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EXTRACTING KNOWLEDGE FROM INTEGRATED EXPERIMENTAL DATA ON THE ADI MANUFACTURE

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Abstract

The problem discussed in this article relates to the integration of knowledge about the design process of products from ADI. Specialised domain knowledge, often resulting from costly experiments, published in the world in a large number of magazines, is an invaluable source of information for its users and researchers. The authors draw attention to the need to develop a system that will facilitate selective access to specific passages of this knowledge, allowing for its automatic processing. The cost of developing such a system is certainly lower than the cost of multiple repetition of the experiments. Proposed under the system, aggregation and centralisation of the results of studies already carried out may be the basis for planning and execution of subsequent experiments, covering areas hitherto unexplored. Another outcome may relate to the creation of new knowledge through the discovery of relationships and dependencies that are not visible in individual, single, experiments, but emerge when the results of a large number of different tests are compared.

This paper proposes the use of artificial neural networks to explore the relations between the properties of ADI and selected heat treatment parameters based on a set of integrated experimental data from various publications. In the future, this form of knowledge representation may be used in intelligent computer systems in the knowledge acquisition module on the manufacturing process of ADI.

Key words: data extraction, manufacture of ADI, table of attributes, decision support systems, artificial neural networks

1. INTRODUCTION

Specialised domain knowledge, often resulting from costly experiments, published in the world in a large number of magazines, is an invaluable source of information for both technologists and researchers. However, getting familiar with all the articles in a particular subject (the production of ADI) and in a particular field of study (metallurgy-founding) is often a great problem arising, among others, from the restricted access to certain databases, language barriers, time constraints, etc.

The creation of a system facilitating selective access to specific passages of domain knowledge and allowing for an automatic processing of this knowledge seems to be the goal deliberate and advantageous. The cost invested in the development of such a system will certainly be lower than the cost of multiple repeating of experiments that have already been carried out. Moreover, this combination of results (centralisation) can be a source of inspiration for the planning and execution of research covering the areas unexplored so far.

With integrated expertise in a particular field, one can attempt to design inference algorithms and systems that will enable automatic processing of the knowledge (Kochański et al., 2010).

2. CHARACTERISTICS OF THE SOURCE MATERIAL

The sphere of the authors' interest includes published knowledge on the manufacturing process of ADI (Austempered Ductle Iron). An overview of

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journals and an analysis of articles relating to this area aimed at the selection of the ADI production parameters ensuring the achievement of certain properties in the final material. Most experimental studies were designed to investigate the effect of selected agent on the properties of the material. For example, on samples of a given chemical composition, several variants of the heat treatment were performed, or for a predetermined variant of the heat treatment, the chemical composition was changed, introducing, e.g., a new element and examining its effect on the structure of the material and hence on the properties (Zahiri et al., 2003; Dymski, 2001; Putatunda, 2001a, 2001b; Lin et al., 1996; Janowak & Morton, 1984; Biel-Gołaska & Kowalski, 1996; Kowalski et al., 1990).

ical composition of the base material, the dimensions of the heat treated product, and the heat treatment parameters, while the resulting variables are the values of selected properties of the examined product. The logical diagram is presented in figure 1. From the examined articles, using the adopted scheme, the experimental data were extracted. An attribute table was developed containing the specific values of the variables, which are used as the premises. These are the following parameters:

- *chemical composition*: C, Si, Mn, Mg, Cu, Ni, Mo, S, P, B, V, Cr, Ti, Sn, Nb, Al;
- *dimensions* (usually these are dimensions of samples according to standards adopted in the experiment);

