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MATHEMATICAL MODELING OF THERMOMECHANICAL TREATMENT PROCESS APPLIED TO ALUMINUM BASE ALLOYS FOR AERONAUTICS

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ABSTRACT

To optimize the thermo-mechanical processing of aluminum base alloys, mathematical modeling was used in a laborious research program by planned experiment of thermomechanical treatment process applied to an Al-Zn system alloy. The paper presents the modeling stages, the type of mathematical model that allows for the analysis of the main influences (technological parameters),their influence size and the type of correlationsbetween them. The simulation of the thermomechanical treatment process by varying the process parameters within the tested values and thermomechanical treatment optimization (getting the optimal complex of strength and plasticity properties in a convenient treatment option) is possible using the mathematical model developed.

KEYWORDS: mathematical model, aluminum alloy, thermomechanical treatments

Introduction

Mathematical modeling means transposing of a real physical process into a mathematized form. The construction of the models associated to processes and systems is a vital part of the simulation process, being absolutely necessary to distinguish between different types of models that can be used by analysts. Process modeling can be considered as consisting of two stages: one that specifies the form under which the model must be expressed, and the second describing how it is used to provide a series of predictions or provide the optimal solution of the problem studied. In this paper we conducted the mathematical model of thermomechanical treatment process applied to alloys studied by statistical methods i.e. regression analysis by active experiment.

Currently, the most effective methods for programming the experiment are those concerning solving extreme problems involving the determination of levels of independent quantities (input), u1, u2,...uk, for which the objective function:

$$y = f(u_1, u_2, ..., u_k) \qquad (1)$$

has extreme values (maximum or minimum) as well as the calculation of these values.

For each basic factor the base levels, u_{01}, u_{02} respectively u_{03}, are determined, whichare actually thecoordinates in the factorial space of the randomlychosen starting point as well as the ranges Δu_1, Δu_2 and Δu_3. By addingthe variation interval to the basic level, the superior level is obtained, and by lowering it the inferior level of the factor is obtained. If the encoded value of ui factor is denoted by xi, resulting from the relationship:

$$x_i = \frac{u_i - u_{0i}}{\Delta u_i}$$

the higher level will be coded with a score, the lower by -1, and the basic level to 0.

Experimental conditions

In the case of high strength aluminum alloy AlZn5.7Mg2.6 processed according to the schedule in Figure 1, in which the solution hardening involves primarily hardening compounds leaching, a process that takes place through activation of diffusion phenomena in solid form, taking into account diffusion laws, it can be said that the solution temperature and the maintaining time at this temperature will have a decisive influence on the effectiveness of treatment by their influence on the diffusion coefficients and on the process dynamics.

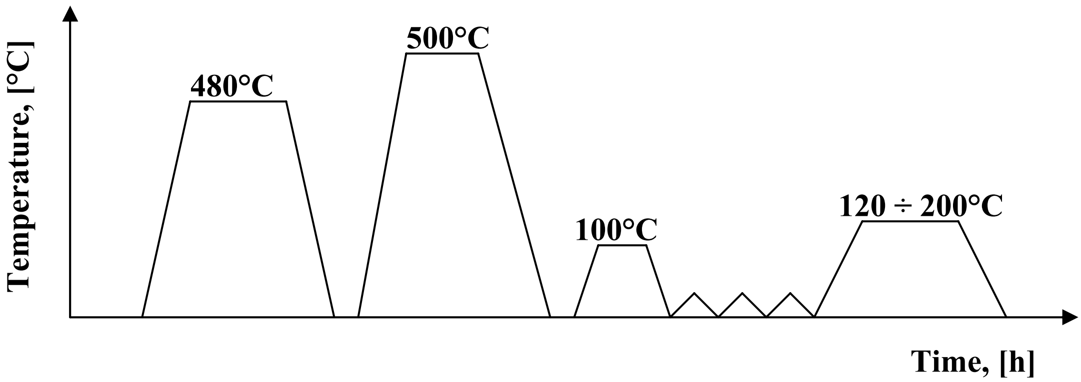

***Fig.1** Technological scheme of achieving experiments*
I-homogenization; II-solution hardening; III -artificial aging;
IV - cold plastic deformation, V - artificial aging

Cold plastic deformation was experimented with three different degrees of deformation, namely: ε1 = 10%, ε2 = ε3 = 20% and 30%. In this way the hard compounds deform (elongate in the direction of the deformation) or crumble.

Given the above, the following factors will be considered as process parameters: 1- artificial aging temperature - T, [° C]; 2- maintaining time – τ [h]; 3- the degree of deformation – ε [%].

