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Prediction of mechanical properties in spheroidal cast iron by neural networks

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Abstract

An artificial neural network-based system is proposed to predict mechanical properties in spheroidal cast iron. Several castings of various compositions and modules were produced, starting from different inoculation temperatures and with different cooling times. The mechanical properties were then evaluated by means of tension tests. Process parameters and mechanical properties were then used as a training set for an artificial neural network. Different neural structures were tested, from the simple perceptron up to the multilayer perceptron with two hidden layers, and evaluated by means of a validation set. The results have shown excellent predictive capability of the neural networks as regards maximum tensile strength, when the variation range of strength does not exceed 100 MPa. © 2000 Elsevier Science S.A. All rights reserved.

Keywords: Artificial neural network; Spheroidal cast iron; Mechanical properties

1. Introduction

The great number of variables that determine the result of a spheroidal cast iron production process has historically led to insuperable difficulties in developing reliable models to predict the mechanical properties of castings on the basis of the process variables only, chemical composition being included. The output characteristics, in fact, depend on both the matrix structure and the shape, size and distribution of the graphite spheroids. Matrix and spheroids, in turn, depend on the chemical composition of the melt, on the desulphurizing, spheroidizing and scorifying methods applied in the treatment ladle, on the inoculation method and finally, on the time elapsing between these events and the casting in the mould [1]. Moreover, the mechanics of spheroid formation itself has not yet been completely understood and many models are still in competition [2,3].

Added to this is the fact that every cast iron production plant has historically developed its own process, differing from those of others in many factors, such as the composition of the charge, the characteristics of the moulding sand and its compacting, the casting method, etc. These production methods are real "hidden variables" of the process, which act through a systematic law on the finished product, making it very difficult to correlate the results between pieces produced in different plants.

For this reason, although finite element analyses (FEM) or finite difference analyses (FDM) can furnish information on cooling rates and on the time elapsing before solidification, the chemical and physical characteristics of all the process elements being perfectly known, they will not be able to successfully correlate this knowledge with the mechanical properties of the casting [4].

An alternative approach to predicting mechanical properties in spheroidal cast iron products is based on the utilization of an artificial neural network (ANN). ANNs consist of many computational elements, operating in parallel, connected by links with variable weights which are typically adapted during the learning process. Although the development of detailed mathematical models began in the 1960s, it is only in recent years that improvements in the science of ANNs have allowed the development of manufacturing applications [5–7].

In the utilization of ANNs, a fundamental step consists of determining the input–output data necessary for the training stage. They can be obtained either from a process model or through actual experimentation. Since analytical correlation between input and output variables in the case study is

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Nomenclature

N_m	number of the melt
N_c	number of the casting
T_m	inoculation temperature (°C)
t_{tm}	time to mould (s)
U_{actual}	ultimate strength (MPa)
Ø	casting diameter (mm)

subject to the above-mentioned limitations, the latter method has been adopted.

This approach attains the goal of eliminating the need to declare to the system all those process variables which are more typical of the foundry than of the particular component produced, must be considered as constants. At the same time, it gives the correlation between process variables and product characteristics which the scientific literature cannot provide. Moreover, to the knowledge of the authors, neural network systems have not yet been used in spheroidal cast iron technology.

In this paper, the production of very simple cylindrical spheroidal iron castings of different diameter has been studied, with the aim of verifying the possibility of predicting the mechanical properties of the castings by means of neural network-based systems with supervised training.

A limited number of castings were produced in 10 melts and the mechanical properties evaluated in order to obtain the input–output patterns used to train the neural networks. The training stage for the neural networks was conducted using the back-propagation algorithm.

Different ANN structures have been tested, from the simple perceptron up to the multilayer perceptron with two hidden layers. For each ANN, different learning rates, iteration numbers, activation functions, and initial random weights have been considered.

Based on the encouraging results of this work, the next step in the research will be to extend the predictive capability of the ANN system to more complex shapes of industrial relevance.

2. Experimental

2.1. Moulding materials and test pieces

The mould consisted of natural sand AFS 60–65, bonded with water and 0.5% bentonite, to give 3–3.5% final moisture content, 40–45 mm compactability and 1500–2000 g/cm^2 green compressive strength. The mould used for the experiments contained the horizontally placed test piece, fed by a central sprue through two lateral gating systems with risers (Fig. 1). This mould design determines a plane of symmetry with respect to plane AB in Fig. 1, so that the two sides of the casting undergo identical filling sequences. This makes it possible to cut from the casting both a tension test specimen and a specimen for metallography, having strictly correlated characteristics.

