THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
N°. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

MATHEMATICAL MODELING OF THE CARBONITRIDING PROCESS FOR OLC 25 STEEL

Marian-Iulian NEACȘU
"Dunarea de Jos" University of Galati
e-mail: mneacsu@ugal.ro

ABSTRACT

The paper is based on research on several experimental carbonitriding regimes of OLC25 steel samples.

Following the experiment for each regime, the HV microhardness values of the treated samples were measured at various points (identical for all samples) along the depth of the carbonitrided layer. The results of these measurements were compiled into a database that was used to create a mathematical model of the carbonitriding process.

The paper presents the results of mathematical modeling based on an active experimental study of the carbonitriding process applied to OLC25 steel samples.

KEYWORDS: steel, carbonitriding, mathematical modeling, simulation

1. Introduction

Thermochemical treatments are technological processes applied to metallic materials, especially steels, with the main objective of modifying the chemical composition of the surface layers of the parts. These treatments consist of introducing active chemical elements (such as carbon, nitrogen, boron, etc.) into the surface layer of the material, by diffusion, at high temperatures. Thus, unlike thermophysical treatments, which produce only internal structural changes without altering the chemical composition, thermochemical treatments simultaneously induce structural and chemical transformations in the surface region of the part [1].

The clear differentiation between the characteristics of the treated layer and the core represents the essence and fundamental purpose of applying thermochemical treatments in industry [2].

For thermochemical treatments to be effective and to lead to the formation of a surface layer with desired properties, it is essential that the three fundamental stages of the process - dissociation of the active substance (Ds), adsorption of active atoms on the surface of the part (A) and their diffusion into the material (D) - are correctly balanced [2].

Carbonitriding is a complex thermochemical treatment aimed at simultaneously enriching the surface layer of metal parts with carbon and nitrogen atoms, thus combining the advantages offered by carburizing (increased hardness through carbon addition) and nitriding (high resistance to wear and corrosion through nitrogen addition). Basically, this process brings together in a single step the effects of the two treatments, resulting in a surface layer that benefits from superior mechanical and chemical characteristics [3, 4].

The treatment is carried out in special environments (solid, liquid or gaseous), which have the capacity to provide active carbon and nitrogen atoms. The temperature at which the process takes place is intermediate between that specific to nitriding (500-550 °C) and that of carburizing (900-950 °C), which allows for an efficient diffusion of both elements into the base material [5].

In the carbonitriding process, a thermochemical treatment used to improve the mechanical properties of metal parts, a gas mixture consisting predominantly of methane (CH_4) in proportions ranging from 65% to 75%, and ammonia (NH_3) in proportions ranging from 25% to 35% is frequently used. The treatment is carried out at temperatures between 600 and 750 °C [3, 6, 7].

To ensure efficient treatment, the gas composition is precisely controlled, using special autonomous installations. These allow maintaining a constant composition of the gas mixture in the retort (the container where the treatment takes place), and regulating the degree of ammonia dissociation, an essential parameter for controlling the nitrogen diffusion process in the steel.

The duration of keeping the parts in the active atmosphere depends directly on the depth of the

THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
No. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

desired layer, but is generally shorter than in the case of classical nitriding. In practice, this duration is not fixed, but is determined experimentally, by testing representative samples until the desired characteristics of the layer are achieved [8].

Process modeling is an essential tool both in the design stage of metallurgical installations and in the analysis of their operation under real conditions. By using mathematical models, in combination with the advantages offered by modern information technology, it becomes possible to identify and establish optimal operating regimes for various metallurgical processes. Progress in the development of the specific mathematical apparatus, as well as in the development and application of advanced statistical methods, has allowed the optimization problem to be approached as not only possible, but also extremely efficient from a technical and economic point of view [9].

