

# MODELING PROPERTIES BASED ON THE CHEMICAL COMPOSITION IN MAGNESIUM ALLOYS

Nikolay Tonchev<sup>1</sup> Hai Hao<sup>2</sup> Emil Yankov<sup>3</sup> Martin Ivanov<sup>4</sup> Ivanka Savova<sup>1</sup>  
tontchev@vtu.bg,

<sup>1</sup>Todor Kableskov Higher School of Transport-Sofia, <sup>2</sup>Dalian University of Technology (DUT): 大连理工大学,

<sup>3</sup>University of Ruse "Angel Kanchev", <sup>4</sup>New Bulgarian University

**Abstract:** The paper presents standard statistical procedures for determining expert assessments for the influence of magnesium alloy components on the controlled mechanical properties: tensile strength and relative elongation. There are obtained neural models describing mechanical characteristics from the amount of aluminum, manganese, nickel, iron and silicon directly related to the exploitation properties of the product. The applied approach makes it possible to determine of compositions ensuring relatively optimal values of the explored quality indicators.

**KEY WORDS:** MODELING PROPERTIES, STATISTICAL CALCULATIONS, MAGNESIUM ALLOYS, ANN, MULTICRITERIA OPTIMIZATION, PARETO FRONT.

## 1. INTRODUCTION

The solution of modern technical problems is related to eliminating a given technical or physical contradiction among the factors describing the problem. In the domain of material science this is the contradiction between the strength  $R_m$  [MPa] and the relative elongation –  $A$  [%]. The set of their alternatives is obtained via respective alloying or thermal treatment. Thus a problem is formulated with input parameters the composition determined by the amount of the specific element and the processing mode parameters. The process of solving such problems is oriented to approaches enhancing the Decision Maker (DM) in the analyses prepared by him/her. The different obtained solutions are related to different determined effect of the achieved benefits. The application of statistical methods in analysis of certain quality indicator requires models for the investigated values in the performed experiment. It is possible to make valuable propositions improving the parameters of the created product and technologies based on rich information from companies [1-4] of various data bases during the research of the dependencies.

The research is a part of a series of evolving approaches and methodologies [5] which on the stage of the solution generation do not use the knowledge accumulated in the domain of metallurgy. This research is a logical continuation of an experiment carried out in connection with the National Program for High Technologies, Research and Development – Program – 863 of China in 2009, project AA03Z525 of the Fund for Science and Technologies of Dalian and an internal project J21DW003/2009.

The cited research [5] is a methodology, a way to design alloys with an a priori given data base. It is the exact place for the possibility to illustrate the usage of modern computational tools to solve specific engineering problems in the area of processing magnesium alloys.

## 2. METHODOLOGY FOR CONDUCTING THE SURVEY

The methodology to conduct the research includes the following steps:

- Preliminary statistical analysis of the survey data with visualization of the dependencies between the observed quantities. This includes the determination of the baseline (descriptive) statistical characteristics, the presence of parametric correlation in the experimental research.

- Approximation of the dependencies between the participating in the chemical compound of the chemical alloy and its mechanical properties using neural models.

The subject of the analysis is a set of experimental data on the composition and properties of magnesium alloys. The data contained 41 experimental observations. The aim of the analysis is to identify the basic statistical characteristics describing the data from the experiment as well as to compile statistical models approximating the relationships between the chemical composition of the alloy and the physico-mechanical parameters of the tensile strength ( $R_m$ ) and the relative elongation ( $A$ ).

The results of the preliminary statistical analysis of the available experimental data, including also the calculation of basic descriptive statistics, are shown in Table 1. These include: average, minimum and maximum, standard deviation.