Table 1 shows the correspondence between different levels of the factors expressed in natural values with those expressed in coded values for the three factors used in the thermomechanical treatment process.

***Table 1.** Correspondence between the values of the factors expressed in natural and coded units [1]*

Factor	Process temperature		Process time		The degree of deformation	
	Natural units, in ° C	Values coded	Natural units, in hours	Values coded	Natural units, in hours	Values coded
Base level	$u_{01} = 160$	$\frac{160-160}{40} = 0$	$u_{02} = 12$	$\frac{12-12}{4} = 0$	$u_{03} = 20$	$\frac{20-20}{10} = 0$
The ranges	$\Delta u_1 = 40$	0	$\Delta u_2 = 8$	0	$\Delta u_3 = 10$	0
Higher	$u_{1s} = 200$	$\frac{200-160}{40} = +1$	$u_{2s} = 20$	$\frac{20-12}{8} = +1$	$u_{3s} = 30$	$\frac{30-20}{10} = +1$
Lower	$u_{1i} = 120$	$\frac{120-160}{40} = -1$	$u_{2i} = 4$	$\frac{12-20}{8} = -1$	$u_{3i} = 10$	$\frac{10-20}{10} = -1$

In the coded representation of the experiment the following notations and symbols were used:
- x1 – artificial aging temperature, T, ° C;
- x2 – mentaining time, τ, [h];
- x3- deformation degree, ε [%];
- Y1 - tensile strength, Rm, [MPa];
- Y2 - yield strength, Rp02 [MPa];
- Y3 – specific elongation at break, A5, [%];
- Y4 - hardness, HB;

Between the natural and coded values of x_i factors there are the following linking relations:

$$x_1 = \frac{t - t_0}{\Delta t}, \; x_2 = \frac{\tau - \tau_0}{\Delta \tau}, \; x_3 = \frac{\varepsilon - \varepsilon_0}{\Delta \varepsilon}, \qquad (2)$$

To determine the dispersion of results reproducibility , six experiments were performed at the basic levels of the factors. In this way a full factorial experiment of the type 2^3 was performed as shown inTable 2.

***Table 2.** Matrix determination for the factorial experiment of the type 2^3 [1]*

Nr. exp.	X_0	X_1	X_2	X_3	$X_1 X_2$	$X_1 X_3$	$X_2 X_3$	Y_1	Y_2	Y_3	Y_4
1	+1	+1	+1	+1	+1	+1	+1	487	424	8,1	135
2	+1	-1	+1	+1	-1	-1	+1	630	591	6,8	194
3	+1	+1	-1	+1	-1	+1	-1	455	384	8,7	122
4	+1	-1	-1	+1	+1	-1	-1	569	516	7,7	155
5	+1	+1	+1	-1	+1	-1	-1	435	391	10,4	121
6	+1	-1	+1	-1	-1	+1	-1	577	531	8,4	171
7	+1	+1	-1	-1	-1	-1	+1	411	377	11,0	109
8	+1	-1	-1	-1	+1	+1	+1	507	468	9,5	135
9	+1	0	0	0	0	0	0	498	452	10.0	123
10	+1	0	0	0	0	0	0	512	473	9,0	145
11	+1	0	0	0	0	0	0	506	459	8,9	143
12	+1	0	0	0	0	0	0	503	456	8,5	140
13	+1	0	0	0	0	0	0	514	475	9,2	148
14	+1	0	0	0	0	0	0	509	462	9,1	144

Considering the function Yi as the analytical expression of the order I model, that is:

$$Y_i = c_0 + \sum_{i=1}^{3} c_i \cdot x_i + \sum_{\substack{i=1 \\ j=1 \\ i \neq j}}^{3} c_{ij} x_i x_j \qquad (3)$$

Equation (3) is written as matrix form:

$$Y = X \cdot C \qquad (4)$$

where: X is the matrix of experimental conditions

$$X = \begin{Vmatrix} x_{01} & x_{11} & x_{21} & \cdots & x_{m1} \\ x_{02} & x_{12} & x_{22} & \cdots & x_{m2} \\ x_{03} & x_{13} & x_{23} & \cdots & x_{m3} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{0n} & x_{1n} & x_{2n} & \cdots & x_{mn} \end{Vmatrix}$$

m - number of terms of equation (3);
n - number of considered experiences;
C – column vector of coefficients c_i
C = [c0, c1,..., cn] T
T – matrix transposition symbol
Y - matrix of experimental results

$$\mathbf{Y} = [\, Y_1 , Y_2 , \ldots , Y_n \,]^T \qquad (5)$$

where : Y_1 = [487 630 455 569 435 577 411 507 498 512 506 503 514 509]
Y_2 = [424 591 384 516 391 531 377 468 452 473 459 456 475 462]
Y_3 = [8,1 6,8 8,7 7,7 10,4 8,4 11 9,5 10 9 8,9 8,5 9,2 9.1]
Y_4 =[135 194 122 155 121 171 109 135 123 145 143 140 148 144]