The mathematical models resulting from these methods not only allow the determination of extreme (optimal) operating conditions, but also constitute a valuable source of useful information for the real-time management and regulation of metallurgical processes. Although several works on mathematical optimization methods have been published in the Romanian technical literature in recent times, few of them deal in an applied manner with the particularities of processes specific to the metallurgical industry [10].

The process of developing a mathematical model based on statistical methods involves two main stages. In the first stage, called the preliminary experiment, essential issues related to the identification and selection of the main factors influencing the analysed process, as well as the possible interactions between them, are resolved. The second stage, known as the basic experiment, consists of the actual construction of the mathematical model and the performance of a detailed statistical analysis thereof [10].

The modeling process itself usually involves two fundamental steps:

• in the first step, the form of expression of the model is established, this can be, for example, in the form of a system of equations, an algorithm or a set of logical rules.

• in the second step, the model is used to make a series of predictions on the behavior of the system, to simulate possible scenarios or to identify the optimal solution to a given problem [9].

An essential aspect of mathematical models is the use of concise and rigorous notations, which allow a clear representation of the possible states of a system and the way in which these states evolve over time, depending on the modification of certain variables. This approach provides a solid basis for making predictions and simulations, as the model can be mathematically manipulated to highlight the behavior of the system in various scenarios [11].

For a mathematical model to be correct and useful, it is necessary to define a formal structure, based on axioms (basic principles accepted as true), theorems (propositions proven based on these axioms), and standardized mathematical procedures. The choice of these elements constitutes a fundamental step in the construction of the model, as they determine the limits of applicability and the degree of precision of the predictions it can generate [11].

An important advantage of mathematical models is the relatively low cost of their use, especially compared to physical models. Once formulated, they can be quickly implemented on a computer, and the analysis can be easily repeated for different data sets or conditions. Additionally, their structure allows for general conclusions to be obtained about the behavior of the system, without the need for expensive physical experiments [10].

2. Experimental conditions and obtained results

In this paper, we developed a mathematical model of the thermochemical carbonitriding treatment process applied to OLC25 steel, using statistical methods, namely regression analysis through an active experiment [12].

This approach to the problem involves experimental programming, that is:

• establishing the necessary and sufficient experiments, as well as the conditions for their implementation.

• determining by statistical methods the regression equation, which represents with a calculable degree of approximation, the process model.

• determining the conditions for achieving the optimal value, i.e., the performance of the analysed process [18].

In the paper, several experimental regimes of carbonitriding of OLC25 samples were studied (researched).

The experimental regimes were the following:

Ammonia/methane ratio = 0.25% at temperatures T_1 = 550 °C, T_2 = 650 °C, T_3 = 750 °C, with a holding time of 150 minutes.

Ammonia/methane ratio = 0.15% at temperatures T_1 = 550 °C, T_2 = 650 °C, T_3 = 750 °C, with a holding time of 150 minutes.

Ammonia/methane ratio = 0.05% at temperatures T_1 = 550 °C, T_2 = 650 °C, T_3 = 750 °C, with a holding time of 150 minutes.

THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
No. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

After carrying out the experiment for each regime, the HV microhardness of the treated samples was measured at various points (identical for all measurements) along the depth of the carbonitrided layer.

The results of these measurements were organized into a database that we used to create a mathematical model of the carbonitriding process.

We considered the following technological parameters as the main influencing factors (independent variables):

- temperature of the thermochemical treatment – t, °C;
- ammonia percentage – NH_3, %;
- depth of the carbonitrided layer – As, mm.

The parameter to be optimized is the HV microhardness.

To establish the base level and the variation range of the influencing factors, we used data from the specialized literature [13].

To establish the base level and the variation range of the influencing factors, we also used values obtained from HV microhardness tests.

In order to encode the experimental design, the following notations and symbols were used:

Independent variables:

x1 - temperature of thermochemical treatment;

x2 - ammonia percentage;

x3 - depth of the carbonitrided layer.

