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STATISTICAL STUDY OF THE DEPENDENCE BETWEEN CONCENTRATION OF METALLIC ELEMENTS MIGRATED FROM STAINLESS STEEL GRADE AISI321 AND WORKING PARAMETERS

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Abstract: *One of the main problems concerning food safety is the possible migration of ions in metallic materials intended to come into contact with food.*
The aim of this paper is to find and apply the mathematical modeling of experimental data which should describe as accurately as possible the dependence between the variables used in the experimental plan. The research made and presented in this study also aims to create a real possibility for rapid intervention in the process control when one of the parameters cannot be maintained at a predetermined value. In this paper we used some experimental data obtained by testing the migration of metal ions from austenitic stainless steel grade AISI 321 samples in solutions with concentrations of 3%, 6% and 9% acetic acid. To find an accurate mathematical model describing the phenomena of diffusion, ANOVA method, known as the variance analysis, was used. In order to obtain the mathematical model we used a polynomial model with independent variables: corrosive environment temperature (X_1), exposure time (X_2), stirring environment (X_3) and the dependent variables Y - concentrations of elements Ti, Cr, Mn, ^{56}Fe and Ni found in solutions. Values of the regression coefficients very close to the value 1 (the dependent variables coefficients are valid) were obtained, which demonstrates the validity of the applied method.

Keywords: *austenitic stainless steel, mathematical modeling, ANOVA method, dependent and independent variables, coded values, validity of the model.*

1. Introduction

Stainless steels are commonly used as metallic materials intended to come into contact with food environments. This widespread use of stainless steels led to increase the importance of studying the diffusion processes of metal ions in food environments, research on the interaction between corrosive environments and stainless steels being the subject of scientific research for a long time [1], [2], [3], [4]. In this context, one of the most used grade of stainless steel is 300 series such as AISI 321, both containing 11wt% Ni [5].

Diffusion of metal ions in foodstuffs is a slow process that occurs in different types of environments, often in acidic environments [6], [7], [8], [9], [10].

In the last decade, based on several scientific researches, the modeling of migration metallic constituents of materials in contact with foodstuffs has played an important part in the quality assurance system in the food industry. By classical methods or by using specialized software, mathematical modeling has become a relatively inexpensive tool for scientists aiming to minimize the number of experiments and to determine the influence of various parameters influencing the safety and quality processes [11-13]. Since the beginning we must analyze if the problem is correctly defined and consistent, if its solution to provide useful information for the study and influence factors correspond to the characteristics that must be satisfied. To find an accurate mathematical model describing the phenomena of diffusion, the ANOVA method, known as the analysis of variance, was used. ANOVA is widely used because it is recommended when studying a larger number of levels of the independent variables, making possible to observe with greater accuracy the effect of the independent variables on the dependent ones and their combined effect.

The aim of this work was to apply the ANOVA method for modeling the experimental data obtained from the migration test, which describes exactly the dependence between the variables used in the experimental plan.

2. Experimental

2.1. Materials and samples preparation

In this study metal samples of AISI 321 stainless steel grade were used. The chemical composition of the steel is given in Table 1 (*EN 10088-2:2005*).

Table 1

Chemical composition of austenitic stainless stell AISI 321 (wt %)

Fe	C	Mn	P	S	Si	Cr	Ni	Ti
68	0.08	2	0.045	0.03	1	18	11	0.4

Metal samples were cut from unused sheet, free from deformation or scratches. Sample sizes were established according to the D.M. 03/21/1973, which stipulates that the ratio of the exposed surface of the sample and the volume of solution should be between 0.5 ... 2. Sample sizes were 40 x 40 x 2.5 mm. Acetic acid is recommended to test metal alloys in contact with foodstuffs. Acetic acid solutions 3%, 6% and 9%, were used as corrosive environments. To avoid contamination of corrosive solutions with foreign compounds, the surface of metal samples was washed with a detergent solution at 40°C and rinsed in double distilled water. Ultrasonic cleaning was performed at 45°C for 15 minutes in the ultrasonic. The samples were dried in oven at 50°C. Profile roughness evaluation, complying with EN ISO 4287, was determined with an optical profilometer (*Nano Focus µscan*) for contactless 2D and 3D measurement of microscopic surface structures. The surface roughness was R_a - *0.7816±0.019µm*.

2.2. Migration test

In the experimental studies the following working parameters were used:

- *Testing temperature -* ***T*** *[°C]*
- *Stirring environment -* ***n*** *[rot/min]*
- *Exposure time -* ***t*** *[min]*

Variation levels of working parameters are given in Table 2.

Table 2

Variation levels of working parameters

Working parameters	Minimum value	Central value	Maximum value
Testing temperature	22	28	34
Stirring environment	0	125	250
Exposure time	30	60	90

In the case of the experiments made in

stationary environment and at different temperatures of the environment, the samples were maintained in the oven while for those requiring temperatures of 28°C and 34°C and stirring environment, a magnetic heating stirrer *Heidolph MR Hei-Tec* was used.

2.3. Chemical analysis of corrosive environments

The concentrations of metal ions Ti, Cr, Mn, ^{56}Fe and Ni from acid solutions were analyzed using mass spectrometry and inductively coupled plasma *ICP-MS - Agilent 7500* model.

