COMPARATIVE ANALYSIS OF MODELS DSAT-16 AND MOTP_VTU TO CALCULATE THE PROPERTIES OF THE LAYER IN THE WELDING AREA

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Abstract: *The paper presents the characteristics of a modern software system for modeling and optimization of technological processes MOTP_VTU. It outlines the possibilities also to use the system at the design stage. A comparative analysis is performed of three characteristics to apply the new software system MOTP_VTU related to a similar existing one – DSAT-16. via similar systems it is possible to expand the basis of constructions and of functional materials in low technological level during exploration of the set of properties of these materials. This process of realization of scientific and technical ideas is a process to search via multi criteria support of decision making between the project task and the actual possibility, determined by the chemical composition and the processing-mode parameters.*

Keywords: DSS, MCDM, MODELING, OPTIMIZATION, TECHNOLOGICAL PROCESSES

1. Introduction

The realization of technical solutions via *Informatics Science & Materials Science* is among prioritized scientific elaborations marked by the absence or a limitation of the possibilities of constructive and functional materials and also by an insufficient technological level in the research of the set of properties of these materials. This process of realization of scientific and technical ideas is a process to search a reasonable compromise between the required in the project and the possible reality; it is proved by the rapid development of these two branches of science and the adjacent industries after the convergence of *Informatics Science & Materials Science*. In this regard, modeling and optimization may be treated as methods of knowledge from the real life, forming the so called information society linked to the intelligent core of rapidly developing technologies [Samarsky, A. A., A. P. Mikhailov] [1].

Modern computer systems allow to create (to collect) huge data arrays to solve problems of processing, analysis and optimization algorithms of data related to materials. In this regard, the improvement of similar approaches, methods and software tools are directly connected to the improvement of the explored technologies via the obtained technological solutions with specific benefits for the materials for aerospace engineering up to biomaterials that save lives

2. Aim and Specifics of the Proposed research

The present research is goal-oriented at a comparative analysis between the already present computational system DSAT-16 and the new one MOTP_VTU created in the University of Transport "T.. Kableshkov" [2] and on this basis to identify the possibilities provided to their users.

The stage of preparation of the numeric solution includes the elaboration of the algorithm and also of a software/system for the direct determination of the solutions. The solutions of models with increased numbers of parameters are always of a multivariate nature. The research of various numeric methods can significantly supplement the results from the analytical research; for lots of models this turns out to be the only realizable solution. The analysis of the numeric results and their usage are related to the adequacy of the models. The mathematical methods for testing/verification can determine if a model is built incorrectly and also they can determine the class of potentially robust models.

All this comprises elements of the system to support the decision making in the domain of analysis and multi criteria optimization of different selected indicators for control, and the optimization of quality parameters of metal-processing technologies.

A validated algorithm is applied. It is associated with the following two classes of problems:

- *Informative with a predefined threshold;*
- *Operative – analytical.*

The system (the software) allows work with a data base with full information for the decision maker about the analysis of the investigated multi parameter space and also the effective solutions for a series of quality indicators in this multidimensional research area. The data base itself is a set of tables that store the data grouped as rows and columns. Part of the data in the rows represent various combinations of the technological parameters that together with other data from the row determine the relation of this combination with the research quality parameters.

The main part for the final decision is quantitative information (as a level of detail and as a degree of reliability) formed at the stage of experimental testing and processing. There is a need to increase the accuracy of such calculations compared to already existing ones. They must provide a reasonable choice of alternatives at the initial stages of the design and the formulation of quantitative data of the criteria (mechanical properties or other indicators) for structural and parametric optimization.

3. The main idea of the proposed software in the field of metallurgy

At the design stage, the process of selection or synthesis of properties of compositions and processing materials gives the sense of the most important field of materials science. Solving problems regarding the relation "structure-properties" is always associated with resolving the contradictions that formulate the complex /set/ by certain characteristics. A good example in this regard is the production of alloys that overcome the contradiction between "strength and plasticity elongation". Deciding such contradiction, as an innovation in the field of steels there have been created TRIP-steels, which in addition to high strength, possess higher plasticity, e.g. more than 6-10% and also more than the ones compared to Mart-steels. The traditional strategy for development of alloys consists of producing numerous samples of varying composition, and variations of elements and mode of treatment for a particular alloy with optimal properties. This approach leads to high costs for experimentation.