Dependent variables (parameters to be optimized):

Y – HV microhardness, [MPa];

There are the following relationships between the natural and coded values of the factors x_i:$x_1 = (t-t_0)/\Delta t$; $x_2 = (NH_3-NH_{30})/\Delta NH_3$; $x_3 = (As-As_0)/(\Delta As)$.

The Yi values are expressed in natural units.

In order to create the mathematical model for the carbonitriding process under investigation, we considered as process parameters: treatment temperature (t1, t2, t3), ammonia/methane ratio and carbonitrided layer depth with the following values:

As = 0.09; 0.17; 0.25; 0.33; 0.47; 0.49; 0.57, for all variants, the treatment time was 150 minutes.

According to this method, the number of experiments taken into account is 2k.

The equation of the mathematical model has the general form: y = f(x_1,x_2,….x_k) where k represents the number of parameters taken into account. In the case of the present work, we considered the equation:

$Y = f(x_1,x_2,x_3,x_4=ct)$, where x_1 is the encoded quantity for temperature, x_2 is the encoded quantity for the ammonia/methane ratio, x_3 is the encoded quantity for the layer depth, x_4=ct is the encoded quantity for the treatment time.

The modeling variant performed shows the dependence of the HV size depending on the three parameters (temperature, ammonia percentage and layer depth).

Before drawing up the experiment matrix, it is necessary to establish the minimum, maximum and base values for the process parameters (Table 1).

Table 1. *Minimum, maximum and baseline values for process parameters*

Coded variable	Maximum value (+1)	Base value (0)	Minimum value (-1)
$x_1 \rightarrow t$	750 °C	650 °C	550 °C
$x_2 \rightarrow NH_3$	25%	15%	5%
$x_3 \rightarrow A_s$	0.57 mm	0.33 mm	0.09 mm
$x_4 \rightarrow \tau$	150 min	150 min	150 min

The relationships between the coded quantities (x_1, x_2, x_3, x_4) and the natural quantities (temperature, ammonia/methane ratio, layer depth and time) are given by the following:

$$x_1 = \frac{t - t_0}{\Delta_t};\ x_2 = \frac{NH_3 - NH_{30}}{\Delta_{NH_3}};\ x_3 = \frac{A_s - A_{s0}}{\Delta A_s}$$

x_4 = treatment time = ct.

For temperature, the minimum value is 550 °C and will be coded with (-1), the maximum is 750 °C and will be coded with (+1), and the value of 650 °C will be considered the "base value", coded with (0).

$\Delta_t = 650-550 = 750-650 \Rightarrow \Delta_t = 100$ °C, which is called the range of variation of the temperature parameter.

For NH_3, the minimum value = 5%, coded with (-1), the maximum value = 25%, coded with (+1), and the "base value" = 15%, coded with (0).

The interval $\Delta_{NH_3} = 15 - 5 = 25 - 15 \Rightarrow \Delta_{NH_3} = 10\%$, is called the variation interval of the NH_3 parameter.

For the layer depth (A_s), the minimum value is 0.09 mm, coded with (-1), the maximum value is 0.57 mm, coded with (+1), and the value of 0.33 will be considered the "base value", marked with (0).

The time for each experiment had a fixed value of 150 min.

THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
N°. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

The equation of the mathematical model has the form: y=f(t°,NH_3,A_s)

Codified we will make the association:

$$x_1 \rightarrow t°C; x_2 \rightarrow NH_3, x_3 \rightarrow A_s; y \rightarrow HV$$

$$y = C_0 + C_1X_1 + C_2X_2 + C_3X_3 + C_{12}X_1X_2 + C_{13}X_1X_3 + C_{23}X_2X_3$$

$$y = -122{,}591 + 0{,}678t - 1633{,}269A + 578{,}039A_s - 1{,}38tA_s + 3{,}637tA - 1119{,}791AA_s$$

Following the application of mathematical modeling, when the dependence of the HV microhardness on three parameters of the carbonitriding process is shown, namely carbonitriding temperature, ammonia percentage, and layer depth - it is found that there are minor differences between the values obtained from the mathematical model calculations and the values measured under the same conditions. The graphical representation of these differences is shown in Figures from 1 to 8.

