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Application of Nonlinear Programming for Identification of Mathematical Models of Corrosive Destruction of Structures

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***Abstract*-- Considered the theorem on the belonging of optimal solutions one or more surfaces of the area permissible decisions. The results of investigations on the comparative evaluation of the identification of models of corrosive destruction with the help of analytical method and by random search method are presented.**

***Keywords*-- Comparative Evaluation, Identification, Mathematical Models of Corrosive Destruction, Method of Least Squares, Random Search Method.**

I. INTRODUCTION

Modern methods of calculation and design of chemical and petrochemical equipment require the use of mathematical models of corrosive destruction, allow to work off various options for the impact on the design of an aggressive environment, temperature, different load combinations, changing the properties of the material, etc. Analitical methods, used in computational practice for finding the extremum of optimized functions , for example, the method of least squares, are determine the extreme values of the control variables, regardless of the size of the area of permissible parameters. In the same case, if the area of permissible parameters has restrictions is limited, search of extreme control parameters is considerably complicated.

Existing mathematical models of corrosion destruction of structures interacting with aggressive media, as a rule, include a set of empirical coefficients whose values are determined by identifying the model to experimental data. On the region of existence of these factors usually are imposed restrictions: physical, geometrical, etc. It is possible that the extreme values of the coefficients belong to the boundary of permissible solutions. Let us investigate this issue in detail on the example of optimal designing of design.

II. THEOREM ON THE BELONGING OF OPTIMAL SOLUTIONS ONE OR MORE SURFACES OF THE AREA PERMISSIBLE DECISIONS

Consider the following theorem: *At the optimal designing of structures the extreme value of the objective function belongs of one or of more surfaces of restrictions of the region of permissible parameters*.

In the proof of the theorem, we'll refer to the manuscript work N.A. Alfutov and P.A. Zinovev "Some features of non-linear programming problems at the designing of structures of minimum weight", where the authors generalize the particular solutions given in [1], [7].

Let's formulate the problem of mathematical programming [3]:

minimize the function:

$$F(\mathbf{X}) = F(x_1, x_2, \ldots\ldots, x_n) \qquad (1)$$

at the performance of restrictions

$$g_j(x_1, x_2, \ldots., x_n) \leq, =, \geq b_j, \qquad (2)$$

where: $\mathbf{X} = (x_1, x_2, \ldots, x_n)$ − vector of control parameters. The problem (1) − (2) is a problem of nonlinear programming, if at least one of the functions $F(\mathbf{X}),\ g(\mathbf{X})$ is non-linear.

Let's imagine the optimized structure as a set of discrete elements and denote the linear dimensions of discrete elements, taken as independent variables in the problem of nonlinear programming through x_{ik}, where the subscript i denotes the number of the element, and k – the index of the linear dimension in the list of sizes, characterizing element i.

The objective function which expresses the weight or volume of the material of construction, consisting of discrete elements, in this case takes the following form:

$$F(\mathbf{X}) = \sum_i \prod_k c_i x_{ik}, (i = 1,2,\ldots,m; k = 1,2,3). \qquad (3)$$

Here: c_i – the constant coefficients.

$$x_{ik} \geq 0. \qquad (4)$$

Restrictions (4) have a geometric meaning and reduce the problem of mathematical programming towards the search of extremum function (1) which satisfy the restrictions (2), in a non-negative octant space E^n ($n = i \times k$)..

International Journal of Emerging Technology and Advanced Engineering
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Consider the problem of nonlinear mathematical programming with inequality constraints:

$$g_j(\mathbf{X}) \geq b_j, (j = 1,2,...,m) \qquad (5)$$

And let's investigate the function (2.3) in the extreme state. For this purpose, we use a generalization of the classical method of Lagrange multipliers in the case where the restrictions are given by inequalities. Transform the restrictions (5) in equalities. To do this, we introduce in the expression (5) auxiliary variables z_j. We get:

$$g_j(\mathbf{X}) - b_j - z_j^2 = 0; (j = 1,2,...,m). \qquad (6)$$

As a result the conditions (5) are tantamount to inequalities:

$$z_j^2 \geq 0; (j = 1,2,...,m). \qquad (7)$$

The problem is reduced to the determination of the global minimum of the function $F(\mathbf{X})$ in a non-negative octant E^{n+m}. We form the Lagrangian:

$$\Phi(\mathbf{X}, z, \lambda) = F(\mathbf{X}) + \sum_{j=1}^{m} \lambda_j (g_j - b_j - z_j^2) \qquad (8)$$

where λ_j – undetermined Lagrange multipliers. Equating partial derivatives on $\Phi(x, z, \lambda)$ of upon all the variables, we obtain the following equation:

$$\frac{\partial \Phi(\mathbf{X}, z, \lambda)}{\partial x_{ik}} = c_i x_{i,k-1} x_{i,k+1} + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j(\mathbf{X})}{\partial x_{ik}} = 0 , \qquad (9)$$

where: k = 1,2,3; k□−1 = 1,2 at k = 2,3; k−□1 = 3 at k = 1; k + 1 = 2.3 when k = 1,2; k + 1 = 1 when k = 3:

$$\frac{\partial \Phi(\mathbf{X}, z, \lambda)}{\partial z_j} = -2\lambda_j z_j = 0 ; \qquad (10)$$

$$\frac{\partial \Phi(\mathbf{X}, z, \lambda)}{\partial \lambda_j} = g_j(\mathbf{X}) - b_j - z_j^2 = 0 . \qquad (11)$$

Conditions (9) - (11) are performed in two cases. In the first of them all $z_j \neq 0, \lambda_j = 0$, which means that all the restrictions (6) are fulfilled as equations.

This case corresponds to the search for the minimum function $F(\mathbf{X})$ in a non-negative octant space E^m, at this the equality restrictions are not considered, since the system of equations (8) for $\lambda_j = 0$ has infinitely many solutions, belonging to a non-negative sites of coordinate axes of space E^n, which as a rule does not satisfy the restrictions (5) and (11). In the second case the system of equations (9) − (11) has a solution if at least part z_j is zero. In this case the relevant restrictions (5) are satisfied with the equality sign.

In the geometric sense this assertion means that the global minimum point of the function $F(\mathbf{X})$ *in the presence of restrictions determined by the inequalities, belongs at least to one of the surfaces of restrictions.*

This conclusion allows be recommended for finding of the extremum of nonlinear problems of mathematical programming the application of the zero-order methods that do not require the analysis of derivatives, for example, probabilistic methods.

Consider the example of the identification of one of the mathematical models of corrosion destruction. We formulate the task of identifying the mathematical model as a mathematical programming problem. As the object of the identification we take the logistic model of Verhulst (MMLV) [4].

$$\delta = \frac{\delta_0}{1 + \eta \cdot \exp(-\vartheta \delta_0 t)} , \qquad (12)$$

where $\delta_0, \eta, \vartheta$ –coefficients taking into account the effect of corrosive environment, □ δ – the current value of the depth of corrosion damage; δ_0 – upper limit of the depth of corrosion damage; *t* – time of corrosion.

Identification of the model is to determine the coefficients of the model $\delta_0, \eta, \vartheta$, which would provide the best approximation of calculated curve described by equation (12), to the experimental curve. We write the expression for the objective function as functional:

$$J = \sum_{j=1}^{n} \left[\delta_{ej} - \frac{\delta_0}{1 + \eta \cdot \exp(-\vartheta \delta_0 t_j)} \right]^2 . \qquad (13)$$

As the restrictions on the area of the changing of control variables, we take the condition of non-negativity of the coefficients of the model $\delta_0, \eta, \vartheta$:

EXPLORING RESEARCH AND INNOVATIONS

International Journal of Emerging Technology and Advanced Engineering

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$$\delta_0^- \le \delta_0 \le \delta_0^+;\ \ \eta^- \le \eta \le \eta^+;\ \ \vartheta^- \le \vartheta \le \vartheta^+, \tag{14}$$

where $\delta_0^-, \delta_0^+;\ \eta^-, \eta^+;\ \vartheta^-, \vartheta^+$ the lower and upper limits of the values of the coefficients δ_0, η and ϑ.

Introducing a vector of control variables $\mathbf{X} = (x_1, x_2, ..., x_n)$ and denoting them $x_1 = \delta_0,\ x_2 = \eta,\ x_3 = \vartheta$, we obtain the following mathematical programming problem:

Find the minimum of the functional

$$F(\mathbf{X}) = \min \sum_{j=1}^{n} \left[\delta_{эj} - \frac{x_1}{1 + x_2 \cdot \exp(-x_3 x_1 t_j)} \right]^2 \tag{15}$$

at the performance of restrictions:

$$\begin{gathered} g_1(\mathbf{X}) = x_1 - x_1^- \ge 0;\ \ g_2(\mathbf{X}) = x_1^+ - x_1 \ge 0; \\ g_3(\mathbf{X}) = x_2 - x_2^- \ge 0;\ \ g_4(\mathbf{X}) = x_2^+ - x_2 \ge 0; \\ g_5(\mathbf{X}) = x_3 - x_3^- \ge 0;\ \ g_6(\mathbf{X}) = x_3^+ - x_3 \ge 0 \end{gathered} \tag{16}$$

The formulated mathematical programming problem (15) − (16) was solved by random search SGEF [5]. Restrictions on the area permitted by decisions taken by the following: $0{,}01 \le \delta_0 \le 5$ mm; $1{,}0 \le \eta \le 1000{,}0; 0{,}01 \le \vartheta \le 10{,}0$. The results of solution are shown in Table 1.