For this case, the linear function (3) has a particular form:

$$Y_i = c_0 + c_1 \cdot x_1 + c_2 \cdot x_2 + c_3 \cdot x_3 + c_{12} \cdot x_1 \cdot x_2 + c_{13} x_1 \cdot x_3 + c_{23} \cdot x_2 \cdot x_3 \qquad (6)$$

Multiplying at the left side each term of the matrix equation by unitary matrix

$$E = [XT\ X]^{-1} \times XT \qquad (7)$$

there follows:

$$C = [XT\ X \times]^{-1} [XT \text{ x } Y] \qquad (8)$$

expression that represents the relationship for calculating the coefficients of regression equation. Using the values in Table 2, based on relation (8), first order models coefficients are obtained, summarized in Table 3.

***Table 3.** Values of first-order models coefficients*

c_i \ Y_i	Y_1	Y_2	Y_3	Y_4
c_0	508.0714	461.3571	8.95	141.7857
c_1	-61.875	-66.25	0.725	-21
c_2	23.375	24	-0.4	12.5
c_3	26.375	18.5	-1	8.75
c_{12}	-9.375	-10.5	0.1	-6.25
c_{13}	-2.375	-8.5	-0.15	-2
c_{23}	-0.125	4.75	0.025	0.5

Therefore the mathematical model of first-order equation (7) for each property in part, is:

$$Y_1 = 508,0714 - 61,875 \cdot x_1 + 23,375 \cdot x_2 + 26,375 \cdot x_3 - 9,375 \cdot x_1 \cdot x_2 - 2,375 \cdot x_1 \cdot x_3 - 0,125 \cdot x_2 \cdot x_3 \quad (9)$$

$$Y_2 = 461,3571 - 66,25 \cdot x_1 + 24 \cdot x_2 + 18,5 \cdot x_3 - 10,5 \cdot x_1 \cdot x_2 - 8,5 \cdot x_1 \cdot x_3 + 4,75 \cdot x_2 \cdot x_3 \quad (10)$$

$$Y_3 = 8,95 + 0,725 \cdot x_1 - 0,4 \cdot x_2 - \cdot x_3 + 0,1 \cdot x_1 \cdot x_2 - 0,15 x_1 \cdot x_3 + 0,025 \cdot x_2 \cdot x_3 \quad (11)$$

$$Y_4 = 141,7857 - 21 \cdot x_1 + 12,5 \cdot x_2 + 8,75 \cdot x_3 - 6,25 \cdot x_1 \cdot x_2 - 2 x_1 \cdot x_3 + 0,5 \cdot x_2 \cdot x_3 \quad (12)$$

By replacing the variables xi with relations (2) and doing the respective calculations in the above equations, the following equations are obtained representing expressions of mathematical first –order models for the four properties considered:

$$Y_1(t,\tau,\varepsilon) = 592,1339 - 1,0766\, t + 7,6406\, \tau + 3,6063\, \varepsilon - 0,0293\, t \cdot \tau - 0,0059\, t \cdot \varepsilon - 0,0016\, \tau \cdot \varepsilon \quad (13)$$

$$Y_2(t,\tau,\varepsilon) = 536,621 - 0,8375 t + 7,0625 \tau + 4,5375 \varepsilon - 0,0328 t \cdot \tau - 0,0213 t \cdot \varepsilon + 0,0594 \tau \cdot \varepsilon \quad (14)$$

$$Y_3(t,\tau,\varepsilon) = 8,125 + 0,0219 \cdot t - 0,1063 \cdot \tau - 0,0438 \cdot \varepsilon + 0,0003 \cdot t \cdot \tau - 0,0004 \cdot t \cdot \varepsilon + 0,0003 \cdot \tau \cdot \varepsilon \quad (15)$$

$$Y_4(t,\tau,\varepsilon) = 137,5357 - 0,1906\, t + 4,5625\, \tau + 1,6 \cdot \varepsilon - 0,0195\, t \cdot \tau - 0,005 \cdot t \cdot \varepsilon + 0,0063\, \tau \cdot \varepsilon \quad (16)$$

First-order mathematical models have been verified statistically, using Fischer criterion to decide if they can be used for studying the analysed process or if it is necessary to determine the higher order models.