3. Results and Discussion

The concentrations of metallic elements Ti, Cr, Mn, ^{56}Fe and Ni obtained by mass spectrometry and inductively coupled plasma were used in mathematical modeling of diffusion phenomena.
Since the literature has not provided a sufficiently accurate mathematical apparatus to describe the interdependencies mentioned we chose to develop a mathematical model with statistical means by ANOVA method.
To achieve this mathematical model *Design Expert®* software and a polynomial model with multiple variables were used:

- *Independent variables*: testing temperature (X_1), exposure time (X_2), stirring environment (X_3);
- *Dependent variables (response functions) Y_1, Y_2, Y_3, Y_4 and Y_5:* concentrations expressed in *ppb* of elements Ti, Cr, Mn, ^{56}Fe and Ni.

3.1. Mathematical modeling of concentration of metallic elements migrated in 3% acetic acid solution.

After having made the analysis of variance ANOVA, a polynomial model with the lowest value of the critical probability *P* for all dependent variables: Ti, Cr, Mn, ^{56}Fe and Ni, was chosen. It is known that the null hypothesis of the dependent variables is rejected if the value of the variables of *P* is less than the chosen significance threshold (*α=0.05*). The statistical summary of mathematical models found to describe dependent variables Ti, Cr, Mn, ^{56}Fe and Ni is given in Table 3. The mathematical models are presented in equations (1), (2), (3), (4) and (5) and comparative graphical representation of measured values and the values obtained by modeling ANOVA are shown in Figures 1-5.

Table 3. Model summary Statistics

Dependent variable	*P*	*Model*	*Standard deviation [σ]*	*R-Squared [R^2]*	*Adjusted R-Squared [R^2 adjusted]*
Y_1	0.033	Cubic	0.24	0.9905	0.9440
Y_2	0.016	Quartic	1.62	0.9925	0.9512
Y_3	0.015	Quadratic	1.20	0.9878	0.8872
Y_4	0.046	Cubic	91.33	0.9898	0.8876
Y_5	0.025	Quartic	4.13	0.9903	0.9812

The mathematical model of the response function Y_1 (*Ti* concentration) is given in the equation (1):

$$Y_1 = 1.71 + 0.97 \cdot X_1 + 0.94 \cdot X_2 - 0.50 \cdot X_3 - 0.22 \cdot X_1^2 - 0.094 \cdot X_2^2 - 0.19 \cdot X_3^2 - 0.17 \cdot X_1 \cdot X_2 - 0.19 \cdot X_1 \cdot X_3 - 0.40 \cdot X_2 \cdot X_3 - 0.33 \cdot X_1^2 \cdot X_2 - 0.17 \cdot X_1^2 \cdot X_3 - 0.23 \cdot X_1 \cdot X_2^2 - 0.36 \cdot X_1 \cdot X_3^2 - 0.05 \cdot X_2^2 \cdot X_3 - 0.13 \cdot X_2 \cdot X_3^2 + 0.05 \cdot X_1 \cdot X_2 \cdot X_3 \quad (1)$$

To check the validity of the mathematical model obtained, the *experimental values* vs *model values* were plotted (Figure 1).

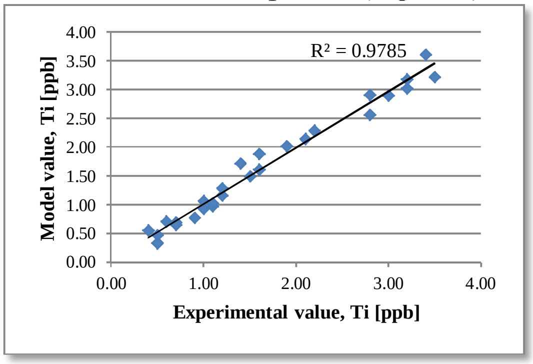

Figure 1. Validity check of the mathematical model obtained

The mathematical model of the response function Y_2 (*Cr* concentration) is given in equation (2):

$$Y_2 = 7.26 + 3.72 \cdot X_1 + 1.44 \cdot X_2 + 2.67 \cdot X_3 + 3.61 \cdot X_1^2 + 8.11 \cdot X_2^2 + 2.11 \cdot X_3^2 + 0.25 \cdot X_1 \cdot X_2 + 2.50 \cdot X_1 \cdot X_3 - 2.00 \cdot X_2 \cdot X_3 + 1.58 \cdot X_1^2 \cdot X_2 + 0.50 \cdot X_1^2 \cdot X_3 - 0.58 \cdot X_1 \cdot X_2^2 + 1.17 \cdot X_1 \cdot X_3^2 + 2.50 \cdot X_2^2 \cdot X_3 + 1.83 \cdot X_2 \cdot X_3^2 + 0.75 \cdot X_1 \cdot X_2 \cdot X_3 - 6.92 \cdot X_1^2 \cdot X_2^2 + 6.50 \cdot X_1^2 \cdot X_2 \cdot X_3 - 0.17 \cdot X_1^2 \cdot X_3^2 - 1.00 \cdot X_1 \cdot X_2^2 \cdot X_3 + 1.00 \cdot X_1 \cdot X_2 \cdot X_3^2 - 0.67 \cdot X_2^2 \cdot X_3^2 \qquad (2)$$

The validity of the mathematical model obtained for *Cr* has been plotted by *experimental values* vs *model values* (Figure 2).

