum of a few components, due to the following phenomena:

Debonding of matrix from the fibres which cross the crack.

Pulling of debonded out of the matrix, the fibre displacement is equal to the crack width.

Passing of the fibres across the crack.

Other possible behaviour for θ close to 90° is not considered here. Detailed description of the assumptions and derivation of proposed formulae is presented in previous papers.[10,11] Final relation for the total energy which is the optimisation criterion has the following form:

$$W(\theta,\beta)=\beta\left\{\frac{1}{2}\frac{1}{D}lv_e\tau_{max}\cos^2\theta+4\frac{1}{D}\tau\left[\frac{l}{4}(v_0-v_e)-\frac{1}{2}(v_0^2-v_e^2)\right]\cos^2\theta+v_0\tau_f\theta\cos\theta+\frac{4}{\pi}Df_m\left(\alpha\frac{f_f}{f_m}\right)^2\left(\cos^2\theta-\theta\frac{\cos^3\theta}{\sin\theta}\right)+\frac{4}{D}l\tau v_0\phi\sin\frac{\upsilon}{2}\cos\theta\right\}, \quad (5)$$

here the following symbols are used:

D and l — diameter and length of a single fibre,

v_e and v_0 — elastic and final displacements of a fibre,

τ_{max} and τ — maximum and mean values of bond stress beween matrix and fibre determined in a pull-out test,

τ_f — ultimate shearing stress in the fibres,

f_f and f_m — strength of fibres and matrix,

ϕ — friction coefficient between fibres and matrix,

α — numerical coefficient.

Another optimisation criterion is the ratio P(θ,β) of the tensile strength of the composite material to the strength of the plain matrix. This ratio is determined from experimental data published by Mindess *et al.*,[22] who considered also discontinuous fibres and the orientation angle y was taken the same for all fibres. The function P(θ,β) is obtained as approximation of the experimental data with the following polynomial:

$$P(\theta,\beta)=A_1+A_2\beta+A_3\theta+A_4\beta\theta, \quad (6)$$

here coefficients A_i, i = 1,..,4 are determined using the least squares method in programme MATHEMATICA and the following values have been found out:

$$A_1=1.51871, A_2=105.277, A_3=-0.619771,$$
$$A_4=-67.1418.$$

The obtained surface $P(\theta,\beta)$ is shown in Fig. 3.

The third optimisation criterion is assumed in the form:

$$K(\beta)=k_cV_c+k_fV_f+g(\beta)V_f, \quad (7)$$

there k_c, k_f, V_c and V_f are specific costs of the cement matrix and reinforcing fibres and their respective volumes. The function $g(\beta)$ determines increased cost of execution of the composite material due to the fibre reinforcement. The proposed form of function $g(\beta)$ is simple:

$$g(\beta)=b_1\beta^2+b_2\beta,$$

here b_1 and b_2 are constants, determined from technological conditions. Because the volumes of the matrix and of the fibres are

$$V_c=(1\text{-}\beta)V;\ V_f=\beta V$$

and finally eqn (7) takes form:

$$K(\beta)=K_1(\beta)V=[(1\text{-}\beta)k_c+k_f\beta+(b_1\beta^2\beta^2+b_2\beta)\beta]V \quad (8)$$

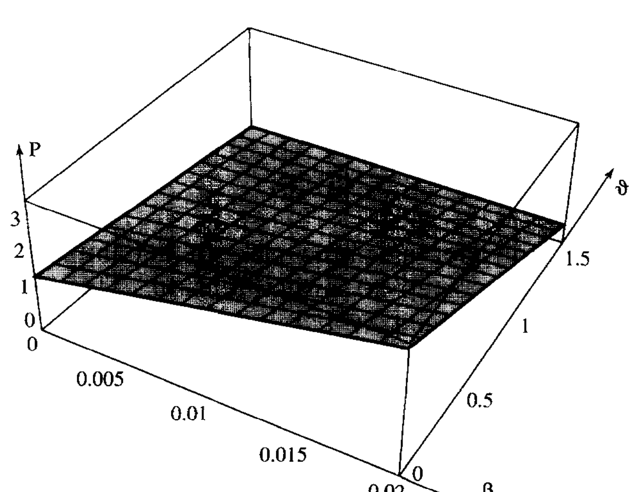

Fig. 3. Function P (θ, β) from equation (6).