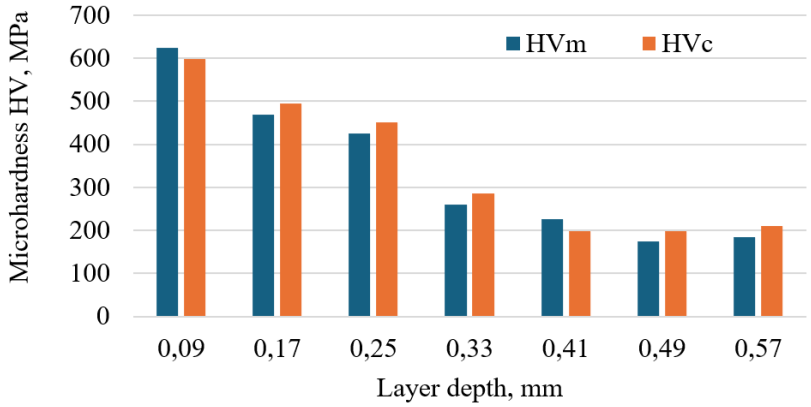

Fig. 1. *Comparison of measured values with those calculated at a temperature of 750 °C, for an ammonia concentration of 25%, HVm = Measured HV, HVc = Calculated HV*

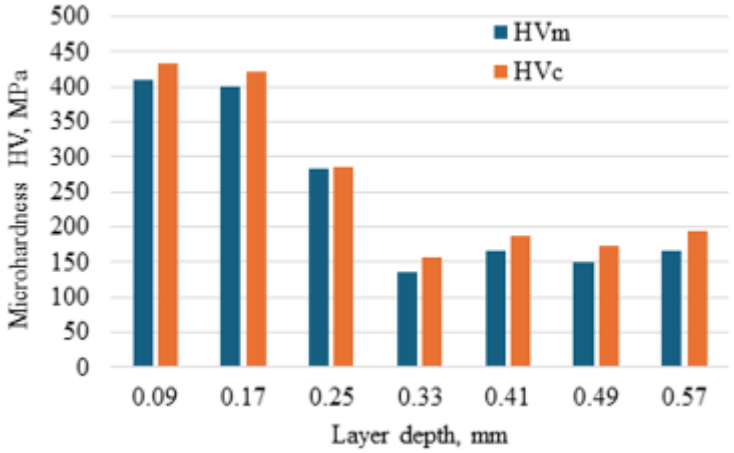

Fig. 2. *Comparison of measured values with those calculated at a temperature of 750 °C, for an ammonia concentration of 15%, HVm = Measured HV, HVc = Calculated HV*

THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
N°. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

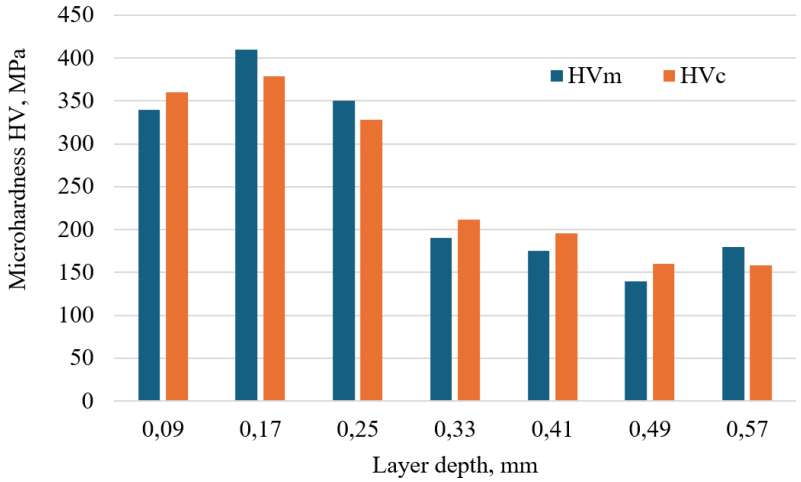

Fig. 3. *Comparison of measured values with those calculated at a temperature of 750 °C, for an ammonia concentration of 5%, HVm = Measured HV, HVc = Calculated HV*