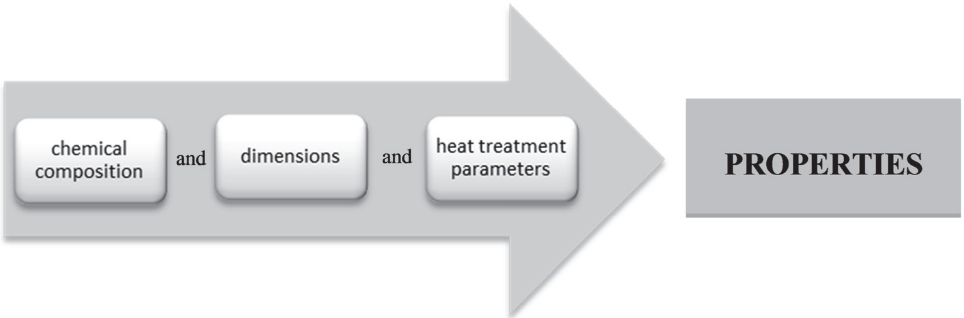


Fig. 1. *Logical diagram used for the presentation of experimental results.*

Table. 1. *Part of the table developed.*

L.p.	chemical composition												austempred		isothermal transformation		tensile strength, MPa	elongation, %	hardness, HRC
	C	Si	Mn	Mg	Cu	Ni	Mo	S	P	B	V	Cr	TA, °C	tA, s	Ti, °C	ti, s			
26	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	350	7200	947	9,8	32,2
27	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	350	14400	912	5,8	25,3
28	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	900	1348	2,8	36,7
29	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	1800	1282	4,1	33,3
30	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	3600	1329	2,7	33,6
31	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	7200	1021	4,7	32,2
32	3,21	2,57	0,28	0,024	0	0,098	0,015	0,01	0,061	0	0	0,036	830	3600	300	14400	973	4	29,3
33	3,4	2,41	0,15	0,064	0	0	0	0,017	0,015	0	0	0	927	7200	260	7200	1528	1,9	
34	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	273	7200	1522	3,1	
35	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	288	7200	1470	3,4	
36	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	316	7200	1326	4	
37	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	357	7200	1105	9,6	
38	3,4	2,41	0,15	0,064	0	0	0	0,007	0,015	0	0	0	927	7200	371	7200	1062	10,5	
39	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	260	7200	1600	3	43
40	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	288	7200	1510	4,8	39,5
41	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	302	7200	1400	7	36
42	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	316	7200	1370	8	35,5
43	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	330	7200	1230	11	28
44	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	343	7200	1200	12,5	28,5
45	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	357	7200	1060	13,8	27
46	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	371	7200	1040	15	26,5
47	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	385	7200	1090	20	23
48	3,45	2,48	0,4	0,15	0	1,5	0,3	0,012	0,013	0	0	0	927	7200	400	7200	1010	16,3	21,5
49	3,85	2,9	0,61	0,08	0	1,5	0,47	0,01	0,05	0	0	0	900	7200	370	7200	875	6,2	28
50	3,85	2,9	0,61	0,08	0	1,5	0,47	0,01	0,05	0	0	0	900	7200	320	7200	1161	3	38
51	3,85	2,9	0,61	0,08	0	1,5	0,47	0,01	0,05	0	0	0	900	7200	270	10800	1275	1,5	44

Logical diagram, observed in most of the reviewed articles, used for the presentation of the results of experiments can be expressed in the form of an implication where the premises include the chem-

- *heat treatment parameters*: temperature of austenitising (T_A), time of austenitising (t_A), temperature of isothermal transformation (T_i), time of the transformation (t_i), and the cooling medium;

The variables which are conclusions include:
- tensile strength (Rm);
- elongation (A_5);
- reduction of area (Z);
- hardness (HRC);
- toughness (KC);
- yield strength (Re).

A model of the table was created taking into account all the variables that have occurred in the described experiments. Since only some of the experiments allow for all the variables, the table also includes areas for which no data are available. Table 1 presents a fragment of the developed table.

The table summarises the results of 260 variants of experiments carried out in the production of ADI. ADI is formed by the properly conducted heat treatment (HT) of ductile iron, which is a starting material for the production of ADI. The heat treatment consists of two stages, i.e. austenitising and austempering. The heat treatment parameters, i.e. the parameters of both austenitising (T_A – temperature of austenitising and t_A – time of austenitising) and austempering (T_i - temperature of isothermal holding and t_i - time of isothermal holding) are selected depending on the properties that are to be obtained in ADI, e.g. high ductility combined with moderate strength and hardness, or vice versa a low ductility at the expense of high hardness and strength. The combination of properties that are required must be optimal from the point of view of later conditions of the casting operation

Table 2 presents the classification of ADI by American ASTM A897 Standard. For ADI the classification is based on properties and not on the chemical composition. Below are the properties obtained by heat treatment that decide about the grade of the material.