The optimisation criteria are the following:

Maximum of the fracture energy absorbed at the limit state given by eqn (5).

Maximum of the ratio of composite to plain matrix tensile strength expressed by eqn (6).

Minimum of the total cost as given by eqn (8).

Design variables θ and β have the following limits:

$$0° \le \theta \le 90°,\ 0 \le \beta \le \bar{\beta}.$$

Value of the upper limit $\bar{\beta}$ may be deduced from the experience in mixing and casting the fresh concrete mix with dispersed fibres.

To solve the optimisation problem with three criteria, the ideal solution should be found out. Then, the Pareto compromise set should be determined and next the preferred solution.

The following numerical values are accepted as in papers Refs 10 and 22: $\tau_{max} = 1.8$ N mm^{-2},$\tau = 0.8$ N mm^{-2},$\tau_f = 105$ N mm^{-2}, $v_e = 0.002$ mm, $v_o = 1$ mm, $\phi = 0.3$, $\alpha = 0.15$, $f_f = 210$ N mm^{-2}, $f_m = 30$ N mm^{-2}, $l = 40$ mm, D = 0.6 mm.

Using eqns (5), (6) and (8) and programme EUREKA the following results have been obtained:

$$\max W(\theta,\beta) = Wo = 2.1038 \text{ for } \theta = 39°07'$$

$$\text{and } \beta = \beta = 0.02 \text{ (point B' in Fig.4)},$$

$$\max P(\theta,\beta) = Po = 3.6242 \text{ for } \theta = 0 \text{ and}$$

$$\beta = \beta = 0.02 \text{ (point C')}, \min K_1(\beta) = k_c$$

$$\text{for } \beta = 0.$$

To obtain the Pareto set of compromises the normalised non-dimensional functions are created:

$$F_1(\theta,\beta) = W(\theta,\beta)/W_o$$

$$F_2(\theta,\beta) = P(\theta,\beta)/P_o$$

$$F_3(\beta) = K_1(\beta)/K_o$$

and K_o is the maximum value of the function $K_1(\beta)$ in the compromise set. The numerical values for functions determining the cost are assumed after the additional calculations of the commercial prices in Poland:

$$k_c = 8.10^5;\ k_f = 64.10^5;\ b_1 = 4.10^{10};$$

$$b_2 = 6.10^8 [zl/m^3].$$

In the nondimentional space of objective functions the ideal point has coordinates (1.0; 1.0; 0.3049). The compromise set is a surface in the space F_1, F_2, F_3 developed on the curves which represent the set of solutions for two-criterial problems, shown in Figs 5–7. The points B, C and H determine maximum F_1, maximum F_2 and minimum F_3, respectively. The two-criterial compromise sets have been

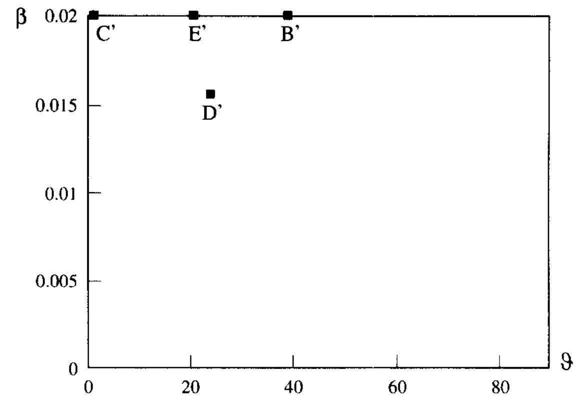

Fig. 4. Feasible region.

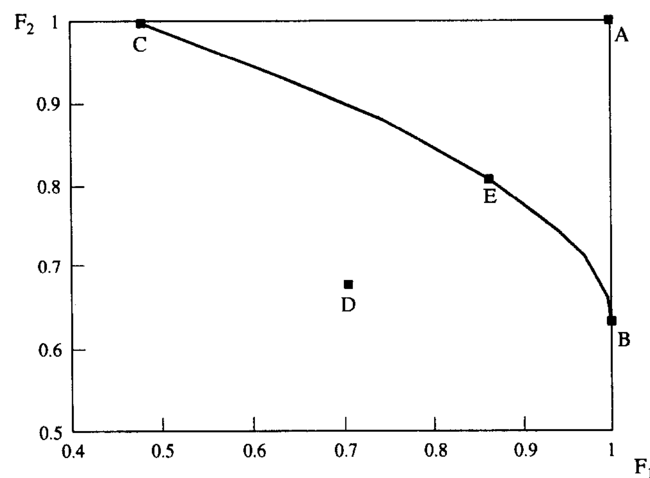

Fig. 5. Compromise set for functions F_1 and F_2.