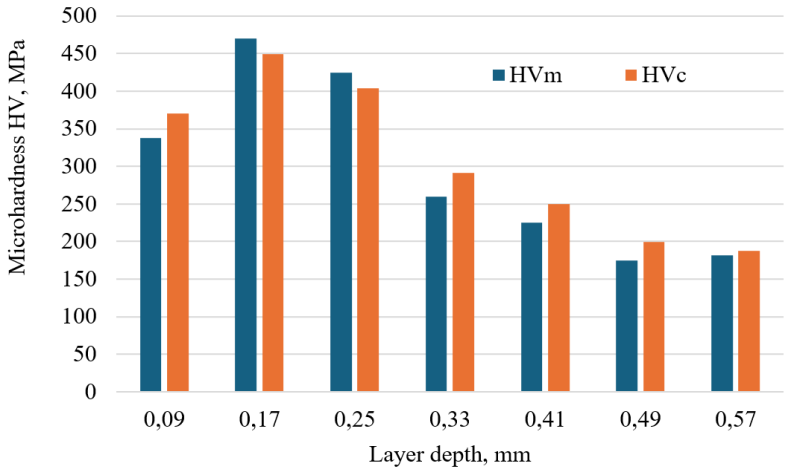

Fig. 4. *Comparison of measured values with those calculated at a temperature of 650 °C, for an ammonia concentration of 25%, HVm = Measured HV, HVc = Calculated HV*

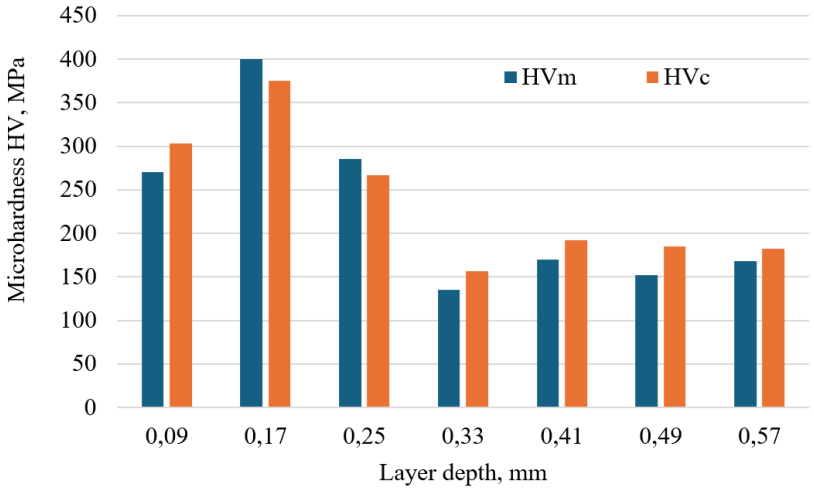

Fig. 5. *Comparison of measured values with those calculated at a temperature of 650 °C, for an ammonia concentration of 15%, HVm = Measured HV, HVc = Calculated HV*

THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
Nº. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

