GENERALIZED ALGORITHM FOR NUMERICAL ANALYSIS AND MULTICRITERIA OPTIMIZATION OF MULTIPARAMETRIC REGRESSION MODELS

ОБОБЩЕН АЛГОРИТЪМ ЗА ЧИСЛЕН АНАЛИЗ И МНОГОКРИТЕРИАЛНА ОПТИМИЗАЦИЯ НА МНОГО ПАРАМЕТРИЧНИ РЕГРЕСИОННИ МОДЕЛИ

Antonia Toncheva, David Stoilkovski, Nikolay Tontchev
Todor Kableshkov University of Transport, 1574 Sofia, 158, "Geo Milev", BULGARIA tontchev@vtu.bg

Abstract: *An algorithm for numerical analysis of multi-parametric regression models is introduced. It is intended for software realization mainly to offer an user-friendly environment for analysis, appropriate to/related to future multi-criteria optimization. The analysis is performed via visualizing various fragments from the domain supported by different tools and editors. The definition of the algorithm is followed by a test sample for analysis in the distribution of hardness of ion nitriding instrumentation, class heat resistant steel.*

KEYWORDS: MODELING, OPTIMIZATION, MCDM, ION NITRIDIG, INSTRUMENTATION STEELS

1. Staging and Purpose of the Task

The design of various equipment and processes requires research and analysis of different quality indicators depending generally on a significant number of parameters [1]. The representation and the analysis of multi-parametric functions is limited for wider use by the existing software on the market [2]. The decision maker (DM) is significantly hampered by the existing products if he/she wishes to analyze a multi-parametric model.

The purpose of the present research is to present an algorithm for analysis of multi-parametric regression models that must be realized in the specialized software MCDA'10 and also to make a test sample to check the operation of the algorithm. The idea of the algorithm is to create a way to represent multi-parametric models as a possibility for an “ad hoc” procedure for decision making. The final goal of the presented research is to reduce the feasible set to reach compromise solutions in various criteria [3]. Since the experimental approach does not use information about the mechanism of the ongoing events, so the idea about a system like MCDA'10 proves [to be] very universal. It is possible to apply the same method for processing experimentally obtained values to many various by their nature processes: chemical, metallurgical, ecological, biotechnological, etc.

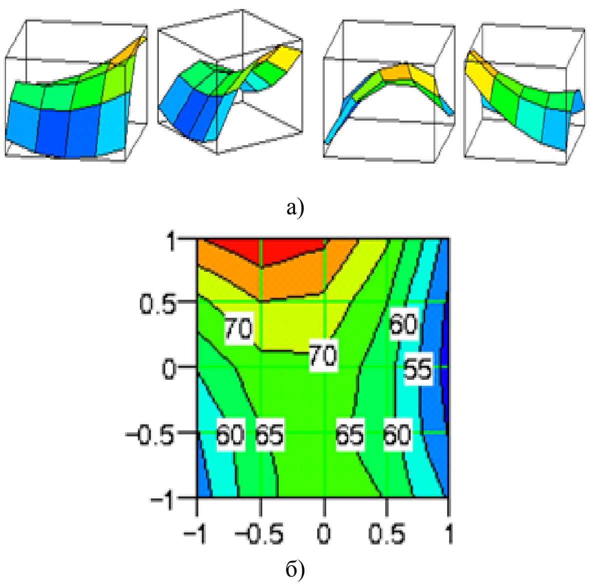


Fig.1. *Ways to visualize the same response surface: a) via space images from different views; b) via a contour diagram with equal-level lines*

During the research of innovative technological processes or processes of dedicated designation, the software makes it possible in the early calculations to code the limits of changes of separate parameters by the concerned researcher to protect the secret of effective solutions.

The specialized calculation software (MATLAB, MCAD, EXCEL, etc.) offers possibilities to visualize the research quantity for analysis of two parametric factors; their changes are located along the ordinate axis and the values of both factors change in the plane of the base. An example of such presentation of the same response surface from different views is made with MCAD; they are presented in Fig.1a. It is possible to obtain from such presentation just a qualitative information; it is not possible exactly to define the address of the input parameters in which the explored quantity obtains a specific value in the research interval.

It is possible to be more useful to the DM the image from the contour diagram during the analysis of the respective response surface with equilevel lines (Fig.1.b); now the value of the research quantity is coded by a certain color in a defined interval. The disadvantage of the specialized software in this case is in the precise fixing of the bounds of the research quantity; thus it is impossible to analyze parts of the diagram for new specific arrangements of the values of the research quantity; also it is impossible to define strictly the address (the combination) of the controlling factors for these values.