3. SELECTION OF TOOLS FOR FORMAL REPRESENTATION OF KNOWLEDGE ABOUT THE ADI MANUFACTURING PROCESS

With integrated knowledge relating to the production of ADI, one can attempt to design inference algorithms and systems enabling automatic processing of this knowledge. A very interesting and promising way to use source materials presented is the ability to create on their basis a new knowledge, i.e. discovering relationships and dependencies that are not visible in the individual experiments, but can occur during the compilation of results provided by a large number of studies.

There are many methods and tools, which are used in the processes of data analysis and creation on this basis of new formal models that describe the studied phenomena. In the industrial engineering, growing popularity are enjoying the intelligent systems that constitute a composition of artificial neural networks (Tadeusiewicz, 1993; Osowski, 1996; Lula et al., 2007), genetic algorithms (Rutkowska et al., 1997; Goldberg, 1998; Michalewicz, 2003) and elements of fuzzy systems (Kluska-Nawarecka et al., 2010; Górny et al., 2013).

The remaining part of this article presents an approach based on the use of collected data to develop a decision support system. The use of such a system provides the ability to determine the effect of selected heat treatment parameters on the specific properties of ADI (strength, elongation, hardness). As a formal tool to develop a model of the phenomenon, artificial neural networks (ANN) were selected.

Table. 2. *ADI classification according to ASTM A897.*

Grade by ASTM A897	Tensile strength R_m[N/mm^2]	Yield strength $R_{p0,2}$ [N/mm^2]	Elongation A_5[%]	Hardness HB	Fracture toughness K_C (unnotched) [J]
ASTM 897 Grade 1	850	550	10	269-321	100
ASTM 897 Grade 2	1050	700	7	302	363
ASTM 897 Grade 3	1200	850	4	341-444	60
ASTM 897 Grade 4	1400	1100	1	388-487	35
ASTM 897 Grade 5	1600	1300	-	444-555	-

4. THE USE OF ANN FOR MODELLING THE MANUFACTURING PROCESS OF ADI

Artificial neural networks are mathematical structures, the operation of which is a simplified representation of the human brain. Artificial neural network consists of a group of interconnected cells (neurons) processing in parallel the received information. Appropriately designed neural network is capable of self-formulating the interdependences between the parameters of a phenomenon during the learning process based on empirical cases. The learning process is an iterative process, repeated many times, step by step, with the primary objective to optimise the network parameters, i.e. the weighting factors. Each of the variables entering the network input gets initially a randomly assigned weight, which is the strength of its impact on the value of the output variable. The weighting factors are determined in a learning process, which is the source of knowledge and the intelligence of a neuron. The higher is the weight value, the more significant is the variable (Lula et al., 2007). The main way to use a neural network is by the creation of models, which are a formalised structure mapping a process or phenomenon. One of the most important issues is an appropriate set of empirical data describing the examined phenomenon.

The collected experimental data on ADI production parameters may give rise to the development of a model of this process. A very important step in the development of intelligent systems (e.g. supporting the decision making process) is to clarify the purpose of the analysis and define its basic assumptions.

The following describes various stages of the work carried out during the construction of a formal model of the phenomenon of the ADI production using artificial neural networks, based on the collected experimental data.

Table 3. The adopted filtering criteria.

C	Si	Mn	Mg	Cu	Ni	Mo	S	P	B	V	Cr	temp. *A*, °C	time *A*, s
3.64	2.53	0.31	0.028	0.031	1.53	0.32	0.008	0.024	0	0	0.049	900	7200

4.1. Stage I - filtering of the global data set according to the adopted criteria

The stated aim of the analysis was to examine the influence of selected parameters of heat treatment (T_i - temperature of isothermal transformation, t_i - time of isothermal transformation) on selected properties of ADI (tensile strength - R_m, elongation - A_5, hardness - *HRC*). Based on the adopted aim of the analysis, appropriate criteria for filtering the global data set were chosen. It was found that among all the analysed cases, only variants with a similar chemical composition (there should be no major differences in the content of individual elements in the base ductile iron) would take part in the analysis, and the values of the austenitisation process parameters should be similar. The criteria adopted in the filtering operation are given in table 3. It was also very important that the set selected by these criteria comprised measured values of all the analysed properties, i.e. the tensile strength - R_m, elongation - A_5, hardness - *HRC*.