Table 1
The results of the identification of the model MMLV of corrosive destruction by random search method

t_j (years)	δ_{ej} (mm)	δ_0 (mm)	η	ϑ (1/mm $\times$ year)	$\delta(t_j)$, mm	Δ, %
0,1643	0,10	2,141	514,0	4,054	0,0179	+82,10
0,5753	0,49				0,4770	+2,65
1,0219	1,95				1,9966	-2,39
1,4410	2,10				2,1369	-1,60
2,0191	2,08				2,1410	-0,02
3,2000	2,25				2,1410	+4,84

Following are comparative assessments model identification MMLV and of some other models of corrosive destruction by random search method and by one of the analytical methods − by the least squares method.

III. Comparative Assessments Of Identification Of Mathematical Models Of Corrosion Destruction By The Analytical Method And The Method Of Random Search

To mathematical modeling of corrosion destruction of designs in recent years devoted a large number of publications [4, 6, 7, 8-10, 11].

As rightly pointed out in one of them [9], the construction of a mathematical model is to create a "...the aggregate of equations describing the deformation and the fracture of structures taking into account the mass transfer equations, of chemical interaction, of corrosive destruction and so on,. of the identification of these equations, i. e. the assessment of values of coefficients on the results of experiments, decision of the aggregate of equations and researching the behavior of structures. "

Consider the definition of the coefficients of the mathematical model of corrosive destruction at the external parameter of damage.

For researching we take the next mathematical models:

IJETAE
EXPLORING RESEARCH AND INNOVATIONS

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 6, Issue 11, November 2016)

1) the fractional-linear model

$$\delta = \delta_0 t/(t+T); \qquad (17)$$

2) the exponential model

$$\delta = \delta_0 \left(1 - e^{-t/T}\right); \qquad (18)$$

3) mathematical model in the form of corrosive wear in view of logistical curve of Verhulst (MMLV):

$$\delta = \frac{\delta_0}{\left(1 + \eta e^{-\vartheta \delta_0 t}\right)} \qquad (19)$$

Here: δ_0 – the maximum depth of corrosion damage; T – parameter of time; η, ϑ – model coefficients (3); t – time. In these models (17) – (19) parameters δ_0, T, η, ϑ represent a sought coefficients.

To evaluate their in [4] is suggested by the method of least squares (LS) with the help of expression

$$J = \sum_{j=1}^{n} \left[\delta_{ej} - \delta(t_j)\right]^2, \qquad (20)$$

Where δ_{ej}, $\delta(t_j)$ – respectively experimental and calculated parameter of damage in time t.

Table 2
The results of the calculation of rates of corrosion deterioration models by least squares (LS)[4] and by the random search method (RS)

Model	J_{min}		δ_0 (mm)		t (years)		η		ϑ (1/mm year)	
	LS	RS	LS	RS	LS	RS	LS	RS	LS	RS
Fractional-linear	2,362	0,713	2,371	3,553	0,218	1,409	-	-	-	-
Exponential	1,287	0,617	2,239	2,519	0,520	1,080	-	-	-	-
Logistical	0,501	0,026	2,250	2,141	-	-	34,00	514,1	1,649	4,054

The coefficients of the model chosen, minimizing the expression (20), we determine, equating the partial derivatives from the functional J over the values of δ_0, T for models (17) and (18) and over the values of δ_0, η, ϑ for the model (19). The result is a system of equations for determining the unknown coefficients.

However, the apparent simplicity of such approach is deceptive . Firstly, this system of equations is time-consuming and is complicated in the decision, for example, for an exponential model (18), and especially for the logistical model MMLV (19). Secondly, the coefficients, which were have been found by minimization of functional (20) by the method of least squares, not always correspond to the physical conditions of the problem. So, for example, in calculating the coefficients of a fractional-linear model (17) (Table 2) this model preliminary leads to linear form [4]

$$y = t/\delta_0 + T/\delta_0. \qquad (21)$$

Here: $y = \frac{t}{\delta}$.

The functional (20) takes the form:

$$J = \sum_{j=1}^{n} \left(y_{ej} - x_j/\delta_0 - T/\delta_0\right)^2, \qquad (22)$$

where: $x_j = t_j$; $y_{ej} = t_j/\delta_{ej}$.