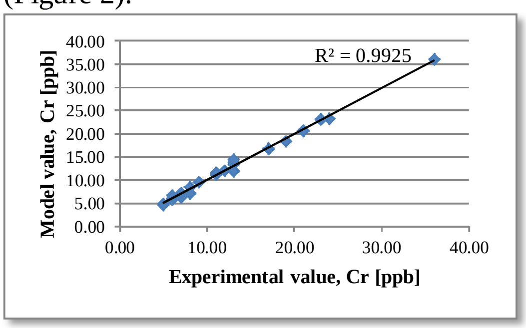

Figure 2. Validity check of the mathematical model obtained for chromium

The mathematical model of the response function Y_3 (*Mn* concentration) is given in equation (3):

$$Y_3 = 8.57 + 1.90 \cdot X_1 + 2.40 \cdot X_2 - 0.92 \cdot X_3 - 0.20 \cdot X_1^2 + 0.33 \cdot X_2^2 - 1.78 \cdot X_3^2 + 1.68 \cdot X_1 \cdot X_2 - 0.60 \cdot X_1 \cdot X_3 - 0.24 \cdot X_2 \cdot X_3 \qquad (3)$$

The validity of the mathematical model obtained for *Mn* has been plotted by *experimental values* vs *model values* (Figure 3).

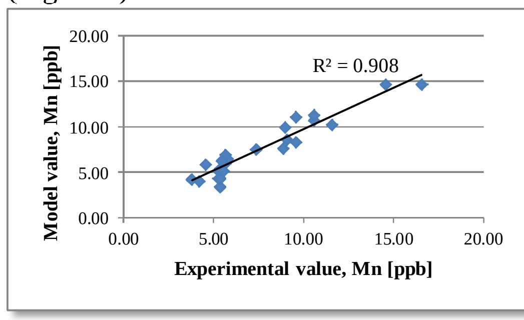

Figure 3. Validity check of the mathematical model obtained for manganese

The mathematical model of the response function Y_4 (^{56}Fe concentration) is given in equation (4):

$$Y_4 = 861.85 + 293.33 \cdot X_1 + 145.56 \cdot X_2 - 50{,}00 \cdot X_3 - 108.89 \cdot X_1^2 - 3.89 \cdot X_2^2 - 310.56 \cdot X_3^2 + 67.50 \cdot X_1 \cdot X_2 - 9.17 \cdot X_1 \cdot X_3 + 28.33 \cdot X_2 \cdot X_3 + 54.17 \cdot X_1^2 \cdot X_2 + 107.50 \cdot X_1^2 \cdot X_3 - 27.50 \cdot X_1 \cdot X_2^2 - 157.50 \cdot X_1 \cdot X_3^2 + 5.00 \cdot X_2^2 \cdot X_3 - 43.33 \cdot X_2 \cdot X_3^2 + 37.50 \cdot X_1 \cdot X_2 \cdot X_3 \qquad (4)$$

The validity of the mathematical model obtained for ^{56}Fe has been plotted by *experimental values* vs *model values* (Figure 4).

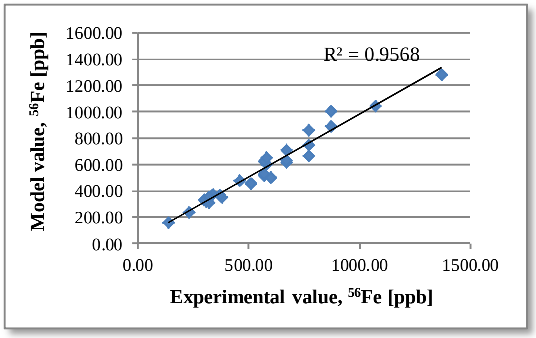

Figure 4. Validity check of the mathematical model obtained for ^{56}Fe

The mathematical model of the response function Y_5 (*Ni* concentration) is given in equation (5):

$$Y_5 = 35.56 + 9.00 \cdot X_1 + 6.33 \cdot X_2 + 3.44 \cdot X_3 - 3.89 \cdot X_1^2 + 0,11 \cdot X_2^2 - 7.89 \cdot X_3^2 + 7.50 \cdot X_1 \cdot X_2 - 2.50 \cdot X_1 \cdot X_3 + 0.002 \cdot X_2 \cdot X_3 + 4.00 \cdot X_1^2 \cdot X_2 - 1.17 \cdot X_1^2 \cdot X_3 + 0.003 \cdot X_1 \cdot X_2^2 - 3.00 \cdot X_1 \cdot X_3^2 - 1.17 \cdot X_2^2 \cdot X_3 + 2.00 \cdot X_2 \cdot X_3^2 + 1.25 \cdot X_1 \cdot X_2 \cdot X_3 + 0.83 \cdot X_1^2 \cdot X_2^2 + 0.50 \cdot X_1^2 \cdot X_2 \cdot X_3 + 7.83 \cdot X_1^2 \cdot X_3^2 + 2.00 \cdot X_1 \cdot X_2^2 \cdot X_3 - 6.50 \cdot X_1 \cdot X_2 \cdot X_3^2 + 0.83 \cdot X_2^2 \cdot X_3^2 \quad (5)$$

The validity of the mathematical model obtained for *Ni* has been plotted by *experimental values* vs *model values* (Figure 5).