One can point out as an another disadvantage of the specialized calculation software the hardness to visualize models with more than two parameters via combinations from 2D contour diagrams for a suitable space arrangement using global and local separations of the variables.

For example the DM orientates himself/herself for the selected discretization on four parameters (X1, X2, X3 and X4) and a single research quantity with nodes [-1, -0.5, 0, 0.5, 1] examining 25 contour diagrams varying globally with X1 and X2 in the defined nodes.

The resulting graphics with the specialized software are built not coordinated relative to one another and therefore the graphics are not normalized to each other. This makes not possible using them for the analysis of decision maker.

2. Tools and Editors in the Execution of the Algorithm

Magnifiers are a basic tool in the intended for development software. They are directed at exactly defined compass parameters. They enclose the endmost (and all) addresses of the variables. Certain definite initial values of the input parameters of the model are fixed hitting a key or [directly] clicking with the mouse. Magnifiers differ by size. They are gradually directed covering the final position of the cooler in a certain way value of the explored quantity.

The research quantity has two values: normed and the real one. The normed value changes in the range of [0-100%]. It is the basic one in the analysis. Using the percentage editor these values are colored in a suitable color depending on their size. The possible coloring interval are six.

The compass determines the range and the step of the research in the domain. The first iterations may be executed via templates by default. These iterations direct the analysis in a certain direction that can be refined afterwards with the step-by-step editor. The step-by-step editor can set uniform or varying steps of discretization during visualization of the explored quantity. When determining the search direction of satisfactory values of the explored quantity, during the analysis it is possible to fix two or four parameters; the rest of them may be explored more in detail. In such cases the explored interval may include more calculation nodes with a constant or varying step.

The template for the first analysis of all up to ten parameters in the range [-1, +] is with a step of 0.5. In analyses of models with up to four parameters in the interval [-1, +1] the template may be set for analysis with a step of 0.25.

Fig.2 presents a graphical interpretation of the parametrical changes in the magnifier movement till its final state.

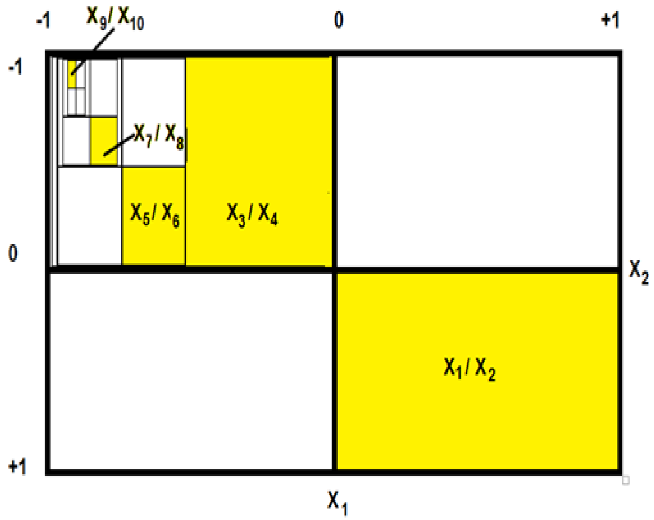


Fig.2. *Ways to display the location of the basic input parameters in analysis with discretization of ten factors in two nodes of change*

The function of the algorithm provides the usage of the following editors during the work with the software:

- Input-Data Editor. The data necessary to realize the analysis and the optimization are input with this editor. The input data are the regression coefficients of the model and the maximal and minimal values for each of the models. The definition of a multi-criteria optimization problem includes the definition of the requirements for various criteria tending to maximum, minimum or in a predefined interval. Besides the editor, the software will provide the input of the required information also from a file.

- Step-by-step editor. This editor makes it possible to define the step of discretization for all explored parameters. Also this editor allows the fixation of certain parameters in the analysis of the model. So the whole domain is digitized with a steady or varying step.

- Percentage editor. This is the basic editor for analysis during ratings of the research value quantities and also for localizing the compromise solution of the defined multicriteria problem. The interval [0, 100%] or parts of it in constantly limited iterations are colored with this editor under freely shifting restrictions with definite colors. The number of the colors may vary from 1 up to 6.

- Editor to set real values. Used to set the minimal and the maximal real values of all factors in the cases when calculations are performed in coded units.