**Table 1.** Basic descriptive statistics for observed variables.

| Variable | Average | Minimum | Maximum | Standard deviation |
|----------|---------|---------|---------|--------------------|
| Al       | 5,2159  | 0,0000  | 10,700  | 3,24134            |
| Mn       | 0,3585  | 0,0800  | 1,5000  | 0,25968            |
| Zn       | 1,2139  | 0,0000  | 6,5000  | 1,78290            |
| Cu       | 0,2510  | 0,0000  | 2,7000  | 0,62465            |
| Fe       | 0,0046  | 0,0000  | 0,0500  | 0,01304            |
| Ni       | 0,0059  | 0,0000  | 0,0300  | 0,00928            |
| Si       | 0,2588  | 0,0000  | 1,0000  | 0,33983            |
| $R_m$    | 228,707 | 150,00  | 295,00  | 37,5887            |
| $A$      | 7,2439  | 2,0000  | 15,000  | 3,50557            |

## 3. STATISTICAL DATA ANALYSIS AND VISUALIZATION

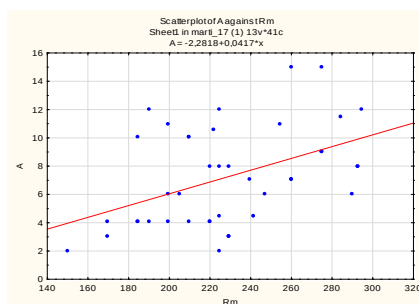
The most important task at this stage is to find an opportunity to find a possible relation between the independent parameters and the dependent characteristics in the experimental research. The statistical analysis allows to determine the uncorrelated input parameters of the experiment that can be used to construct a regression model – the percentage of elements in the magnesium alloy composition. The limited number of observations does not make it possible to draw conclusions on the statistical distribution of the observed variables.

**Table 2.** Correlation coefficients between the variables.

| Variables | Al        | Mn        | Zn        | Cu        | Fe        | Ni        | Si        | Rm        | A         |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Al        | 1,000000  | -0,620126 | -0,471530 | -0,446552 | 0,367573  | 0,180073  | -0,013168 | -0,021270 | -0,324544 |
| Mn        | -0,620126 | 1,000000  | 0,289916  | 0,229913  | -0,047708 | -0,216358 | -0,100364 | 0,030075  | -0,021431 |
| Zn        | -0,471530 | 0,289916  | 1,000000  | 0,863515  | -0,111306 | -0,006764 | -0,255629 | 0,157414  | -0,034116 |
| Cu        | -0,446552 | 0,229913  | 0,863515  | 1,000000  | -0,043246 | 0,064104  | -0,117705 | 0,022081  | -0,159779 |
| Fe        | 0,367573  | -0,047708 | -0,111306 | -0,043246 | 1,000000  | 0,201250  | 0,062923  | -0,270441 | -0,224916 |
| Ni        | 0,180073  | -0,216358 | -0,006764 | 0,064104  | 0,201250  | 1,000000  | 0,285475  | -0,075156 | -0,087665 |
| Si        | -0,013168 | -0,100364 | -0,255629 | -0,117705 | 0,062923  | 0,285475  | 1,000000  | -0,324950 | -0,229324 |
| Rm        | -0,021270 | 0,030075  | 0,157414  | 0,022081  | -0,270441 | -0,075156 | -0,324950 | 1,000000  | 0,446598  |
| A         | -0,324544 | -0,021431 | -0,034116 | -0,159779 | -0,224916 | -0,087665 | -0,229324 | 0,446598  | 1,000000  |

The values of the statistically determined correlation coefficients between the observed variables (two in two) are shown in Table. 2. Generally, they have low values, most of which are statistically insignificant (at p-level = 0.05). Exceptions make several of the values in Table 2 which are marked with a bold + italic font.

A matter of interest is the correlation coefficient between the variables Rm and A due to the possibility to include them in a joint model. This correlation coefficient is positive and statistically significant with a value of 0.4446598. In Fig.1. a diagram of the mutual correlation between the values of the parameters Rm and A is shown.

**Fig. 1.** Diagram of the correlated values of the variables Rm and A.

#### 4. MODELING STATISTICAL DEPENDENCIES WITH LINEAR REGRESSION MODEL

The attempt to compile a linear multidimensional regression model binding the predictors to the resultant variables Rm and A did not give satisfactory results and meaningful statistical evaluations of the model coefficients and also of the overall significance of the regression model – most likely due to the limited number of observations and the absence of clear linear relationships between the predictors and

the result variables in the model. The coefficient values obtained in both models for the most part, as well as the overall ANOVA analysis of the models, proved to be statistically insignificant (at p-level = 0.05). The construction of a linear regression model is not a suitable solution for approximating the relationships between variables in the experiment.