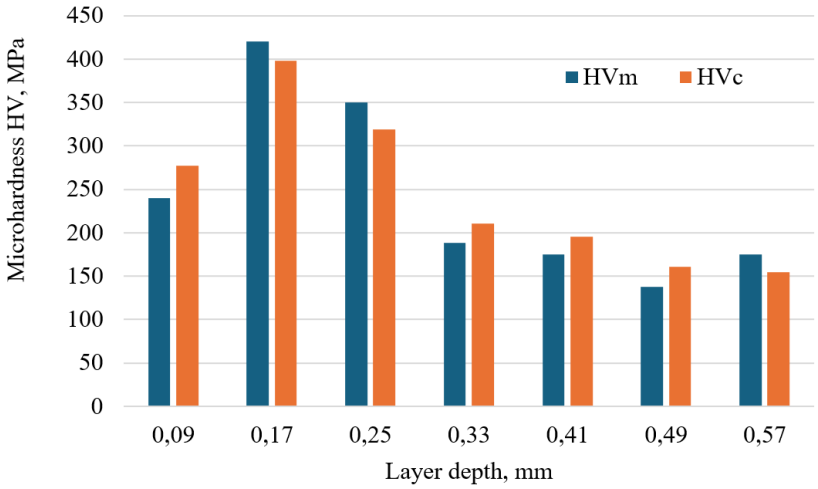

Fig. 6. *Comparison of measured values with those calculated at a temperature of 650 °C, for an ammonia concentration of 5%, HVm = Measured HV, HVc = Calculated HV*

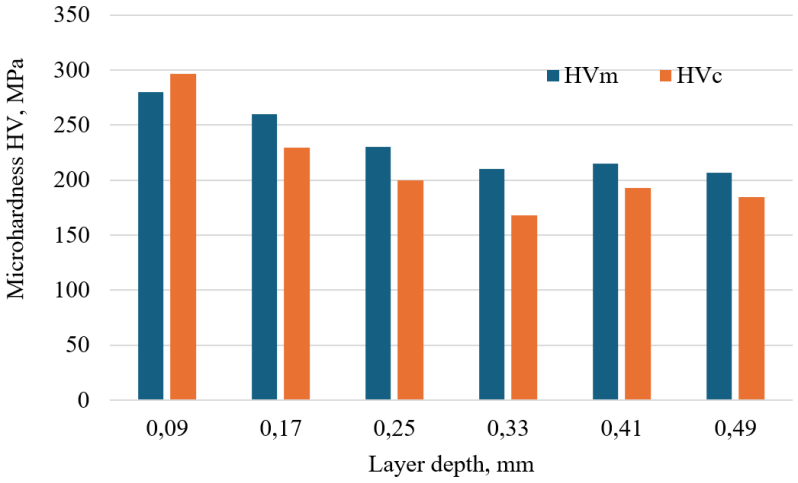

Fig. 7. *Comparison of measured values with those calculated at a temperature of 550 °C, for an ammonia concentration of 25%, HVm = Measured HV, HVc = Calculated HV*

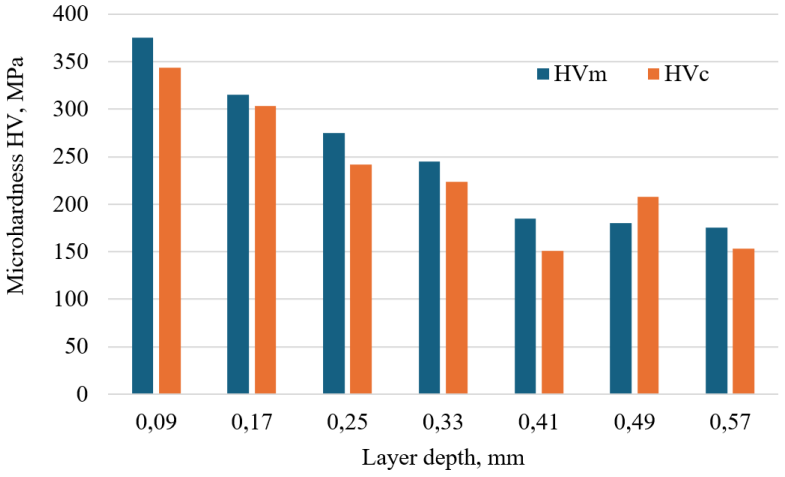

Fig. 8. *Comparison of measured values with those calculated at a temperature of 550 °C, for an ammonia concentration of 5%, HVm = Measured HV, HVc = Calculated HV*