- Editor for analysis at the same base. Used to allow changes of the extreme values in an analysis that is performed for at least two models.

3. *Description of the Algorithm*

The proposed numerical approach is designed to solve single-criteria and multi-criteria problems with many parametric variables. It is applied after derived regression models and for defined extreme (maximal and minimal) values for them. The algorithm is designed to create software to automate calculations to enhance the definition of effective solutions for formulated multi-criteria problems. First a discretization is determined of the variables with a certain step. The algorithm can construct a generalized function from the normed values of several criteria. So it is possible to determine the values of the control factors and their respective values of the individual goal parameters. For the implementation of the multi-criteria optimization the analysis of the research quantity is made in a normed form according to formula –

$$Ns = \frac{100*(x-a)}{b-a}$$

Where:

Ns - Normed value of the research quantity;
x - Real value of the research quantity;
a - Minimal value of the research quantity;
b - Maximal value of the research quantity;

So it is possible in the future to fulfill requirements for the criteria matching mini-max, average arithmetic or geometric average effective points.

The proposal to the user (DM) to work not in the criteria plane but in the variables' plane instead and the use of various up to five-six color delimiting intervals proves to be rather untraditional. These two prerequisites, however, are capable to realize some very useful analysis for various processes.

4. *Test Example from the Field of Material Science.*

The approbated approach is realized at the methodical level.

The purpose of the cited authors' works is to cover the following problem :

- Creation of nonlinear analytical models for control of the properties of steels, depending on the ion nitriding treated condition. For this purpose there has been developed a procedure and software for analysis of the research parameters.

The research methodology includes the following stages:

1. Conducting planned experimental research with the chosen object for exploration aiming at establishing the relationship between the input and output parameters.
2. The research may be directed at a priori preparative unplanned sufficient in number data about the research object.
3. Regression models are output and a test for the model adequacy is performed.

The object of this study – the chemical composition of tested steels – is shown in the table.

4. An experimental check for the adequacy of the models is also performed with exceptional and different from the plan of the experiment investigations.
5. Each model defines a relevant respective criterion of the multicriteria problem. Various multicriteria problems are defined that must be solved from which there are defined the values of all combinations of input parameters which in turn suggest a priori requirements of the output parameters related to maximal and minimal values or of values in a defined interval.

Below is described an example of a study of microhardness of ion nitriding heat–resistant alloys of the same class.

The object of this study with the specific chemical composition and mechanical propretes of the tested steels is shown in the table 1 and table 2.

The data from the experimental plan are taken from the thesis of Zyumbilev, A. (1992), Effect of low temperature plasma nitriding on the properties of tool steels for hot working.

In order to ensure the management of the object, there must be control parameters (degrees of freedom) that are being modified independently from each other. Table 3 indicated the range of variation of the ruling parameters for the mode of thermal and chemicothermal processing. With the variation of the technological factors on the process a planned experiment is run which resulted in the output models checked for adequacy. Zyumbilev's dissertation has defined the relationship between the goal parameters and the technological factors of the modes for processing.

Based on bibliography data and preliminary experiments, the following input (control) factors are defined in Zyumbilev A. (1992): the nitriding temperature, the pressure, the duration of the process, and the temperature of tempering. The following requirements are satisfied during the selection of these factors: independence from each other, compatibility between them and the ability to drive them.

To determine the nitriding modes there have been used mathematical and statistical methods of the planned experiment. A characteristic of this approach is that a compulsory change of input factors is performed within certain limits. Minimum number of trials and simultaneous adjusting of all factors is used. The main problem is reduced to determining the mathematical form of the research, which can be expressed in the given process.

Based on the influence of various factors on the nitriding and the objectives pursued, the following parameters were selected for optimization (matching factors): maximal micro-hardness of the layer HV, relative degree of wear Kv and toughness of destruction K1c (Kq).