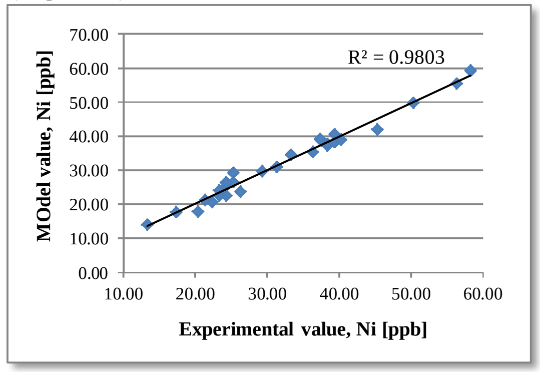

Figure 5. Validity check of the mathematical model obtained for nickel

3.2. Mathematical modeling of concentration of metallic elements migrated in 6% acetic acid solution.

Statistical summary of mathematical models found to describe dependent variables Ti, Cr, Mn, ^{56}Fe and Ni in 6% acetic acid solutions is given in Table 4.

The mathematical models are presented in equations (6), (7), (8), (9) and (10) and comparative graphical representation of measured values and the values obtained by modeling ANOVA are shown in Figures 6-10.

Table 4. Model summary Statistics

Dependent variable	*P*	*Model*	*Standard deviation [σ]*	*R-Squared [R^2]*	*Adjusted R-Squared [R^2 adjusted]*
Y_1	0.0001	Cubic	0.23	0,9931	0,9820
Y_2	0.0061	Cubic	1.29	0,9803	0,9488
Y_3	0.0670	Quartic	0.61	0,9949	0,9669
Y_4	0.0145	Quartic	13.79	0,9988	0,9921
Y_5	0.0516	Quartic	28.65	0,9952	0,9688

The mathematical model of the response function Y_1 (*Ti* concentration) is given in equation (6):

$$Y_1 = 1.44 + 1.03 \cdot X_1 + 0.58 \cdot X_2 + 0.31 \cdot X_3 + 1.25 \cdot X_1^2 + 0.017 \cdot X_2^2 - 0.05 \cdot X_3^2 + 0,42 \cdot X_1 \cdot X_2 + 0.75 \cdot X_1 \cdot X_3 + 0.45 \cdot X_2 \cdot X_3 + 0.85 \cdot X_1^2 \cdot X_2 + 0.47 \cdot X_1^2 \cdot X_3 - 0.06 \cdot X_1 \cdot X_2^2 - 0,12 \cdot X_1 \cdot X_3^2 - 0,03 \cdot X_2^2 \cdot X_3 + 0.81 \cdot X_1 \cdot X_2 \cdot X_3 \quad (6)$$

The validity of the mathematical model obtained for *Ti* has been plotted by *experimental values* vs *model values* (Figure 6).

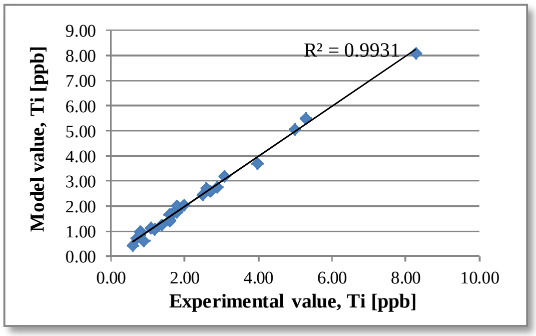

Figure 6. Validity check of the mathematical model obtained for titanium

The mathematical model of the response function Y_2 (*Cr* concentration) is given in equation (7):

$$Y_2 = 10.33 + 3.83 \cdot X_1 + 8.06 \cdot X_2 + 2.83 \cdot X_3 - 0.17 \cdot X_1^2 + 0.17 \cdot X_2^2 - 0.83 \cdot X_3^2 - 0{,}75 \cdot X_1 \cdot X_2 + 0.083 \cdot X_1 \cdot X_3 + 1.08 \cdot X_2 \cdot X_3 - 3.08 \cdot X_1^2 \cdot X_2 - 1.75 \cdot X_1^2 \cdot X_3 - 0.75 \cdot X_1 \cdot X_2^2 - 0{,}25 \cdot X_1 \cdot X_3^2 + 1.25 \cdot X_2^2 \cdot X_3 - 1.58 \cdot X_2 \cdot X_3^2 - 0.25 \cdot X_1 \cdot X_2 \cdot X_3 \quad (7)$$

The validity of the mathematical model obtained for chromium has been plotted by *experimental values* vs *model values* (Figure 7).