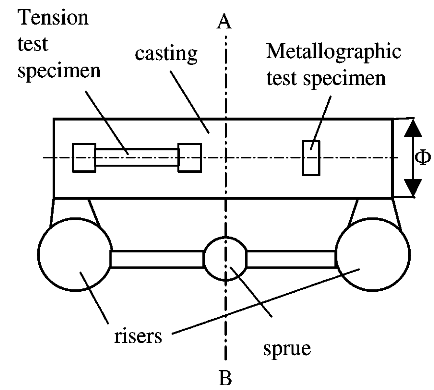

Fig. 1. Casting geometry and location of the specimens.

2.2. Charge materials

The charge materials, including the percentages used for the production, are listed in Table 1. The charge materials were melted in a cupola, from which the melt was then poured into the treatment ladle. Ten melts were produced for the actual investigation.

2.3. Desulphurizing and spheroidizing

Desulphurizing and spheroidizing treatments were carried out in the ladle by means of the Gazal method, which uses the mixing action of preheated nitrogen flux from the bottom. Desulphurizing was performed by means of 0.8% of CaC, and spheroidizing by means of 2.1% of FeSiMg5. After spheroidizing, the top of the ladle was removed and the melt was deslagged and poured into the casting ladle.

2.4. Inoculation

The casting ladle was preheated to avoid temperature losses. Inoculation was performed by means of 0.35% of FeSi75. After inoculation the temperature was measured and part of the melt was poured into the chill mould for spectro-

Table 1
Details of the charge materials

Charge materials	Percentage
Pig iron	25.8
Mild steel	21.5
Ductile iron scrap	38.7
Coke	9.0
$CaCO_3$	2.5
Desulphurizing agents	2.4
Graphite	0.1

Table 2
Composition of the melts

Melt number (N_m)	C (%)	Si (%)	Mn (%)	P (%)	S (%)	Cr (%)	Ni (%)	Cu (%)	Sn (%)	Mg (%)	Mo (%)
1	3.326	2.086	0.131	0.022	0.012	0.021	0.007	0.532	0.030	0.045	0.010
2	3.471	2.225	0.140	0.020	0.022	0.022	0.008	0.052	0.079	0.042	0.013
3	3.330	2.230	0.090	0.020	0.009	0.020	0.005	0.850	0.020	0.050	0.012
4	3.270	2.290	0.087	0.021	0.008	0.021	0.004	0.057	0.077	0.047	0.009
5	3.400	1.980	0.063	0.018	0.012	0.054	0.003	0.490	0.017	0.054	0.010
6	3.320	3.570	0.140	0.017	0.014	0.024	0.007	0.083	0.047	0.076	0.014
7	3.570	3.560	0.135	0.013	0.018	0.025	0.012	0.100	0.019	0.118	0.228
8	3.250	2.590	0.099	0.029	0.009	0.019	0.007	0.055	0.053	0.040	0.010
9	3.230	2.410	0.094	0.027	0.005	0.017	0.007	0.136	0.028	0.035	0.010
10	3.485	2.355	0.119	0.015	0.005	0.038	0.007	0.051	0.025	0.039	0.012

graphic analysis of the SG cast iron produced. The results of the analysis are summarized in Table 2 for the 10 melts produced.

2.5. Casting

The melt was then poured into the moulds. For each ladle, different moulds were poured (from two to four), in order to consider the time between the ladle temperature evaluation and the beginning of mould pouring as a process parameter. Each casting was marked for identification both in the sand and in the box, in order to allow the time to mould to be measured. All of the filling times were kept within a narrow range for each casting diameter: 16–20 s for Ø140 mm; 7–9 s for Ø70 mm; 5–6 s for Ø35 mm. After one day of cooling, the moulds were carefully broken.

2.6. Tension tests

Tension test specimens were extracted from the axis of the castings and tested on an INSTRON 8033 machine, with 0.056 mm/s ram speed. Ultimate load and elongation were recorded. The results are shown in Table 3.

2.7. Metallography

In a position symmetrical to the tension test specimen, a second specimen was extracted for metallography and hardness measurements.