Selected in this way, the factors and intervals are used to design experiments also on the basis of a plan of the various combinations of processing-mode parameters with which the experiments were conducted. In order to reduce the errors it is recommended that every attempt is done twice and the combinations of zero-level factors five times. All samples were ion nitrided in an installation of type ION-20. The impregnation gas during nitriding in glow discharge was gaseous ammonia. After nitriding the samples were cooled in air

Table 1. *Chemical composition of steel from the class of scope, [%]* (GOST, Tool steel, 2010)

Steel	**C**	**Si**	**Mn**	**Cr**	**Mo**	**W**	**V**
4H5MFS	0.32 - 0.4	0.9 - 1.2	0.2 - 0.5	4.5 - 5.5	1.2 - 1.5	–	0.3 - 0.5
3H3M3F	0.27 - 0.34	0.1 - 0.4	0.2 - 0.5	2.8 - 3.5	2.5 - 3.0	–	0.4 - 0.6
3H2V8F	0.3 - 0.4	0.15 - 0.4	0.15 - 0.4	2.2 - 2.7	Up to 0.5	7.5- 8.5	0.2 - 0.5

Table 2. *Characteristics of the steels in scope* (GOST, 2007-2013)

Steel	**Yield strength** **Rm**, [MPa]	**Tensile strength Re,**[MPa]	**Elongation,** **A**[%]	**Reduction of area Z** , [%]	**Impact strength** **KCU**, [kJ/m^2]
4H5MFS	1750	1480	–	–	570
3H3M3F	1670	1470	–	50	220
3H2V8F	1530	1390	12	36	200

Table 3 Variation range of the input parameters

Factors	**T_{nit}** [°C]	**P** [Pa]	**τ** [h]	**T_{tem}** [°C]
Levels X	X_1	X_2	X_3	X_4
Zero level (0)	530	300	7	650
Interval of variation	20	150	3	50
Upper level (+I)	550	450	10	700
Lower level (-I)	510	150	4	600

Table 4. Connection between input outputs parameters

N o	X_1	X_2	X_3	X_4	4Х5МФС	3Х3М3Ф	3Х2В8Ф
					$HV_{0,1}$	$HV_{0,1}$	$HV_{0,1}$
					MPa	MPa	MPa
1	- 1	- 1	- 1	- 1	10970	11140	11310

2	+1	-1	-1	-1	10800	10800	11310
3	-1	+1	-1	-1	10200	10970	12060
4	+1	+1	-1	-1	12060	11860	11080
5	-1	-1	+1	-1	11490	11490	12660
6	+1	-1	+1	-1	12250	11300	11680
7	-1	+1	+1	-1	10170	12060	11680
8	+1	+1	+1	-1	11490	11300	10970
9	-1	-1	-1	+1	9980	10970	10480
10	+1	-1	-1	+1	10480	10480	10170
11	-1	+1	-1'	+1	10170	11000	10640
12	+1	+1	-1	+1	11310	10640	11000
13	-1	-1	+1	+1	11240	11000	10000
14	+1	-1	+1	+1	10970	10480	10970
15	-1	+1	+1	+1	10170	10320	9320
16	+1	+1	+1	+1	10500	10480	10480
17	+1,414	0	0	0	12060	11680	11310
18	-1,414	0	0	0	11680	11000	11140
19	0	+1,414	0	0	10970	10640	10970
20	0	-1,414	0	0	10480	12060	10640
21	0	0	+1,414	0	11490	11310	10170
22	0	0	-1,414	0	11680	10640	11680
23	0	0	0	+1,414	12060	11140	11000
24	0	0	0	-1,414	11310	10970	10640
25	0	0	0	0	11680	11860	11410
26	0	0	0	0	11000	11680	11140
27	0	0	0	0	11490	11860	11310
28	0	0	0	0	12060	11680	11310
29	0	0	0	0	11490	11680	11410
30	0	0	0	0	11680	11860	11410

The levels of the input parameters of the research are shown in the tab. 5.

Table 5. *Variation range of the input parameters*

Factors	$\mathbf{T_{nit}}$ [°C]	**P** [Pa]	**τ** [h]	$\mathbf{T_{tem}}$ [°C]
Levels X	X_1	X_2	X_3	X_4
Zero level (0)	530	300	7	650
Interval of variation	20	150	3	50
Upper level (+I)	550	450	10	700
Lower level (-I)	510	150	4	600