Of the 260 cases included in the global table, the established criteria were met by 70 cases, which in further course of the study were adopted as a base set for analysis using the ANN.

4.2. Stage II - design of a neural network and choice of the environment for its implementation

With explicit nature of the problem and established set of data for analysis, the design of the network has begun. The process of model building consisted of the following stages: defining the explanatory variables and the explained variables; type selection and determination of the neural network structure; learning of the neural network; evaluation of the network model. The input (explanatory) variables were:
- T_i – the temperature of isothermal transformation,
- t_i – the time of isothermal transformation.

The dependent (explained) variables were:
- R_m – tensile strength,
- A_5 – elongation,
- *HRC* - hardness.

To determine the detailed, yet optimal, network architecture, the STATISTICA software and its *Automatic Neural Networks* module were used. Several architectures with different number of hidden neurons (arbitrarily it was assumed that the number of neurons should not be less than 4 and more than 10) and different activation functions (linear, sigmoidal, tangesoidal and exponential) were tested. The STATISTICA Generator allows implementing only one hidden layer, so this parameter was not subjected to analysis. At the time when the learning process was initiated, the neurons between layers were interconnected with each other. Of all the networks generated by the programme, three MLP type networks, which gave the best answers, were finally selected. Networks had 2 input neurons and 3 output neurons, and differed in the number of hidden neurons. Summary of the learning process of selected neural networks and their specific characteristics are given in table 4.

Table 4. *Summary of the network learning process.*

Network name	MLP 2-7-3	MLP 2-5-3	MLP 2-6-3
Quality (learning)	0,970961	0,972785	0,973469
Quality (testing)	0,963774	0,957228	0,956306
Quality (validation)	0,904937	0,922499	0,932627
Error (learning)	424,604	379,930	298,828
Error (testing)	1202,007	1420,773	1472,218
Error (validation)	1828,513	1525,045	1887,503
Learning algorithm	BFGS 84	BFGS 67	BFGS 129
Error function	SOS	SOS	SOS
Activation (hidden)	Logistic	Tanh	Logistic
Activation (output)	Tanh	Tanh	Linear

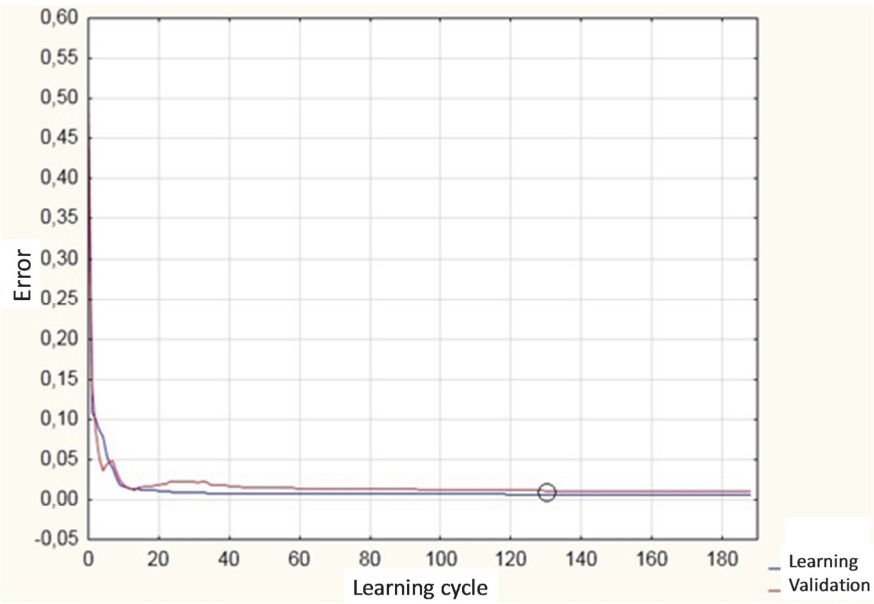


Fig. 2. *Changes in errors (learning and validation) depending on the epoch number for the MLP2-6-3 network.*

4.3. Stage III - analysis of the network parameters

There are many algorithms for learning the MLP networks widely described in the literature (Tadeusiewicz, 1993; Rutkowska et al., 1997; Lula at al., 2007). One of the groups are methods based on Newton's algorithm. These methods include the BFGS (Broyden-Fletcher-Goldfarb-Shanno) method used in the designed networks. The numbers, shown in the description of the applied learning algorithm, in table 4, indicate in which epoch the network learning has been completed. In the case of MLP2-6-3 networks, termination of the learning process took place in epoch 129.