That is why within the group of methods for directed search, the "trial and error" method is the least preferred and it stands lowest in the hierarchy of methods.

An alternative and effective approach is to use data from previous experience, processed up to a statistical model, based on a large amount of data related by composition, processing and properties.

The design of the alloy composition and the optimization of the technological-process parameters are directly related to the resolution of the compromise between the measured values related to certain selected indicators of the quality of a set of materials for a test group or a class [1].The most characteristic for these approaches is that they do not use the principles of metallurgy and metal physics. It is relied mainly only on an a priori information about the relation "composition and processing and their influence on the properties". Compared with physical models, the advantage of statistical models is their ability to explore a complex of properties and to obtain information in a timely and effective manner, even when there are no well-established physical theories and models. These approaches are created for ease of the DM. After determining the composition such that they meet the formulated requirements, an expert and experimental verifications carried out.

Metallurgical design is not only the design on a base with alloying elements by type, number and amount of the elements, but it includes taking into account also their synergistic effect. It is necessary to select such a synergistic effect by the combination of elements in which the more expensive elements must be in lesser amounts.

Along with the execution of this task, the metallurgical design must meet also the sought compromise between the properties of the product, depending on the processing parameters. These several groups of parameters should form the general parameters of the metallurgical design. The complexity of the so defined problem consists in the large number of input parameters, and the fact that the chemical composition is involved implicitly by the synergistic effect in the system "composition-structure-processing-properties-price". Multicriteria genetic algorithms (MCGA) have proven to be effectivein finding Pareto-optimal solutions of multicriteria optimization problems.

There are many MCGA capable of approximating Pareto - fronts with a set of points. One of the biggest difficulties in implementing MCGA to solve the described problem is the large amount of calculations of the computing functions of the criteria, because the order is several thousand. Reducing the number of these calculations is an important issue. Finding good approximation methods is particularly difficult due to the number of criteria and the possible interactions between them.The goal of this study is to propose an approach by which to determine optimal compositions corresponding to the precisely specified properties, a priori defined by the user, in accordance with the system "composition-structure-processing-properties-price."

The main goal of the research is to apply the approach to a specific task.

In this work a solution is proposed, based on the use of software model with applied techniques from the field of multi-criteria analysis and optimization, and the establishment of regressions between the mechanical properties of the alloy and its chemical composition based on neural models.[4]

4. Mathematical Model MOTP_VTU

General Characteristics of the Model

Data processing for an experiment begins with its formation into a table (matrix). The result from experiment "Y" we call output data (*data functions*). The values of "Y" depend on a series of other values "X" which we shall call input data (*factors*). These names are specified because the programs contain questions and guidelines for them. Every matrix is characterized by its number of rows and by its number of columns. It is accepted in the elaborated software that the number of factors cannot exceed 10 and that the output values cannot exceed 200, but there are no constraints like the ones for the number of factors. The matrix must be refined at messages for shortage of memory ("out of memory") for the problem to find the model coefficients.

For example, the case with 5 numbers "X" and 3 numbers "Y" needs the following form of matrix formulation: X_1, X_2, X_3, X_4, X_5, Y_1, Y_2, Y_3. We begin with the factors and we end with the outputs.

We remember the meaning of every "X" and "Y". The so formed matrix is used for a further processing and search of solutions**.**

Data Input

Data input is the next stage of processing the results from the experiment. The input must be performed in rows, starting from the first and ending with the last line. There will be questions about the number of the rows, the number of the factors and the number of the outputs. The sum of the number of the factors and the number of the outputs determines the number of the columns in the matrix.