By minimizing the functional (22) over $\delta_0^{-1} = a$ and $T/\delta_0 = b$, we obtain the system of equations:

$$\begin{aligned} a\sum_{j=1}^{n} x_j^2 + b\sum_{j=1}^{n} x_j &= \sum_{j=1}^{n} x_j y_j \\ a\sum_{j=1}^{n} x_j + bn &= \sum_{j=1}^{n} y_j, \end{aligned} \qquad (23)$$

After decision of this system we find:

IJETAE
EXPLORING RESEARCH AND INNOVATIONS

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$$\delta_0 = \frac{\left(\sum_{j=1}^{n} x_j\right)^2 - n\sum_{j=1}^{n} x_j^2}{\left(\sum_{j=1}^{n} x_j\right)\left(\sum_{j=1}^{n} y_j\right) - n\sum_{j=1}^{n}\left(x_j y_j\right)};\ T = n^{-1}\left(\delta_0 \sum_{j=1}^{n} y_j - \sum_{j=1}^{n} x_j\right) \qquad (24)$$

Calculation by the experimental data (Table 2) at number of observations $n = 6$ gives such values of parameters: $\delta_0 = -357{,}653$ mm, $T = -383{,}528$ years, that not corresponds to the physical conditions of task. At the same time are known [4] the quite real results: $\delta_0 = 2{,}3713$ mm, $T = 0{,}218$ years (Table 2.1.). Obviously, these results have been received not across the entire spectrum of experimental data, but only by part of it. If for determination of the coefficients we take observations № 3, 4, 5 and 6 (Table 2), i.e. on the upper portion of the experimental curve (Fig.1), the model parameters $\delta_0 = 2{,}406$ mm, $T = 0{,}2471$ years are quite close to values adduced in [4].

A similar pattern occurs in the calculation of the coefficients for the exponential model (18). Parameters δ_0 and T are determined on the points only № 3-□6, but were extended to the whole range of observations. As a result, we get a big error on the initial stage of corrosive destruction, which reaches 506% for the exponential model (Table 4) and 920% for fractional-linear model (Table 3).

Table 3
The coefficients of fractional-linear model (RS method)

№ Obser-vations	t_j, years	δ_{ej}, mm	δ_0, mm	T, years	$\delta(t_j)$, mm	Error, % RS	Error, % LS
1	0,1643	0,10			0,371	-210,00	-920,00
2	0,5753	0,49			1,030	-110,20	-251,00
3	1,0219	1,95	3,553	1,409	1,494	+24,41	0,00
4	1,4410	2,10			1,796	+14,46	+1,90
5	2,0191	2,08			2,03	-0,61	-2,88
6	3,2000	2,25			2,467	-9,64	+1,33

Table 4
The coefficients of exponential model (RS method)

№ Obser-vations	t_j, years	δ_{ej}, mm	δ_0, mm	T, years	$\delta(t)$, mm	Error, % RS	Error, % LS
1	0,1643	0,10			0,355	-255,00	-506,00
2	0,5753	0,49			1,040	-112,30	-206,00
3	1,0219	1,95	2,519	1,08	1,541	+29,97	0,00
4	1,4410	2,10			1,856	+11,64	-0,20
5	2,0191	2,08			2,131	-2,43	-4,30
6	3,200	2,25			2,388	-6,17	+1,20

International Journal of Emerging Technology and Advanced Engineering
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Analysis of the results of calculation of coefficients of fractional-linear model throughout the spectrum of observations allows us to conclude the feasibility of imposing restrictions on the area of permissible parameters in order to avoid getting physically incorrect data. Introduction of restrictions casts doubt on the applicability of the method of least squares to determine the coefficients selected mathematical model. The solution is offered to perform by one of the numerical methods of nonlinear programming − by random search method (RS).

In this case, the problem of mathematical programming is formulated as follows: find a minimum of the functional

$$J=\sum_{j=1}^{n}\left[\delta_{ej}-\delta(t_j)\right]^2,(j=1,n) \quad (25)$$

at the performance of restrictions:

$$g_q=\left(x_i-x_i^-;x_i^+-x_i\right)\geq 0,(q=1,s). \quad (26)$$

Here: $\delta(t_j)$ – a function that takes the form (17) − (19); x_i − coefficients of mathematical models (17) − (19) δ_0, T, η, ϑ; x^-, x^+ − accordingly the lower and upper limits of the sought coefficients.

The solution of the task is performed by the method of random search SGEF described in [5].