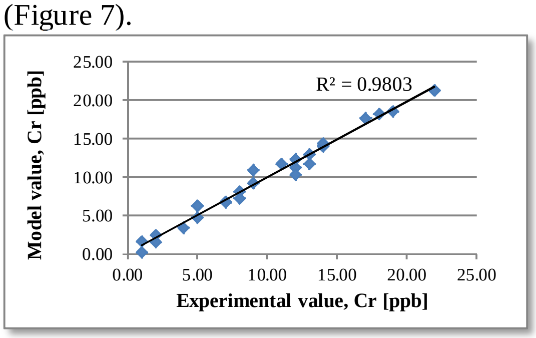

Figure 7. Validity check of the mathematical model obtained for chromium

The mathematical model of the response function Y_3 (*Mn* concentration) is given in equation (8):

$$Y_3 = 6.46 + 1.36 \cdot X_1 + 1.57 \cdot X_2 - 0.17 \cdot X_3 - 0.39 \cdot X_1^2 - 0.99 \cdot X_2^2 - 0.29 \cdot X_3^2 + 1.37 \cdot X_1 \cdot X_2 - 1.07 \cdot X_1 \cdot X_3 - 0.075 \cdot X_2 \cdot X_3 + 0.68 \cdot X_1^2 \cdot X_2 + 1.37 \cdot X_1^2 \cdot X_3 + 0.84 \cdot X_1 \cdot X_2^2 - 0.058 \cdot X_1 \cdot X_3^2 + 0.23 \cdot X_2^2 \cdot X_3 + 0.77 \cdot X_2 \cdot X_3^2 + 1.13 \cdot X_1 \cdot X_2 \cdot X_3 + 1.06 \cdot X_1^2 \cdot X_2^2 + 1.72 \cdot X_1^2 \cdot X_2 \cdot X_3 + 0.21 \cdot X_1^2 \cdot X_3^2 + 0.40 \cdot X_1 \cdot X_2^2 \cdot X_3 + 0.075 \cdot X_1 \cdot X_2 \cdot X_3^2 + 1.16 \cdot X_2^2 \cdot X_3^2 \quad (8)$$

The validity of the mathematical model obtained for manganese has been plotted by *experimental values* vs *model values* (Figure 8).

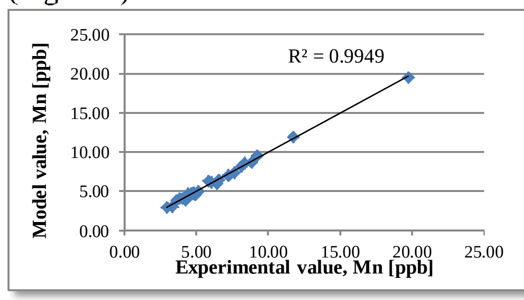

Figure 8. Validity checkof the mathematical model obtained for manganese

The mathematical model of the response function Y_4 (^{56}Fe concentration) is given in equation (9):

$$Y_4 = 298.89 + 120.56 \cdot X_1 + 108.89 \cdot X_2 + 93.33 \cdot X_3 + 11.67 \cdot X_1^2 - 3.33 \cdot X_2^2 + 66.67 \cdot X_3^2 + 47.50 \cdot X_1 \cdot X_2 + 2.50 \cdot X_1 \cdot X_3 + 5.00 \cdot X_2 \cdot X_3 + 19.17 \cdot X_1^2 \cdot X_2 - 32.50 \cdot X_1^2 \cdot X_3 + 14.17 \cdot X_1 \cdot X_2^2 - 30.83 \cdot X_1 \cdot X_3^2 + 5.00 \cdot X_2^2 \cdot X_3 - 8.33 \cdot X_2 \cdot X_3^2 + 37.50 \cdot X_1 \cdot X_2 \cdot X_3 + 42.50 \cdot X_1^2 \cdot X_2^2 + 27.50 \cdot X_1^2 \cdot X_2 \cdot X_3 - 67.50 \cdot X_1^2 \cdot X_3^2 + 27.50 \cdot X_1 \cdot X_2^2 \cdot X_3 - 25.00 \cdot X_1 \cdot X_2 \cdot X_3^2 + 0.001 \cdot X_2^2 \cdot X_3 \quad (9)$$

The validity of the mathematical model obtained for ^{56}Fe has been plotted in (Figure 9).

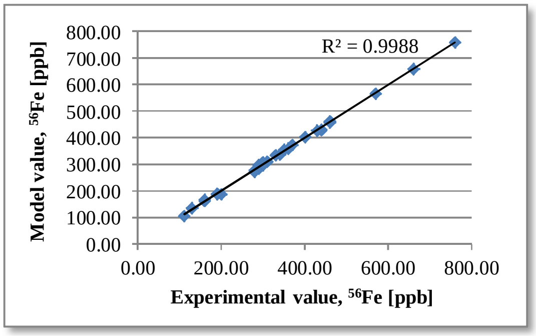

Figure 9. Validity check of the mathematical model obtained for ^{56}Fe

The mathematical model of the response function Y_5 (*Ni* concentration) is given in equation (10):

$$Y_5 = 603.04 + 151.11 \cdot X_1 + 83.33 \cdot X_2 + 117.22 \cdot X_3 - 95.56 \cdot X_1^2 + 54.44 \cdot X_2^2 - 100.56 \cdot X_3^2 + 22.50 \cdot X_1 \cdot X_2 + 30.00 \cdot X_1 \cdot X_3 + 7.50 \cdot X_2 \cdot X_3 - 30.00 \cdot X_1^2 \cdot X_2 - 85.83 \cdot X_1^2 \cdot X_3 - 1.67 \cdot X_1 \cdot X_2^2 + 0.83 \cdot X_1 \cdot X_3^2 + 16.67 \cdot X_2^2 \cdot X_3 + 10.00 \cdot X_2 \cdot X_3^2 - 18.75 \cdot X_1 \cdot X_2 \cdot X_3 - 46.67 \cdot X_1^2 \cdot X_2^2 - 21.25 \cdot X_1^2 \cdot X_2 \cdot X_3 + 135.83 \cdot X_1^2 \cdot X_3^2 - 6.25 \cdot X_1 \cdot X_2^2 \cdot X_3 - 1.25 \cdot X_1 \cdot X_2 \cdot X_3^2 - 26.67 \cdot X_2^2 \cdot X_3^2 \quad (10)$$

The validity of the mathematical model obtained for nickel has been plotted in (Figure 10).