THE ANNALS OF "DUNAREA DE JOS" UNIVERSITY OF GALATI
FASCICLE IX. METALLURGY AND MATERIALS SCIENCE
No. 4 - 2025, ISSN 2668-4748; e-ISSN 2668-4756
Article DOI: https://doi.org/10.35219/mms.2025.4.17

3. Conclusions

The objective of this work was to develop a mathematical model capable of describing the carbonitriding process applied to OLC25 steel, more precisely to show the dependence of the HV microhardness on the process parameters.

During the work, the following main conclusions were highlighted:

• Importance of the carbonitriding treatment: By combining the diffusion of carbon and nitrogen at controlled temperatures, carbonitriding allows the achievement of a hard and wear-resistant surface layer, without negatively affecting the toughness of the core. This is particularly valuable in the case of low-alloy steels, such as OLC25.

• Mathematical modelling: A model was developed based on an active experiment that assumed a finite number of experiments with the variation of the carbonitriding process parameters. Four variants of specific mathematical equations were developed, which show the dependence of the HV microhardness as a function of the values of the carbonitriding process parameters. The model allows the estimation of HV microhardness values depending on the treatment temperature, ammonia concentration and carbonitrided layer depth.

• Model validation: The results obtained through numerical simulation were compared with experimental data obtained during the experiments performed and showed a good correlation, which confirms the validity of the theoretical approach.

• Process optimization: The use of the mathematical model allows rapid testing and optimization of technological parameters (temperature and ammonia concentration) without resorting to expensive experiments. Thus, efficient treatments can be obtained, tailored to the functional requirements of the part.

• Industrial applications: The proposed model has a high potential for application in industry, especially in digitally assisted thermochemical treatment processes, contributing to improved precision and reduced material losses.

In conclusion, the mathematical modelling of the carbonitriding process for OLC25 steel represents a valuable tool both theoretically and practically, providing support for efficient technological decisions, based on rigorous predictive calculations. The present work represents a step towards the integration of mathematical methods in the control and optimization of modern thermochemical treatments.

References

[1]. Crainic N., *Tratamente termochimice*, Editura MatrixRom, București, 2007.
[2]. Gîrbea I. D., *Tratamente termice și termochimice – Ghid de laborator*, Editura Universității Tehnice din Cluj-Napoca, 2018.
[3]. Țugui A., *Oțeluri și tratamente termice*, Editura Didactică și Pedagogică, București, 2002.
[4]. Allen J. Fuller Jr., *Introduction to Carburizing and Carbonitriding*, in ASM Handbook, 2013.
[5]. Mitelea I., Tîțu I., Giurgiu L., *Tratamente termice – Teorie și aplicații*, Editura Universității „Lucian Blaga" din Sibiu, 2016.
[6]. Marin N., *Tratamente termice ale oțelurilor aliate*, Editura Universitaria, Craiova, 2014.
[7]. Popescu L. G., *Modificări structurale în oțeluri supuse tratamentelor termice*, Editura Politehnica, Timișoara, 2011.
[8]. Totten G. E., *Tratamentul termic al oțelului: Metalurgie și tehnologii*, CRC Press, Taylor & Francis, 2007.
[9]. Crainic N., *Tratamente termochimice*, Editura MatrixRom, București, 2007.
[10]. Ionescu V., *Bazele modelării matematice în inginerie*, Editura Politehnica Press, București, 2007.
[11]. Bălan C., *Modelare matematică și simulare numerică în inginerie*, Editura MatrixRom, București, 2009.
[12]. Dowden John M., *The Mathematics of Thermal Modeling: An Introduction to the Theory of Laser Material Processing*, Editura: CRC Press, 2001.