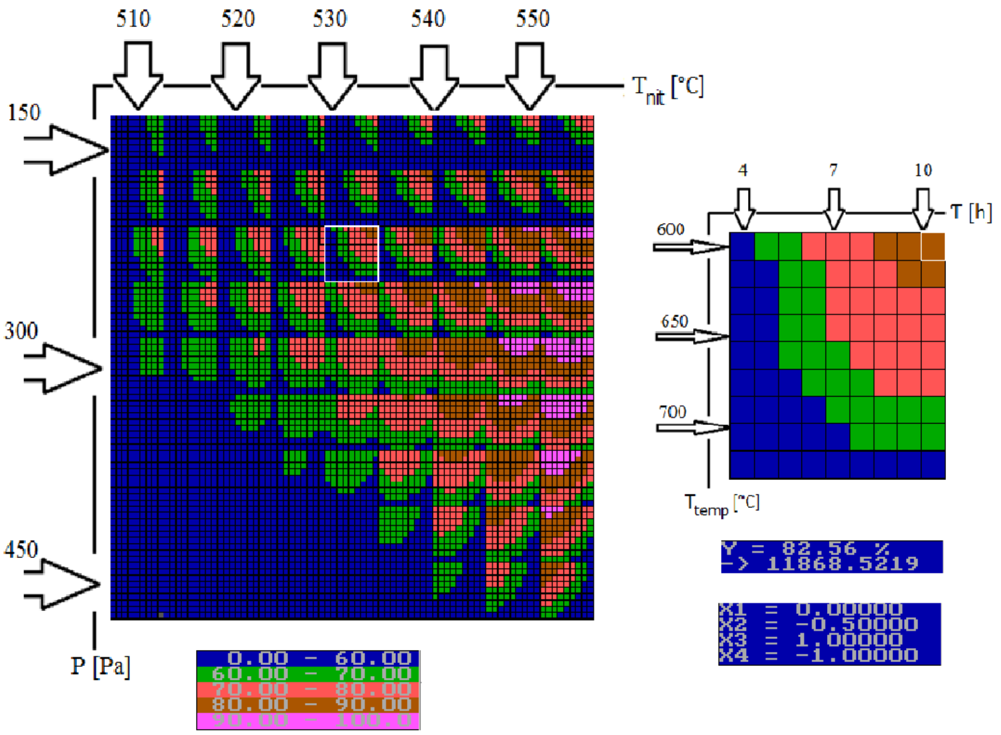
The output parameter is of the explored steels and the multi-criteria problem which we set ourselves to solve is the definition of the input parameters for which the whole class of steels has a relative maximal hardness.

The regression models are micro-hardness as it follows:

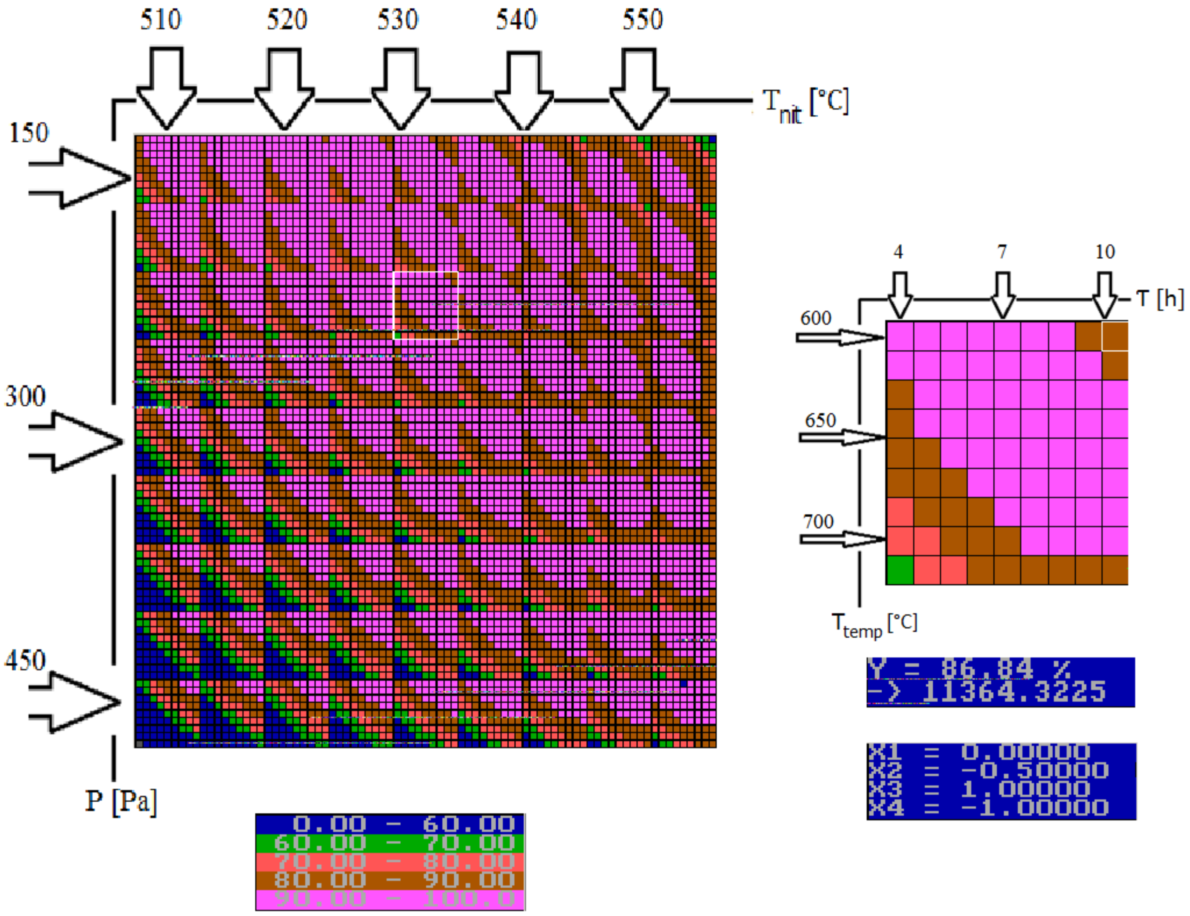
parameters	$\mathbf{H_{\mu V}}$ $\mathbf{(HV_{0,1})}$ **for steel**		
	4H5MFS	3H3M3F	3H2V8F
Free	11675.26	11813.49	11232.81
x_1	300.3842	462.604	-12.78176