Table 5
The coefficients of logistical model (RS method)

№	t_j, years	δ_{ej}, mm	δ_0, mm	η	ϑ 1/mm year	$\delta(t)$, mm	Error, % RS	Error, % LS
1	0,1643	0,10	2,141	514,07	4,054	0,0179	+82,10	-15,50
2	0,5753	0,49				0,4770	+2,65	+8,45
3	1,0219	1,95				1,9966	-2,39	+34,63
4	1,4410	2,10				2,1369	-1,60	+7,73
5	2,0191	2,08				2,1410	-2,93	-6,19
6	3,200	2,25				2,1410	+4,84	0,00

When calculating the coefficients of mathematical models (Tables 2−5) random search carried out under the following restrictions in the region permissible solutions:

$0{,}01\leq\delta_0\leq 5$ mm; $1{,}0\leq\eta\leq 1000{,}0$;

$$0{,}01\leq\vartheta\leq 100{,}0\,\frac{1}{mm\cdot year}.$$

Along with the coefficients of fractional-linear, exponential and models and MLKF model are defined error of calculated results compared with the experimental data. The low percentage of error calculated curves corresponding to the fractional-linear and exponential models [4], is explained because the method least squares operated only with the upper portion of experimental curve.

When taking into account all points of the experimental curve the method least squares does not provide the correct results. Application of the random search to the definition of the coefficients in the closed domain of permissible solutions leads to models whose graphs are shown below in the form of curves (Fig. 1−3). These curves are situated below the curves obtained earlier in [4], and more exactly describe the average-quadratic deviation of the calculated values from experimental. From the logistic curves constructed by least square and by the random search method the the last curve practically concurs with experimental curve. The error except the lowermost point does not exceed 5% (Table 5).

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 6, Issue 11, November 2016)

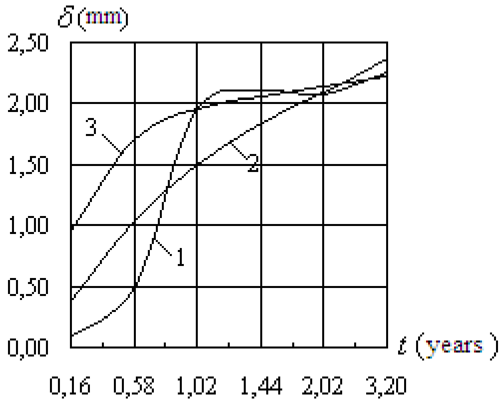

Fig.1. The graphs of fractional-linear model.

1 – experimental curve; 2 – calculated curve (method RS);
3 – calculated curve (method LS).

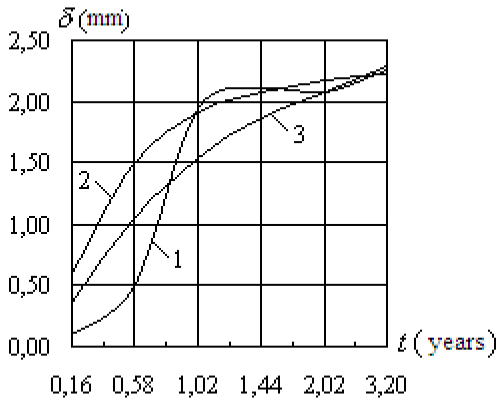

Fig.2. The graphs of exponential model.

1 – experimental curve; 2 – calculated curve (method RS);
3 – calculated curve (method LS).

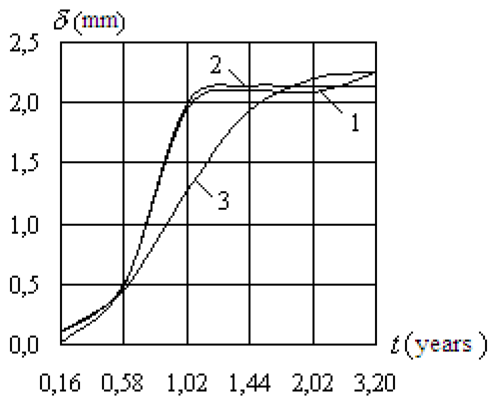

Fig.3. The graphs of logistical model (MMLV).

1 – experimental curve; 2 – calculated curve (method RS);
3 – calculated curve (method LS).

IJETAE
EXPLORING RESEARCH AND INNOVATIONS

International Journal of Emerging Technology and Advanced Engineering

Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 6, Issue 11, November 2016)

Thus, the random search method proposed for estimation coefficients of mathematical models of corrosion damage is invariant to the type of model and allows to avoid serious mathematical difficulties encountered when using of determinative search methods, and provides solutions that enough accurately describe the actual processes of corrosive wear.

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