The values calculated using Fischer criterion for the four first order mathematical models are summarized in Table 4.

Table 4 shows that all models are consistent with the experimental data and can be used in process optimization.

To verify the significance of coefficients for the appropriate model, the following ratio is determined for each coefficient:

$$F_{csi} = \frac{PM_{bi}}{PM_{rez}}$$

Table 4. *Calculation data for checking model adequacy*

Calculated values	Y_1	Y_2	Y_3	Y_4
SP_{rez}	224.1752	478.2142	1.525	419.3571
PM_{rez}	32.025	68.316	0.22	59.90815714
SP_{er}	176	430.8333	1.2283	401.5000
PM_{er}	35.2	86.16666	0.2457	80.3
SP_{in}	48.1752	47.3809	0.2967	17.8571
PM_{in}	24.0876	23.69045	0.1484	8.92855
F_{ci}	0.6843	0.275	0.60388	0.11118991
Accordance	Concorde	Concorde	Concorde	Concorde

Where PMrez is the average square of reziduals calculated in Table 4 PM_{bi} is the average square of the coefficients which are calculated with the matrix relation

*PM*bi = *D (X ^{t} Y)*, where D is the diagonal matrix with the model coefficients as the main diagonal elements, the other elements of the matrix being null.

X is the matrix of experimental conditions at the considered levels (-1, 0, 1)

Y – the matrix of experimental results at the levels considered (-1, 0, 1) Using equation (17) we obtain the values of the Fcsi ratio for the model coefficients shown in Table 4.

Coefficients c_i for which Fcsi> FT [1, frez, (1-α)%] are considered significant; in this case FT (1, 7, 95%) = 5.79.

Thus the four equations become:

$$Y_1(t,\tau,\varepsilon) = 611,51 - 1,195 \cdot t + 7,609 \cdot \tau + 2,64 \cdot \varepsilon - 0,029 \cdot t \cdot \tau \quad (18)$$

$$Y_2(t,\tau,\varepsilon) = 590,371 - 1,262 \cdot t + 8.25 \cdot \tau + 1,85 \cdot \varepsilon - 0,032 \cdot t \cdot \tau \quad (19)$$

$$Y_3(t,\tau,\varepsilon) = 8,65 + 0,018 \cdot t - 0,05 \cdot \tau - 0,1 \cdot \varepsilon \quad (20)$$

$$Y_4(t,\tau,\varepsilon) = 189,535 - 0,525 \cdot t + 1,562 \cdot \tau + 0,875 \cdot \varepsilon \quad (21)$$

Equations (in t, τ and ε) (18), (19), (20) and (21) are valid for t = 120 ... 200 °C, τ = 4 ... 20 hours and ε = 10 .. .30%. Using relations (18), (19), (20) and (21) for examplification, we have drawn graphs of variation of each property function of time for a treatment temperature of 160 ° C, in the case of the deformed alloy where the degree of deformation is - 20%.

As shown in Figures 2 ÷5 mechanical property values determined by calculations using mathematical models are close to the experimentally determined values. This is the proof that the mathematical modeling achieved allow for simulation of thermomechanical treatment process con- ducted according to the scheme in Figure 1.