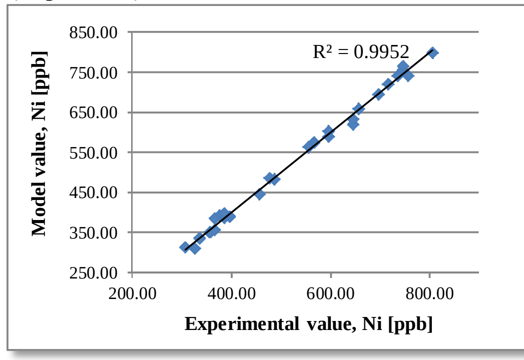

Figure 10. Validity check of the mathematical model obtained for nickel

3.3. Mathematical modeling of concentration of metallic elements migrated in 9% acetic acid solution.

Statistical summary of mathematical models found to describe dependent variables Ti, Cr, Mn, ^{56}Fe and Ni in 9% acetic acid solutions is given in Table 5, the mathematical models are presented in equations (11), (12), (13), (14) and (15), and comparative graphical representation of measured values and the values obtained by modeling ANOVA are shown in Figures 11-15.

Table 5. Model summary Statistics

Dependent variable	*P*	*Model*	*Standard deviation [σ]*	*R-Squared [R^2]*	*Adjusted R-Squared [R^2 adjusted]*
Y_1	0.042	Quartic	0.032	0.9920	0.9948
Y_2	0.017	Cubic	3.78	0.9850	0.9746
Y_3	0.009	Quartic	0.11	0.9996	0.9975
Y_4	0.052	Cubic	23.76	0.9921	0.9794
Y_5	0.048	Quadratic	4.56	0.9885	0.9365

The mathematical model of the response function Y_1 (*Ti* concentration) obtained using ANOVA methodis is given in equation (11):

$$Y_1 = 1.39 + 0.36 \cdot X_1 + 0.43 \cdot X_2 + 0.24 \cdot X_3 - 0.072 \cdot X_1^2 + 0.028 \cdot X_2^2 + 0.028 \cdot X_3^2 + 0,10 \cdot X_1 \cdot X_2 - 0.075 \cdot X_1 \cdot X_3 + 0.075 \cdot X_2 \cdot X_3 - 0.12 \cdot X_1^2 \cdot X_2 - 0.058 \cdot X_1^2 \cdot X_3 - 0.017 \cdot X_1 \cdot X_2^2 - 0,042 \cdot X_1 \cdot X_3^2 + 0.042 \cdot X_2^2 \cdot X_3 + 0.001 \cdot X_1 \cdot X_2 \cdot X_3 - 0.017 \cdot X_1^2 \cdot X_2^2 - 0.025 \cdot X_1^2 \cdot X_2 \cdot X_3 + 0.008 \cdot X_1^2 \cdot X_3^2 + 0.10 \cdot X_1 \cdot X_2^2 \cdot X_3 + 0.025 \cdot X_1 \cdot X_2 \cdot X_3^2 - 0.092 \cdot X_2^2 \cdot X_3^2 \quad (11)$$

The validity of the mathematical model obtained for titanium has been plotted in (Figure 11).

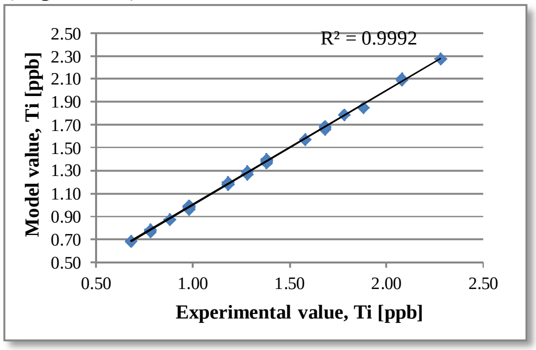

Figure 11. Validity check of the mathematical model obtained for titanium

The mathematical model of the response function Y_2 (*Cr* concentration) obtained using ANOVA methodis is given in equation (12):

$$Y_2 = 13.93 + 2.39 \cdot X_1 + 13.17 \cdot X_2 + 0.50 \cdot X_3 - 4.44 \cdot X_1^2 + 4.06 \cdot X_2^2 - 0.11 \cdot X_3^2 + 4.75 \cdot X_1 \cdot X_2 + 4.67 \cdot X_1 \cdot X_3 + 3.42 \cdot X_2 \cdot X_3 - 4.75 \cdot X_1^2 \cdot X_2 + 7.00 \cdot X_1^2 \cdot X_3 + 3.42 \cdot X_1 \cdot X_2^2 - 0{,}33 \cdot X_1 \cdot X_3^2 + 2.75 \cdot X_2^2 \cdot X_3 - 2.25 \cdot X_2 \cdot X_3^2 + 2.75 \cdot X_1 \cdot X_2 \cdot X_3 \quad (12)$$

To check the validity of the mathematical model obtained, the *experimental values* vs *model values* were plotted (Figure 12).