Data set describing the phenomenon modelled was divided into learning set (70%), validation set (15%) and test set (15%). At the stage of the network learning, the learning set is used and then the validation set, which allows control of the learning process by examining the level of learning of neurons. In fact, learning consists of two phases: selection of weights for the learning set and testing of weights on samples from a validation set. Modification of weight values continues until it reaches a minimum approximation error, or if an error in the validation set begins to grow. The network improves its action solely on the basis of data from the learning set, so if in the course of learning it is observed that the decline of validation error has stopped or the error begins to grow, it indicates that the network has started to be too fit to the learning data and loses its ability to generalise the learning outcomes. Figure 2 shows the change in errors (both learning and validation) in successive epochs for the MLP2-6-3 network.

The final form of the model (trained by the learning set and validated by a validation set) is further tested by a test set. The error is the sum of squared deviations between the setpoint and the output of the network (indicated in table 4 as SOS). After completion of the learning process, the testing process starts using a test set which contains the values not used previously in the network learning process.

Table 4 shows the summary done for the three selected networks giving the best results. The given errors (learning, validation and test) refer to the total network error calculated as a mean squared residue for all output variables. The large values of these errors are the result of the order of magnitude of the source data. The magnitude of the validation and testing errors is much larger than that of the learning error - this is due to the low power of the available data set. In the future, the prospect of completing and augmentation of data set will allow reducing this difference.

A detailed analysis of errors for each output variable (*Rm*, *HRC*, A_5) was performed on the MLP2-6-3 network and is presented in tables 5-7. The network consists of 6 neurons in the hidden layer and the adopted activation functions are: in the hidden layer – a logistic function, in the output layer - a linear function.

The most reliable results include the last three columns, i.e. the relative mean squared error, the relative average deviation and the correlation coefficient, which are independent of the unit of measurement of individual variables, and thus can be mutually compared. In all cases, the relative mean squared error and the relative average deviation are lower for testing than for validation.

4.4. Stage IV - Analysis of the results obtained during the modeling

Table 8 presents several examples of the resulting values of properties estimated by the designed model of an artificial MLP 2-6-3 neural network, compared with actual results.

Figure 3a presents the graph of *Rm* (tensile strength) dependence on the time and temperature of austempering plotted with the use of a neural

Table 5. *Summary of the goodness of the network fit for the observed variable Rm.*

Rm	Mean squared residues	Mean absolute error	Relative mean squared error	Relative average deviation	Correlation coefficient
Learning	800,9871	22,9545	0,00056	0,01911	0,98573
Validation	3135,553	39,928	0,00207	0,03272	0,95999
Testing	2159,686	34,940	0,00108	0,02600	0,97055

Table 6. *Summary of the goodness of the network fit for the observed variable HRC.*

HRC	Mean squared residues	Mean absolute error	Relative mean squared error	Relative average deviation	Correlation coefficient
Learning	0,663496	0,646506	0,000576	0,018563	0,988960
Validation	2,146784	1,067628	0,001700	0,029661	0,955731
Testing	1,205280	0,848841	0,000965	0,023558	0,983516

Table 7. *Summary of the goodness of the network fit for the observed variable A_5.*

A5	Mean squared r esidues	Mean absolute error	Relative mean squared error	Relative average deviation	Correlation coefficient
Learning	0,929752	0,781211	0,034597	0,132726	0,943441
Validation	2,036721	1,048208	0,050089	0,170100	0,874410
Testing	1,257630	0,927432	0,029869	0,153821	0,938395