#### Using neural models to approximate the relations between the predictors and the resulting variables Rm and A.

The problems encountered with the construction of the statistical models, approximating the influence of the predictors on the values of the Rm and A values resulted in the need to look for modeling of the investigated relationships with other means. To solve the specific problem, the approach was chosen using neural models of the multilayer perceptron (MMP) type. This approach is not a novelty, but it proves to be too effective in cases where classical statistical methods do not work. It allows for the compilation of approximation models in cases where the relations between the observed values are considerably more complex and sometimes implicit. Generally, neural models are not related to statistical techniques, but are regarded as self-contained outcomes of machine learning. However, many authors note the computational similarity of these models with the methods of statistical analysis.

The compilation of neural models describing adequately the relations between the predictors and physico-mechanical parameters Rm and A was performed with the Automatic Neural Network Module of the popular Sstatistica package Statistica 12. An experiment was carried out with over 2000 models for each of the approximations sought, the selection being performed according to the value of the correlation coefficients between the observed and calculated result values (respectively for the learner, the test and the validation set). The defined as the best neural models, as well as the quality indicators, are shown in Table 3.

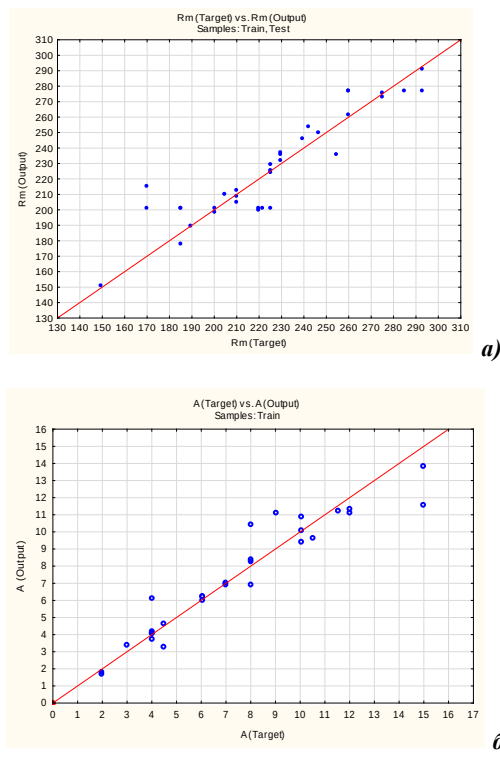
**Table 3.** Quality indicators of selected neural models for approximation of Rm and A.

| Approximated parameter | Network type | Learning | Test[ing] | Validation | Algorithm | Error | Activation function Hidden layer | Activation function Output |
|------------------------|--------------|----------|-----------|------------|-----------|-------|----------------------------------|----------------------------|
| Rm                     | MLP 7-6-1    | 0,947569 | 0,8861244 | 0,80383108 | BFGS 93   | SOS   | Logistic                         | Identity                   |
| A                      | MLP 7-10-1   | 0,952151 | 0,9030694 | 0,90535722 | BFGS 70   | SOS   | Logistic                         | Tanh                       |

The following steps and assessments are included in the analysis of the results of the numerical experiment on modeling the investigated links:

- Compilation of two-dimensional diagrams for distribution of observed (horizontal axis) and model (vertical axis) values. The visual interpretation of the diagram shows a significant linear

correlation between these values for both models (tensile strength and relative elongation) corresponding to the values of the correlation coefficients in Table 3.



**Fig. 2.** Diagrams for distribution of observed (along the horizontal axis) and modeled (along the vertical axis) values, a) – Rm, b) – A.

**Table 4.** Sensitivity analysis for models, approximating Rm and A.

|    | Model      | Zn     | Si     | Cu      | Al     | Fe      | Mn       | Ni       |
|----|------------|--------|--------|---------|--------|---------|----------|----------|
| Rm | MLP 7-6-1  | 92,063 | 37,877 | 21,068  | 11,916 | 6,6961  | 6,467061 | 4,927017 |
| A  | MLP 7-10-1 | 12,926 | 9,3068 | 5,54604 | 16,482 | 6,70571 | 2,58310  | 12,1877  |

Based on the sensitivity analysis of the data, it can be concluded that the strongest influence on the Rm parameter is the zinc element, and for A the most influential element is Aluminum.