Metallographic specimens were polished and etched in 3% nickel solution. The microstructures were examined optically to observe the morphology and nodularity of the graphite. The amounts of the different phases were measured, in order to assess the quality of the casting produced.

3. Neural networks

3.1. General

ANNs are mathematical models constituted by several neurons, arranged in different layers (input, hidden and output), interconnected through a complex network. They solve a problem by means of learning rather than by specific programming based on well-defined rules. In a feed-forward ANN, each input node transmits a signal to each input neuron which after processing, passes on the results to all the neurons belonging to the hidden layer(s). The hidden layer neurons process such signals and then send their outputs to the output layer neurons which lastly, after processing these inputs, generate the output signals of the network. No connections exist among neurons belonging to the same layer. Although each neuron can have several inputs it gives only one output signal which depends on the input signals, the weights of connections, the threshold value and the activation functions.

Table 3
Details of the experimentation

N_m	T_m	N_c	Ø	t_{tm}	U_{actual}
1	1365	1A	140	145	568
		1B	140	170	583
		1C	70	101	570
2	1327	2A	140	111	464
		2B	140	133	462
		2C	70	72	509
		2D	70	86	489
3	1338	3A	140	115	590
		3B	140	143	566
4	1345	4A	140	57	549
		4B	140	92	503
5	1342	5A	140	130	593
		5B	140	165	606
6	1292	6A	70	96	526
7	1280	7A	70	140	458
		7B	70	155	436
8	1327	8A	35	128	523
		8B	35	113	536
9	1352	9A	35	144	521
		9B	35	127	539
10	1373	10A	70	75	569
		10B	70	94	553

The output X_i produced by the neuron i in the layer l is given by the following relationship:

$$X_i = f\left(W_{i,0} + \sum_{j=1}^{n} W_{i,j} X_j\right) \tag{1}$$

where f is the activation function, n the number of elements in the layer $l-1$, and $W_{i,j}$ the weight associated with the connection between the neuron i in the layer l and the neuron j in the layer $l-1$ whose output is X_j. Usually, the threshold value X_0 is constant and equal to 1 so that the corresponding weight $W_{i,0}$ (offset or bias) shifts the activation function along the abscissa axis.

In supervised learning, a data set containing the input patterns and the corresponding output patterns is used to train the network. An iterative algorithm adjusts the weights of connections so that the responses y to the input patterns generated at output neurons, according to Eq. (1), are as close as possible to their respective desired responses d. This is achieved by minimizing the learning error, defined by the mean square error (MSE)

$$\mathrm{MSE} = \frac{1}{QN_0} \sum_{m=1}^{Q} \sum_{n=1}^{N_0} [d_n(m) - y_n(m)]^2 \tag{2}$$

where N_0 is the number of outputs and Q the number of training sets.

Since the desired responses are known at the output level, the local error $d-y$ can be easily calculated for output neurons; conversely, the desired responses at the hidden layer level are unknown so that the local error for hidden layer neurons cannot be determined. This problem was overcome by the back-propagation algorithm [8]. It works by back-propagating the error signals from the output layer neurons to those of the hidden layer, with one pattern presentation at a time. At each presentation cycle K, a forward phase to determine the output errors is followed by a backward one to propagate the error signals among the hidden layer neurons. The weights of connections are adjusted using the following equation:

$$\Delta W_{i,j} = W_{i,j}(K+1) - W_{i,j}(K) = -\eta D_j X_i \tag{3}$$

where η is the learning rate, is the parameter controlling the stability and the rate of convergence, and D_j the derivative of the MSE. This, when j is an output neuron, is given by

$$D_j = (d_n[m] - y_n[m]) f'(P_j) \tag{4}$$

where $f'(P_j)$ is the derivative of the activation function, and when j is a hidden layer neuron and k an output neuron, it is

$$D_j = f'(P_j) \sum_{k=1}^{N_0} D_k W_{k,j} \tag{5}$$

The weights of connections are repeatedly adjusted until the least MSE is obtained. A back-propagation iteration is completed when Eq. (3) is applied to all of the neurons in the network; then the process starts again with a new input–output pattern presentation.

Once the weights are adjusted, the performance of the trained network can be tested by applying input patterns not included in the training set. To this purpose, the generalization error, defined as the MSE between the output generated in response to an input not presented during training and the desired one, is used to quantify the predictive performance of neural networks.