Programming language BASIC used for the realization of the algorithms operates with numbers with seven significant digits but it allows use also numbers with sixteen significant digits (*double precision*). There will be a question about this detail. This is particularly important for processing huge matrices. In our case of limitations this means a matrix with big number of rows. Numbers with up to seven significant digits (*single precision*) require half of the memory. The data input may be aborted at any time followed by an exit from the program for data input. At the end of the input there is a possibility to correct the detected errors. The matrix obtained in this way is saved as a .DAT file with a specific name.

After the end of the input a primary analysis is provided. At this stage, for every column there will be determined the estimates of the mathematical mean, the variance, the minimal and maximal values. These estimates are also saved and they are used later.

Processing and Internal Links

The further processing of entries may continue to search for linear and non-linear relationships between them. It allows each column of the matrix to be presented as a function of another column in the form:

(1) $Y = A_1 + A_2.X$ to $Y = A_1 + A_2.X + A_3.X^2 + \ldots\ldots + A_{11}.X^{10}$

It is possible in this way to establish relations for every column, regardless of the "X" or "Y" with other columns and to draw respective conclusions for further processing.

To relieve the further work there have been elaborated two programs for interpolation: Newton interpolation with unequally spaced nodes, and Eitken interpolation with up to 6 nodes. They can be used to obtain mussing table values**.**

Forming a Mathematical Model

As it has been already said, the number of factors is limited to 10. For every specific case from 2 to 10 factors, there have been elaborated separate programs, because in the case with 2 factors in the mathematical model there are 6 coefficients, in the case with 3 factors they are already 10 coefficients and for 10 factors they are 66 coefficients.

For example for the case with 4 factors the mathematical model has the form:

(2) $Y = A_1 + A_2.X_1 + A_3.X_2 + A_4.X_3 + A_5.X_4 + A_6.X_1.X_2 + A_7.X_1.X_3 + A_8.X_1.X_4 + A_9.X_2.X_3 + A_{10}.X_2.X_4 + A_{11}.X_3.X_4 + A_{12}.X_1^2 + A_{13}.X_2^2 + A_{14}.X_3^2 + A_{15}.X4^2$.

This is the complete and best operating model of mathematical form. After finding the coefficients, the program shows the results from the statistical estimate of the model and the estimate for its ability to predict.

Digital Optimization

In the case with a positive assessment of the adequacy of the mathematical model to predict, there can be sought a desired extremum – min or max.

This problem is solved with 3 programs for digital optimization:

1. Method of Hook and Dzhivs – the configuration method (for up to 10 factors);
2. Method of Nelver and Mid – the deformable-polyhedron method (for up to 6 factors);
3. The method of golden section to find an extremum of functions of a single variable.

The extremum is sought calculating the function value without using derivatives. The optimization is performed within the factor constraints. It is possible to find the extremum with these 3 programs for each case determined by the number of factors. Within the organization of the calculations every program "calls" internally the model coefficients, then it "asks" for min and max factor values and other necessary values**.**

Taguchi Assessments

The calculation of Taguchi assessments starts with calculating matrix (27.*) where "*" is the number of rows of the input matrix. This is done by the first program of the two programs. The calculated matrix is saved in a file. Though that the effect from Taguchi estimates is manifested for greater number of factors, this program is designed for versions from 2 up to 10 factors. The second program calculates Taguchi estimates from the already calculated (27.*) matrix.

Entering the Coefficients of a Model and Calculation of the Model

In cases with multi criteria problems, it is necessary to calculate a function based on the results from the extremum of another problem. This program makes it possible to enter the coefficients of the mathematical model and the values to calculate with. The program is elaborated in the version from 2 to 10 factors.

Sorting in Ascending Order

It is possible to sort a set of values with this program. Sorting is performed in ascending order: after the sorting is over, then the first value is the smallest, and the last value is the greatest one.

5. Analysis of the results obtained via the two software systems for a concrete example in the domain of welding

This analysis was necessary after the originally formulated problem to find the extremum of obtained mathematical models from DSAT for HRC, the "carbon equivalent and cost" for weld metal. The obtained mathematical models are of second degree with interactions on four factors: X_1 – carbon, X_2 – silicon, X_3 – chromium, X_4 – tungsten. The mathematical models can predict.