## 5. ALGORITHM FOR CONSTRUCTING PARETO-FRONT OF THE PROPERTIES OF MANGANESE ALLOYS

The realization of this experimental-computational approach requires the preliminary research of experimental data in order to obtain approximating quantitative relationships between them and subsequently to include the established dependencies in a suitable optimization algorithm.

The steps to perform the research are as follows:

- Compilation of approximation models connect with the parameters of the alloy composition to the resulting physico-mechanical parameters;
- Selection of a suitable algorithm for building a Pareto front;
- Incorporating the approximation models in the algorithm and realization as a programming tool.

On the first step are used the designed neural models of the 'multilayer perceptron' type, providing a reliable and adequate approximation of the experimental results. The input parameters of the model are the percentages of the observed elements in the

They were composed of histograms of residual distribution (differences between observed and modeled values). The statistical parameters of these distributions are respectively: for Rm – mean value  $-1,03232$  and standard deviation  $14,21009$ ; For A – an average value of  $-0.14856$  and a default deviation of  $1.36316$ .

The trials, and the statistical distributions of the residues for approximation with normal distribution did not give satisfactory results. Applying the Chi-square criterion showed values below the standard level of significance  $p\text{-level} = 0.05$ , which is a statistical sign of a significant difference between the observed and the theoretical distributions

The analysis of the results of the approximation with the introduced neural models was supplemented with a sensitivity analysis. The latter shows the relative importance of the predictors in the formation of the values of the resultant variables. For elaborated models these results are shown in Table. 4. A significant influence of the predictor is if its value is greater than 1.

composition of the material. The output parameters are the measured mechanical characteristics (Rm and A). The approximation is performed separately for each of the mechanical parameters. The selection of a suitable model is made by playing a variety of versions, observing a suitable criterion for assessing their quality. The classical approach to assess the quality of the neuronal model takes the value of the correlation coefficient between the data observed in the experiment and the model values. The models used in this research achieve comparatively high values of this criterion. For the model approximating Rm it is 0.92, and for that approximating A – 0.94, respectively.

The algorithm for constructing Pareto's front must take into account the non-linearity of the relationships between the control parameters in the problem and the criteria, as well as the need to simultaneously support a set of non-dominated solutions. These requirements are best matched by the non-dominated sorted genetic algorithm NSGA II, which is iterative, based on genetic optimization with random population generation and tournament selection of individuals, and it maintains non-dominated solutions in the form of several sorted Point fronts (non-dominated decisions).

The incorporation of the approximate models in the overall optimization model is done in the program code. The application was written in Java and showed good solution search efficiency.

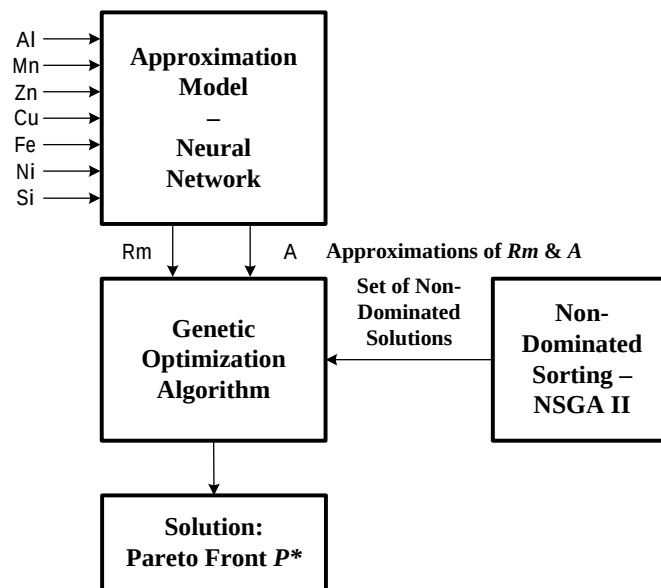


Fig.3. A general block-diagram of the software model for building the Pareto front.