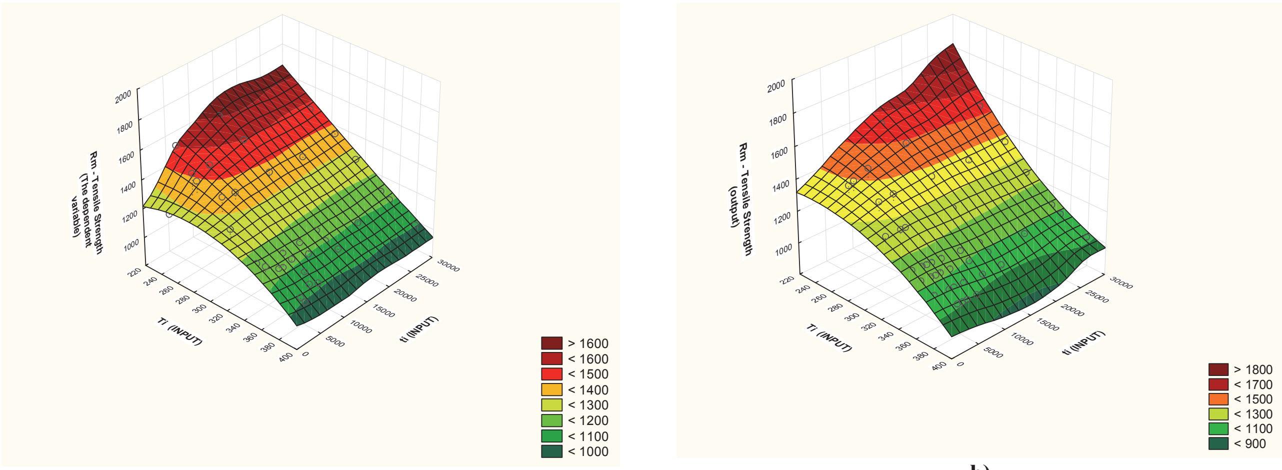
Table 8. *Summary of examples of real results compared with the results obtained by selected neural network.*

Input parameters		Values computed by the MLP 2-6-3 network			Real cases in the learning set		
T_i [°C]	t_i [s]	R_m	A_5	HRC	R_m	A_5	HRC
230	3600	1106	1.2	50.8	1120	1	51
230	21600	1609	3.2	46.8	1590	3.0	46
290	1800	1381	3.3	40.9	1410	3.2	42

network model. Figure 3b shows the course of this relationship when developed from actual data. Figures 4a and 4b show the dependence between hardness and the examined parameters when derived from a neural network model and real data, respectively.

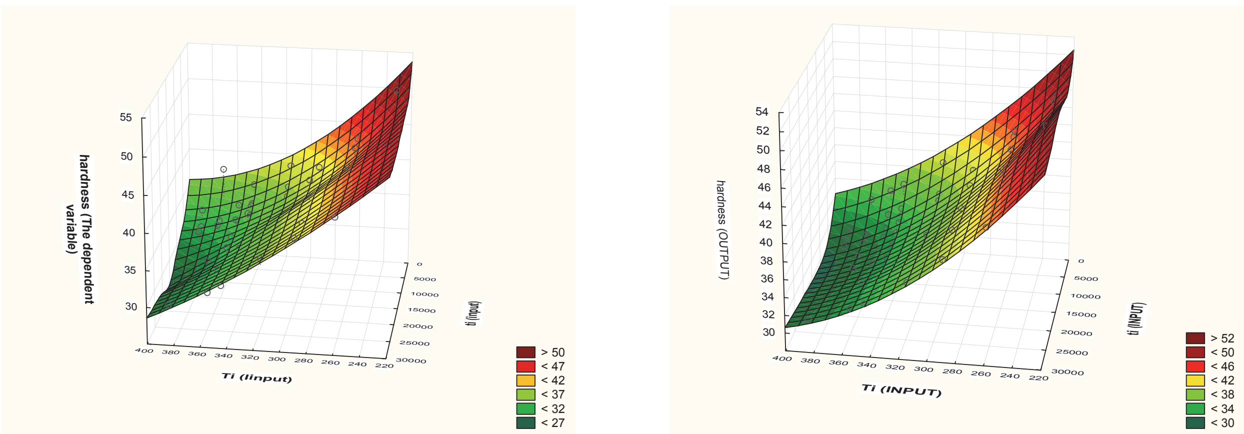
two parameters, significant differences were observed.