When the results were obtained then it was decided that this problem must be solved again with new mathematical models and programs developed in the University of Transport (see pt.4). The statistical analysis of the models shows the following properties:

DSAT Model

HRC	Carbon Equivalent	Cost
R = 0,6635	R = 0,9990	R = 0,9298
F = 2,3032	F = 1456,21	F = 18,6973

MOTP_VTU *Model*

HRC	Carbon Equivalent	Cost
R = 0,7828	R = 1.0	R = 0,9213
F = 4,6327	F = 14,771 E+11	F = 18,6973

In the cases with mathematical models for carbon equivalent and cost, both programs give approximately the same result, because they are analytically calculated values and there is no randomness. The results from both models are very good: the coefficient of multiple correlation *R* is near to 1.

As noted, the mathematical models are able to predict, because the calculated value of Fisher criterion is greater than the value in the table for the case of *F* with (0,05, 14,41) = 1.9465.

This is not so for HRC. The VTU model has a greater coefficient of multiple correlation R = 0,7828 related to R = 0,6635 for the model DSAT. This difference is not small; it shows that the VTU model gives a better approximation to the experimental data.

The desired extrema of the mathematical models are: for HRC – maximum, for carbon equivalent and cost – minimum. The extrema are sought with the method of Hook and Dzhivs; in all cases the starting point is: $X_1 = 1$, $X_2 = 1$, $X_3 = 1$, $X_4 = 1$.

Results

HRC (max)

DSAT Models	*MOTP_VTU Models*
Ye = 11338,05	Ye = 11638,74
X_1 = 3,5	X_1 = 2,0
X_2 = 4,0	X_2 = 4,0
X_3 = 0	X_3 = 6,15
X_4 = 8,1	X_4 = 9,5

The MOTP_VTU model gives a little bit greater value for the obtained extremum.

Carbon equivalent (min)

DSAT Models	*MOTP_VTU Models*
Ye = 3,59	Ye = 8,00
X_1 = 8,00	X_1 = 0,00
X_2 = 0,00	X_2 = 0,00
X_3 = 0,00	X_3 = 0,00
X_4 = 0,00	X_4 = 8,00

In this case, the model DSAT gives a smaller value.

Cost (min)

DSAt Models	*MOTP_VTU Models*
Ye = - 42434,89	Ye = 5,71
X_1 = 8,00	X_1 = 0,08
X_2 = 4,00	X_2 = 1,83
X_3 = 30,00	X_3 = 0,00
X_4 = 9,50	X_4 = 3,31

In this case, DSAT gives as an extremum a negative number which is unacceptable as value whilst MOTP_VTU gives an acceptable value.

The second problem was to formulate HRC, the carbon equivalent and the cost as one-dimensional functions of the given X_1, X_2, X_3, X_4. This was achieved building mathematical models from 2^{nd} to 10^{th} degrees. Then a statistical analysis was performed and the best choice was related to *R*, the coefficient multiple correlation [3].

- Model HRC – the best performance is with variable X3 with a polynomial of 8^{th} degree, R = 0,8406.
- The carbon equivalent model – the best performance is with a variable X1 with a polynomial of 4^{th} degree, R = 0,9847.
- The cost model – the best performance is with a variable X4 with a polynomial of 9^{h} degree, R = 0,8606

The obtained results show that HRC, the carbon equivalent and the cost of weld metal may be represented as single-factor models; in them the better models are in the beginning, taking into account the simultaneous influence of 4 factors.

6. Conclusion

The realization of specific technical solutions with modern tools expands the possibilities at the design stage.

This was demonstrated by the comparative analysis of three characteristics during the application of the new software system MOTP_VTU.

It is possible to expand the basis of constructs and the functional materials for a low technological level of research for the set of properties of these materials**.**

This process of realization of scientific and technical ideas is a process to search a reasonable compromise between the design goal and the possible reality.

Reference

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