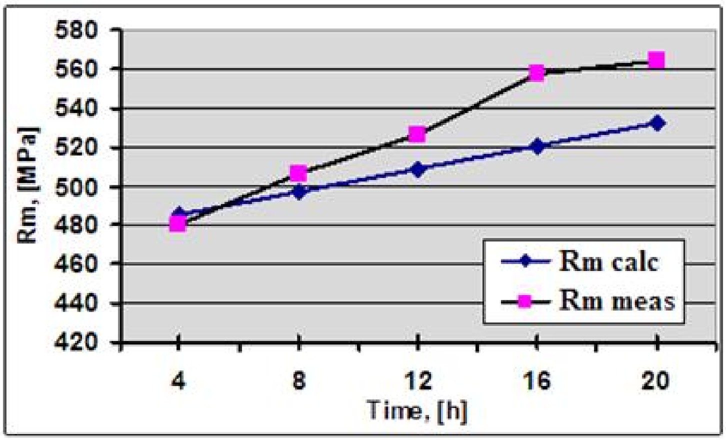

Fig.2. *Variation of mechanical resistance according to treatment time.*

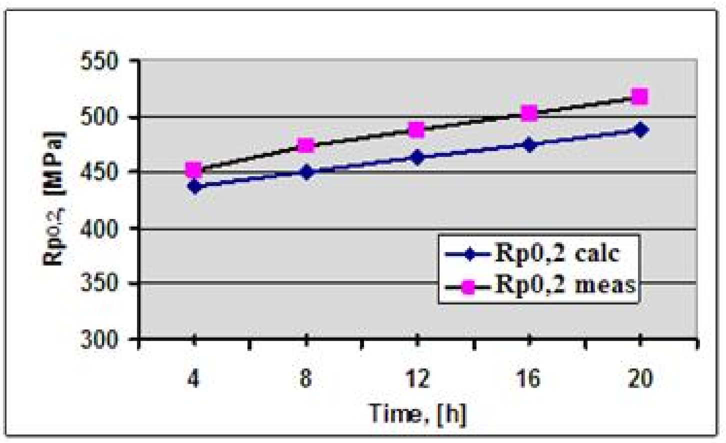

Fig.3. *Variation of yield stress with treatment time.*

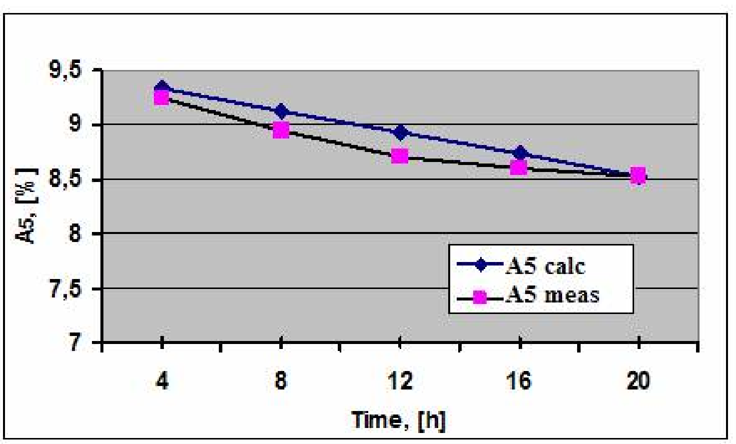

Fig.4. *Variation of elongation at break with treatment time.*

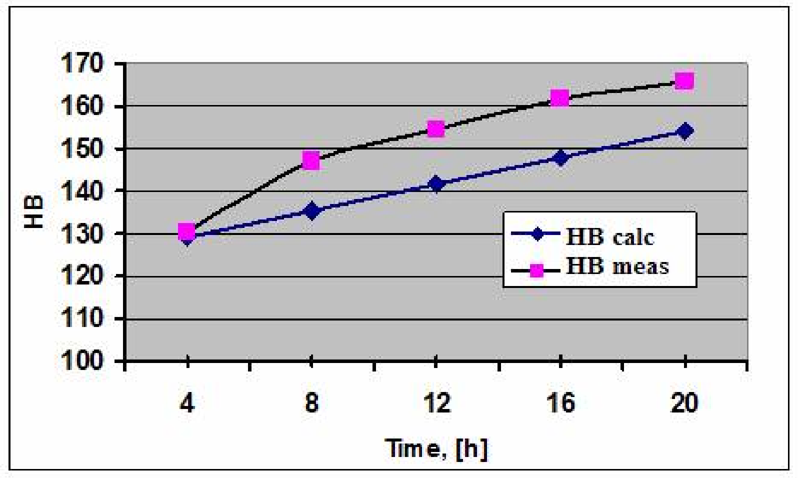

Fig.5. *Brinell hardness variation with treatment time.*

Conclusions

The mathematical model presented in the set of equations (30)÷(33) allows simulation of thermomechanical treatment process, by varying the process parameters values, within experimental limits.

The aging factor has the biggest influence on the increase of mechanical strength as the value of the influence factor coefficient is positive and of the highest value. The next important influencing factor is the degree of cold plastic deformation, as the coefficient of this factor shows, mechanical strength properties increase as the degree of deformation value increases. The value of the temperature parameter coefficient indicates that when the temperature increases, there is a decrease in strength properties.

Elongation at break is influenced according to the model, first by treatment temperature, meaning that as treatment temperature increases, the elongation increases too. From the analysis of the regression equations obtained, it results that an increase in the final aging temperature, in the range considered, above 180 C will lead to lower strength characteristics (tensile strength, yield strength and hardness); instead the plasticity increases (relative elongation increases to some extent with increasing aging temperature).

Mechanical strength depending on aging time increases with time, and elongation at break decreases.

Regarding the influence of the degree of deformation on the properties of resistance (Rm, Rp02 and hardness) that they have higher values than those prescribed by EN 485-2-2007, for all three degrees of deformation.

The mathematical model presented allows for establishing the technological conditions that can lead to obtaining the optimal properties complex of strength and plasticity, in alternative technology involving minimal costs.

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