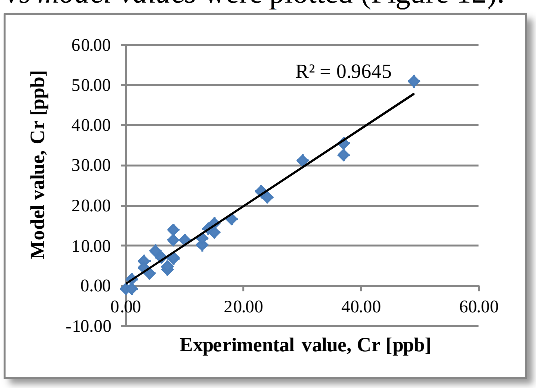

Figure 12. Validity check of the mathematical model obtained for chromium

The mathematical model of the response function Y_3 (*Mn* concentration) obtained using ANOVA methodis is given in equation (13):

$$Y_3 = 5.64 - 0.78 \cdot X_1 + 1.83 \cdot X_2 + 0.46 \cdot X_3 - 1.73 \cdot X_1^2 + 1.12 \cdot X_2^2 + 0.37 \cdot X_3^2 + 0{,}57 \cdot X_1 \cdot X_2 - 0.53 \cdot X_1 \cdot X_3 + 0.10 \cdot X_2 \cdot X_3 + 0.30 \cdot X_1^2 \cdot X_2 + 0.48 \cdot X_1^2 \cdot X_3 + 0.75 \cdot X_1 \cdot X_2^2 + 0.40 \cdot X_1 \cdot X_3^2 + 0.058 \cdot X_2^2 \cdot X_3 - 0.17 \cdot X_2 \cdot X_3^2 - 0.41 \cdot X_1 \cdot X_2 \cdot X_3 + 0.42 \cdot X_1^2 \cdot X_2^2 + 0.31 \cdot X_1^2 \cdot X_2 \cdot X_3 - 0.23 \cdot X_1^2 \cdot X_3^2 - 0.24 \cdot X_1 \cdot X_2^2 \cdot X_3 + 0.24 \cdot X_1 \cdot X_2 \cdot X_3^2 - 0.46 \cdot X_2^2 \cdot X_3^2 \quad (13)$$

To check the validity of the mathematical model obtained for the Y_3 variable, the *experimental values* vs *model values* were plotted (Figure 13).

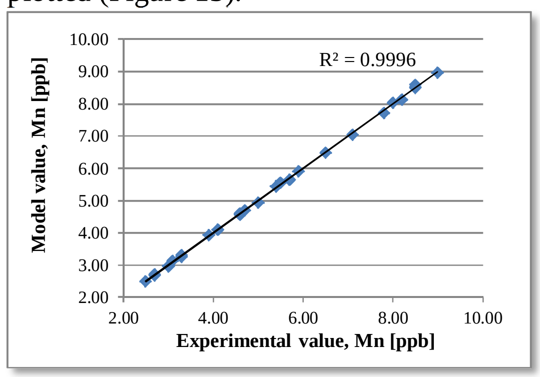

Figure 13. Validity check of the mathematical model obtained for manganese

The mathematical model of the response function Y_4 (^{56}Fe concentration) obtained using ANOVA methodis is given in equation (14):

$$Y_4 = 522.96 + 123.33 \cdot X_1 + 58.33 \cdot X_2 + 96.67 \cdot X_3 - 103.89 \cdot X_1^2 - 13.89 \cdot X_2^2 - 12.78 \cdot X_3^2 + 16.67 \cdot X_1 \cdot X_2 - 5.83 \cdot X_1 \cdot X_3 + 6.67 \cdot X_2 \cdot X_3 + 5.00 \cdot X_1^2 \cdot X_2 + 12.50 \cdot X_1^2 \cdot X_3 + 0.001 \cdot X_1 \cdot X_2^2 + 42.50 \cdot X_1 \cdot X_3^2 - 15.00 \cdot X_2^2 \cdot X_3 - 15.00 \cdot X_2 \cdot X_3^2 - 17.50 \cdot X_1 \cdot X_2 \cdot X_3 \quad (14)$$

The validity of the mathematical model obtained has been plotted by *experimental values* vs *model values* (Figure 14).

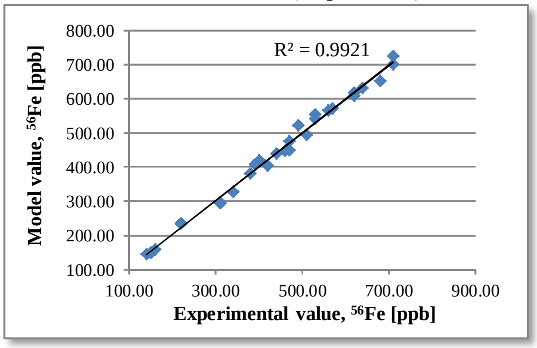

Figure 14.Validity check of the mathematical model obtained for ^{56}Fe

The mathematical model of the response function Y_5 (*Ni* concentration) obtained using ANOVA method is given in equation (15):

$$Y_5 = 21.29 + 12.72 \cdot X_1 + 10.72 \cdot X_2 + 10.78 \cdot X_3 + 3.72 \cdot X_1^2 + 2.72 \cdot X_2^2 + 3.22 \cdot X_3^2 + 3.25 \cdot X_1 \cdot X_2 + 5.50 \cdot X_1 \cdot X_3 + 5.83 \cdot X_2 \cdot X_3 \quad (15)$$

To check the validity of the mathematical model obtained for Y_5 variable, the *experimental values* vs *model values* were plotted (Figure 15).