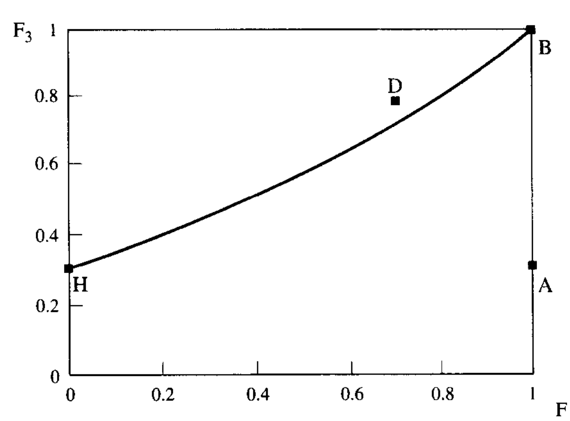

Fig. 6. Compromise set for functions F_1 and F_3.

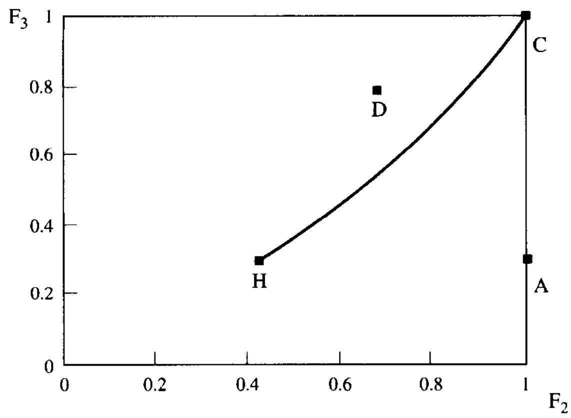

Fig. 7. Compromise set for functions F_2 and F_3.

determined using the method of weight coefficients (4), again using the programme EUREKA.

As the preferred solution the point of the compromise set which was closest to the ideal point was adopted. Its coordinates satisfied the condition of minimum of the following equation

$$\phi(\theta,\beta) = [F_1(\theta,\beta)-1]^2+[F_2(\theta,\beta)-1]^2 +[F_3(\beta)-0.3049]^2.$$

The coordinates of the preferred solution (point D) are: $F_1 = 0.7050$, $F_2 = 0.6762$, $F_3 = 0.7882$. In the space of the design variables the corresponding point D′ has following coordinates: $\theta = 24°\ 03'$ and $\beta = 0.0155$ (Fig. 4). Projections of the preferred point on the planes $F_1 = 0$, $F_2 = 0$, $F_3 = 0$ are shown in Figs 5–7.

In the considered problem the solution is a composite material reinforced with 1.55% of steel fibres inclined at the angle of 24°03′. When the cost is neglected and not included as optimization criterion, then two other mechanical criteria lead to the preferred solution with coordinates $F_1 = 0.8666$, $F_2 = 0.8070$, $F_3 = 0$ (point E in Fig. 5). Therefore, in the space design variables the solution is given at the point $\theta = 20°26'$ and $\beta = 0.02$ (point E′ in Fig. 4). It is obvious, that if the cost of fibres is neglected, then the optimum solution for two mechanical criteria is related to the maximum admissible reinforcement.

CONCLUSIONS

In the paper basic formulae for the application of methods and notions of optimization to design of concrete-like composites are presented. Next, a problem is formulated and solved to show how the formulae may be applied. Because of selecting angle ϑ as one of the independent variables, the problem concerns only composites with one-dimensional reinforcement. For other cases, two-dimensional and three-dimensional, this variable should not be used.

The principal difficulty in such problems is their correct formulation from which effective and useful solutions may be derived. Another difficulty in such problems is the determination of analytic relations between objective functions and variables. Such relations may be established from various test results available from publications or it is necessary to execute experimental research to collect appropriate data.

The last difficulty in these problems is effective solution of obtained equations.

Further development of optimization approach for cement based composites should be directed at various realistic objective functions and variables and at better expressions for objective functions. The generalization for random variables and considerable improvements of mechanical models assumed should be also introduced to the optimization approach.

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