Table 5. Magnesium alloy compositions optimized by properties.

| Al [%]   | Mn [%]   | Zn [%]   | Cu [%]   | Fe [%]   | Ni [%]   | Si [%]   | Rm [MPa] | A [%]    |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 3,51268  | 0,557133 | 3,642975 | 0,004866 | 0,043808 | 0,005287 | 0,025582 | 293      | 7,619694 |
| 4,36030  | 0,219954 | 4,835791 | 0,047128 | 0,045818 | 0,002579 | 0,122034 | 293      | 9,220627 |
| 5,848844 | 0,337508 | 5,056425 | 0,056994 | 0,039052 | 0,011206 | 0,131066 | 292,9999 | 11,13535 |
| 0,271841 | 0,578693 | 4,406906 | 0,249543 | 0,039151 | 0,014401 | 0,003857 | 292,9995 | 13,96775 |
| 6,453005 | 0,167483 | 6,251246 | 0,083834 | 0,048756 | 0,014193 | 0,09249  | 293      | 14,21138 |
| 2,3160   | 0,167483 | 6,251246 | 0,083834 | 0,049552 | 0,014193 | 0,09249  | 293      | 14,73484 |
| 2,1272   | 0,0853   | 3,92513  | 0,417189 | 0,002182 | 0,021437 | 0,188809 | 292,0306 | 14,7719  |
| 1,0797   | 0,531217 | 1,310215 | 0,306018 | 0,021915 | 0,029793 | 0,033673 | 290,1839 | 14,79963 |
| 1,0797   | 0,531217 | 1,310215 | 0,306018 | 0,018621 | 0,029793 | 0,033673 | 284,3487 | 14,86131 |
| 0,7495   | 0,650233 | 1,312941 | 0,018628 | 0,004774 | 0,025723 | 0,131576 | 249,7833 | 14,95381 |
| 2,1488   | 0,11675  | 1,148111 | 0,284934 | 0,008992 | 0,024215 | 0,132072 | 257,1124 | 14,91524 |
| 0,9256   | 0,218758 | 0,856158 | 0,02395  | 0,015513 | 0,029933 | 0,204648 | 227,4298 | 14,96082 |

The result from the implementation of the program is shown in Figure 4 and in Table 5. The compositions of the optimal properties of the magnesium alloys are shown. The graph of algorithm-derived non-dominated solutions referring to the co-maximized values of parameters Rm and A is shown.

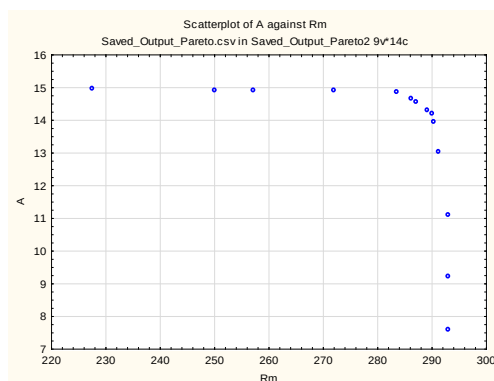


Fig.4. Pareto-front of non-dominated solutions for parameters Rm and A

## 6. CONCLUSION.

Neural models are established describing mechanical characteristics of the amounts of alloying elements in magnesium alloys, substantial for the exploitation properties of the product. The proposed approach is suitable to determine a composition with relatively best meanings of the values of the selected mechanical indices. A multi-criteria approach is applied to expertly assess the influence of alloy composition elements on pre-selected quality indicators to improve the mechanical properties of the products. The total sensitivity of the approximation models is determined by two basic mechanical indicators of a set of networks with varying degrees of complexity, mathematical description and with different degrees of correspondence between the predicted and the real value for a wide variation range of the alloying elements. This allows a more accurate automated prediction of alloy properties depending on the composition and thermal treatment of the alloy. New means confirmed facts already known in science and practice.

**REFERENCES:**

- [1] Friedrich H.E., Mordike B.L. Magnesium Technology: Metallurgy, Design, Data, Applications, Springer-Verlag Berlin Heidelberg, 2006. 647 p.
- [2] Kainer K.U. (Ed.) Magnesium Alloys and Technologies Wiley-VCH, 2003. 285.
- [3] Monteiro W.A. (Ed.) New Features on Magnesium Alloys, InTech, 2012. 174 p.
- [4] Czerwinski F. (Ed.) Magnesium Alloys: InTAe, 2014, 176 p.
- [5] Tontchev N. Materials Science, Effective solutions and Technological variants, 2014/3/3, LAMBERT Academic Publishing.