The construction of more complex structures, and thus the introduction of new input variables to the neural network, is further objective of the authors' activities. Work is underway to complete the



a) b)

Fig. 3. Plotted relationship between the tensile strength Rm and the time and temperature of austempering, based on selected neural model (a), based on real data (b).



a) b)

Fig. 4. Plotted relationship between hardness and the time and temperature of austempering: based on selected neural model (a), based on real data (b).

5. SUMMARY AND CONCLUSIONS

The manufacturing process of ADI is a complex process and the resulting mechanical parameters depend on a lot of factors. Building a neural network model, the authors have established a goal of the analysis, which is to study the effect of two selected parameters (T_i, t_i) on selected mechanical properties (*Rm, A_5, HRC*). The choice of only two variables to build the network was due to the fact that in the whole global set, only between the values of these

global database. Its development will enable the achievement of this goal.

However, despite a significant reduction in the amount of input parameters adopted in this study, this project can still bring utilitarian benefits. Modelling the effect of isothermal transformation parameters (T_i, t_i) on the properties of cast iron of defined chemical composition and constant austenitising conditions (filter installed) may be an excellent tool supporting the work of technologist or researcher in determining the optimum parameters of this treatment (even for a single composition) and helping in future elimination of expensive material-involving experiments.

The article presents the developed and tested basic version of a concept, which is based on the integration of experimental results relating to the production of ADI, and the ability to use this concept in the design of inference algorithms and systems enabling automatic processing of the knowledge acquired.

The development and provision of such a system will in the future prevent the multiple repetition of experiments that have already been carried out and can be a source of inspiration to:

- search for new areas of studies;
- search for these fragments of knowledge that can be used to solve a specific problem;
- create new knowledge (discover relationships and dependencies that are not visible in the individual experiments but can occur during the compilation of results obtained in a large number of studies).

The possibility of using the collected data to develop a formal model of the phenomenon of the ADI production based on specific assumptions and with the use of artificial neural networks was presented.

The obtained results should be regarded as preliminary, indicating the possibility of using Artificial Neural Networks to build a model of the ADI manufacturing process. Further work aimed at improving this model will be connected with the process of network optimisation and the introduction of more learning data obtained from the subsequent published experimental data. There is also the possibility of building a neural network for another configuration of the dependent and independent variables based on the sets of learning data filtered from a global set by criteria other than those specified in this study.

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WYDOBYWANIE WIEDZY ZE ZINTEGROWANYCH DANYCH EKSPERYMENTALNYCH DOTYCZĄCYCH PRODUKCJI ŻELIWA ADI

Streszczenie

Podejmowany w artykule problem dotyczy integracji wiedzy o procesie projektowania wyrobów z żeliwa ADI. Specjalistyczna wiedza dziedzinowa, często będąca wynikiem kosztownych eksperymentów, opublikowana na świecie w dużej liczbie czasopism, stanowi bezcenne źródło wiedzy dla jej użytkowników i dla badaczy. Autorzy zwracają uwagę na potrzebę opracowania systemu informatycznego ułatwiającego selektywny dostęp do poszczególnych fragmentów tej wiedzy, pozwalającego na jej automatyczne przetwarzanie. Koszt opracowania takiego systemu jest z pewnością niższy niż koszty wielokrotnego powtarzania eksperymentów. Proponowana, w ramach systemu agregacja i centralizacja wyników przeprowadzonych już badań, może być podstawą do planowania i wykonania kolejnych eksperymentów, pokrywających obszary dotąd niezbadane. Innym rezultatem może być wytworzenie nowej wiedzy, poprzez odkrycie relacji i zależności, które nie są widoczne w poszczególnych, pojedynczych eksperymentach, ale można je ujawnić podczas zestawienia wyników dużej liczby zróżnicowanych badań.

W artykule zaproponowano wykorzystanie sztucznych sieci neuronowych do odkrywania zależności występujących pomiędzy własnościami żeliwa ADI a wybanymi parametrami obróbki cieplnej w oparciu o zestaw zintegrowanych danych eksperymentalnych, pochodzących z różnych publikacji. Taka forma reprezentacji wiedzy może w przyszłości być wykorzystana w inteligentnych systemach komputerowych w module pozyskiwania wiedzy o procesie wytwarzania żeliwa ADI.

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