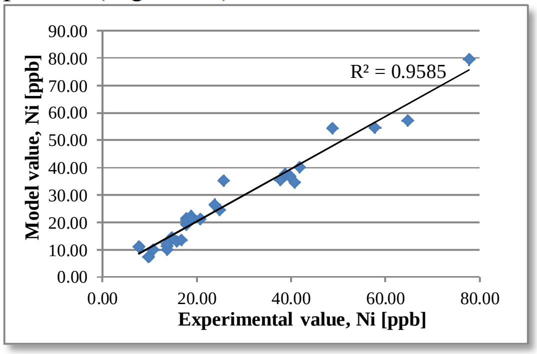

Figure 15. Validity check of the mathematical model obtained for nickel

4. Conclusions

The aim of this study was to find and apply a method for modeling the experimental data obtained by migration test, which describes how exactly the dependence between variables used in the experimental design is.

In order to establish the dependences between the working parameters of migration test and the metal concentrations of Ti, Cr, Mn, ^{56}Fe and Ni, found in corrosive solutions using mass spectrometry ICP-MS inductively coupled plasma, the ANOVA method was used;

By utilizing this statistical method to obtain mathematical models that gives dependence of the working parameters and Ti, Cr, Mn, ^{56}Fe and Ni concentrations, these models can be used to estimate the objective function values. So, the simulation process may be obtained by using mathematical models, but they are produced with certain approximations and assumptions, allowing however, a description of processes for a wide range of values;

For the mathematical models we obtained values of the regression coefficients very close to the value 1 (the dependent variables coefficients are valid), which demonstrates the validity of the applied statistical method;

The comparative graphical representation of the experimental values vs values obtained by modeling shows that the deviation is less than 5%. These small differences give a real opportunity to use mathematical models in real intervention in production processes.

5. References

[1]. ASAMI K., HASHIMOTO K., Surface analytical study of atmospheric corrosion of stainless steel, Proc. 13th International Corrosion Congress, paper 038, Melbourne (1996);

[2]. BEDDOES J., BUCCI K., The Influence of Surface Condition on the Localized Corrosion of 316L Stainless Steel Orthopaedic Implants,

Journal of Materials Science: Materials in Medicine, 10, 389 (1999);

[3]. HUDSON R. M., FREEMAN P. F., ALLAN G. K., Corrosion of Stainless Steel Above and Below Ground Level, Proc. 4th European Stainless Steel Science and Market Congress, Paris, France (2002);

[4].WALLINDER D., ODNEVALL WALLINDER I., LEYGRAF C., Influence of surface treatment of Type 304L Stainless steel on Atmospheric Corrosion Resistance in Urban and Marine Environments, Corrosion, 59, 220 (2003);

[5]. ASTM A321-90, Standard Specification for Steel Bars, Carbon, Quenched and Tempered (2001);

[6]. HERTING GUNILLA, WALLINDER I. O., LEYGRAF C., Factors that influence the release of metals from stainless steels exposed to physiological media, Corrosion Science, 48 2120-2132 (2006);

[7]. BARNES K. A., SINCLAIR C. R., WATSON D.H., Chemical migration and food contact materials, CRC Press, Woodhead Publishing Limited, Cambridge, England, 180-202 (2007);

[8]. HERTING G., Bioaccessibility of Stainless Steels-Importance of Bulk and Surface Features, Doctoral Thesis, Division of Corrosion Science School of Chemical Science and Engineering Royal Institute of Technology Stockholm, Sweden (2008);

[9] HERTING G., WALLINDER I. O., LEYGRAF C., Corrosion-induced release of chromium and iron from ferritic stainless steel grade AISI 430 in simulated food contact, Journal of Food Engineering 87 291-300 (2008);

[10] OKAZAKI Y., GOTOH E., Metal release from stainless steel, Co-Cr-Mo-Ni-Fe and Ni-Ti alloys in vascular implants, Elsevier, Corrosion Science 50, DOI: 10.1016/j.corsci.2008.09.002 3429-3438 (2008);

[11] SANCHES SILVA A., CRUZ J. M., SENDOR GARCIA R., FRANZ R., PASEIRO LOSADA, P., Kinetic migration studies from packaging films into meat products, ScienceDirect, Meat Science 77 238-245 (2007);

[12].TEHRANY E. A., DESOBRY S., Partition coefficient of migrants in food stimulants/polzmers systems, ScienceDirect, Food Chemistry 101 1714-1718 (2007);

[13]. SOOJIN J., IRUDAYARAJ J.M., Food Processing operations modeling - Design and Analysis, Second Edition, CRC Press-Taylor&Francis Group, 1-2 (2009).