x_2	-70.86131	-546.9271	-44.17166
x_3	102.0732	570.9035	-121.2643
x_4	-177.4857	-760.527	-459.0758
$x_1.x_2$	239.375	710.625	9.375
$x_1.x_3$	-74.375	-681.875	85.625
$x_1.x_4$	-129.375	568.125	303.125
$x_2.x_3$	-320.625	544.375	-273.125
$x_2.x_4$	66.875	-740.625	61.875
$x_3.x_4$	-26.875	481.875	-171.875
x_1^2	15.95109	-269.4298	70.23389
x_2^2	-556.7208	-264.4267	-139.8285
x_3^2	-126.592	-451.9834	-79.80983
x_4^2	-76.57547	-411.9729	-132.3259
R^2 =	0.85549	0.819219	0.8211649
Fcalc > Ftabl	2.92458 > 2.4244	2.18637 > 2.4244	2.2183 > 2.4244

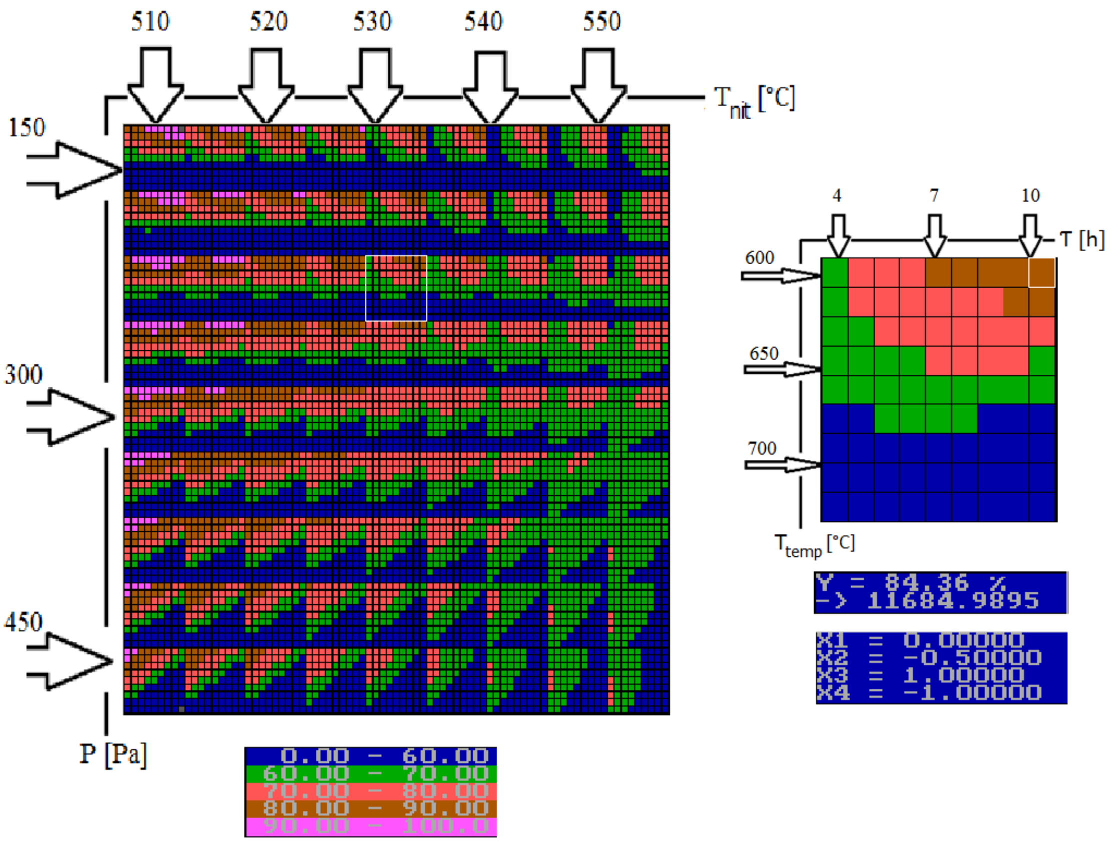
It is possible to make analysis via the graphical interpretation of the results. This analysis determines the influence of the input parameters for the explored steels 4H5MFS, 3H3M3F, 3H2V8F. The percentage interval of the explored micro-hardness parameter is colored in the relevant due way along the chosen scale /right below in the image/.



a)



b)

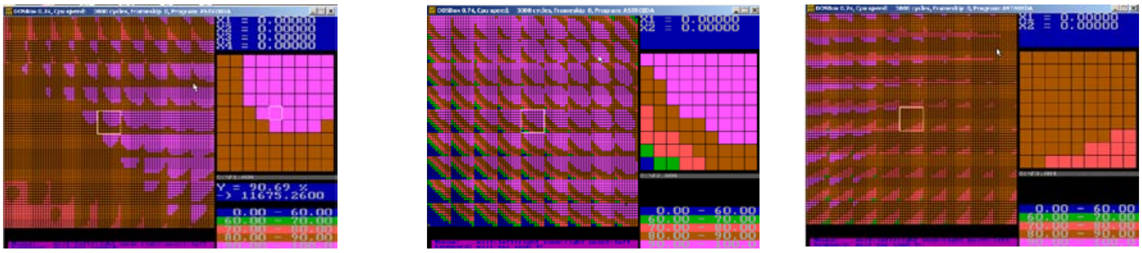


c)

Fig. 3. *Distribution of microhardness in the test domain of input parameters - a) - 4H5MFS, b) - 3H3M3F, c) - 3H2V8F.*

In the presented in Fig.3 images the parameters change horizontally or vertically as it follows: in the horizontal direction and globally X_1, locally X_3; in the vertical direction and globally X_2, locally X_4.

It is possible to determine a common basis comparing minima and maxima of the three models so that the images from Fig.3 change in the way shown in Fig.4.



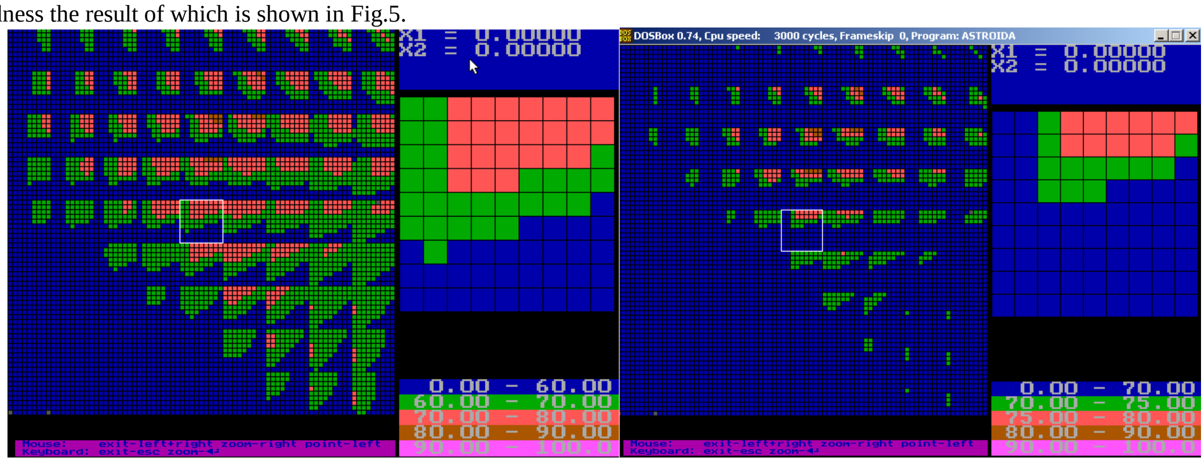
a) b) c)

Fig. 4. *Distribution of microhardness against common basis, in the test domain of input parameters - a) - 4H5MFS, b) - 3H3M3F, at) - 3H2V8F.*

From the analysis of FIG. 2 one can draw the following conclusions:

1. The widest range of variation in hardness in the test domain of input parameters occurs in steel 4H5MFS and 3H3M3F;
2. The most sustainable is the behavior of the hardness of steel 4H5MFS in the research domain of the input parameters. There is a coincidence of the maximal values of microhardness in the same modes of the input parameters for steels 4H5MFS and 3H3M3F
3. There is a sustainable change of hardness of steel 3H2V8F in the research domain of the input parameters but there are no signs for coincidence of the maximal values of microhardness in the same modes for the input parameters of steels 4H5MFS and 3H3M3F.

After this analysis the next task is define the input parameters for which the whole class of the three steels possesses the maximal hardness the result of which is shown in Fig.5.



a) b)

Fig. 5. *Distribution of simultaneous high values of micro-hardness of steel**s** from the whole class in the test domain of input parameters - a) - iteration starting coloration from 60% b) - iteration beginning coloring from 70%.*

From the analysis of Fig.5 it is clear that the processing mode for the maximal values of all three steels is concentrated in the “brown” interval of 80 – 90%. This may be visualized via defining the percentage editor of values shown in Fig.4 where the final decisions are shown, too.

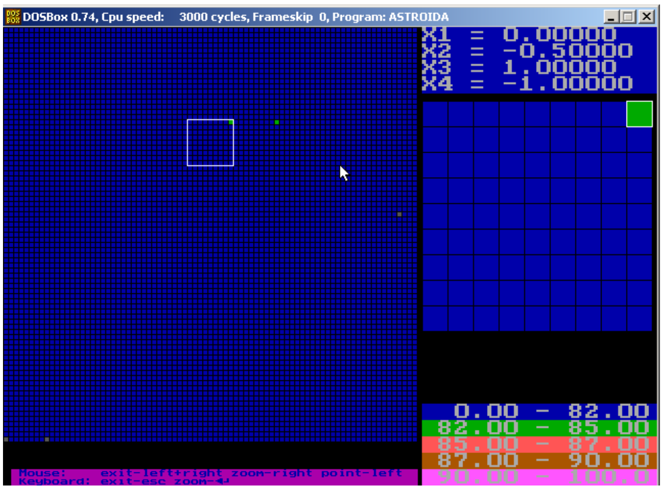


Fig. 6. *Location of the decision of simultaneous high values of micro-hardness of steel**s** from the whole class in the test domain of input parameters.*

The relatively maximal values of hardness for the investigated class of steels for the chosen processing is with the mode of X_1 = 0.0, X_2 =-0.5, X_3 =1.0, X_4 = - 1.0.

4. Conclusion.

This research is an algorithm for numerical analysis of multi-parametric regression models is introduced. It is intended for software realization mainly to offer user-friendly environment for analysis, appropriate to/related to future multi-criteria optimization. The analysis is performed via visualizing various fragments from the domain supported by different tools and editors. The definition of the algorithm is followed by a test sample for analysis in the distribution of hardness of ion nitriding instrumentation, class heat resistant steels. This design concept was tested using experimental data. Thus it was shown that the approach has the potential to identify new technological parameters with significantly improved defined properties.

ACKNOWLEDGEMENT: This work was partially supported by the Bulgarian National Science Fund – H 07/29.

References:

1. Tontchev N., (2014) Materials Science, Effective solutions and Technological variants, LAMBERT Academic Publishing, 142 p.

2. Tontchev N., Z. Cekerevac, (2014): Approach and Application in Multicriteria Decision Support in the Field of Materials Science. MEST Journal, (MEST) 2, no. 118-29.

3. Tontchev N., (2012): Effective solutions to the processing of metallic materials on iron bases, Publishing house of University of Transport “Todor Kableshkov”, Sofia, (in Bulgarian).

4. Tontchev N., L. Kirilov, (2007): Two Approaches for Solving Multiple Criteria Decision Making MCDM Problems with an Illustrative Example. Problems of Engineering, Cybernetics and Robotics, 58, 53-63.