3.2. Training of neural networks

Before training, the network architecture must be defined. As a general rule, the number of neurons must be large enough to form a map region that is as complex as necessary for a given problem. However, it must not be so large that many of the necessary weights of connections cannot be accurately estimated from the available training data. Furthermore, a trained ANN is very effective only if high generalization performance is achieved.

In the problem considered, 14 input neurons were used in order to predict the value of ultimate strength in the single output neuron. The meanings of the input neurons are given in Table 4. Normalization of the values was obtained by dividing each value of the training set by the maximum value of the specific variable considered.

Several feed-forward fully connected ANNs were investigated, considering different topologies (number of layers), activation functions, learning rates and initial random weights. Each network was trained to different number of iterations. The summary of the investigated topologies is represented in Table 5.

3.3. Validation of the neural network

The capability of ANNs to correctly generalize was checked using some input–output data not included in the training set. They have been chosen among the entire

Table 4
Input neurons to the ANN

Neuron number	Process variable
1	Carbon (%)
2	Silicon (%)
3	Manganese (%)
4	Sulphur (%)
5	Phosphorus (%)
6	Copper (%)
7	Tin (%)
8	Nickel (%)
9	Molybdenum (%)
10	Magnesium (%)
11	Chromium (%)
12	Ladle temperature (°C)
13	Time to mould (s)
14	Module (volume/surface) of the casting (mm)

Table 5
ANN topologies investigated

Single layer perceptron (*SLP*)
Activation function, linear (AFL) and sigmoidal (AFS)
Learning rate (LR)=0.03
Connection weights (CW): 0.1 and <1.0
Number of iterations (NI): 20 000 and 100 000

Multilayer perceptron (*MLP*) *with one hidden layer* (1*HL*) *with* 14 *neurons*
Learning rate (LR)=0.03, 0.07
Activation functions, linear (AFL) and sigmoidal (AFS) for the HL, sigmoidal for output neuron
Connection weights (CW): <0.1
Number of iterations (NI): 20 000, 40 000, 60 000, 80 000 and 100 000

Multilayer perceptron (*MLP*) *with two hidden layers* (2*HL*) *with* 14 *neurons each*
Learning rate (LR)=0.03, 0.07
Activation functions, linear (AFL) and sigmoidal (AFS) for the HLs, sigmoidal for output neuron
Connection weights (CW): <0.1
Number of iterations (NI): 20 000, 40 000, 60 000, 80 000, 100 000

experimental set on the basis of the following considerations:

1. Each input neuron variable of the validation set must be within the range defined by the entire training set for that variable.
2. In the training set there is no sample of the same casting number and diameter, which thus differs only in the time to mould.

The latter condition has been introduced for the purpose of avoiding undesirable good results induced by the presence of "similar" samples in the training and validation sets. As a result, the samples used for validation of all the investigated topologies are those indicated in Table 6.

The validation set is thus mainly suited to verify the ability of the ANN to predict mechanical properties in castings of different melt composition. Nevertheless, it is still possible to verify the predictive capability of the network on the time to mould parameter, by considering the results of the samples which belong to the same melt namely, 4A–4B and 9A–9B. It is worth noting that the sign of strength variation with the time to mould parameter is not consistent throughout the experiments, but depends on the melt and on the diameter of the casting; thus, it is of particular relevance in the context of strength prediction.

The possibility of directly verifying the network capability on castings of various diameters (or cooling rates) is not so easy because it is impossible to pour two moulds at the same time with the same ladle. Nevertheless, the importance of this parameter is such that good results will implicitly validate it.

Table 6
Results (selected)

ANN topology	N_c	$U_{predicted}$	U_{actual}	Δ (%)
SLP-AFL, CW: 0.1, NI: 20 0000, LR: 0.03	4A	575	549	4.8
	4B	537	503	6.7
	1C	551	570	−3.3
	9A	583	523	11.5
	9B	599	536	11.8
SLP-AFS, CW: 1.0, NI: 20 000, LR: 0.03	4A	518	549	−5.7
	4B	494	503	−1.9
	1C	558	570	−2.0
	9A	547	523	4.6
	9B	557	536	4.0
MLP-1HL, AFS, CW: 0.1, NI: 20 000, LR: 0.07	4A	551	549	0.4
	4B	517	503	2.9
	1C	560	570	−1.7
	9A	534	523	2.0
	9B	548	536	2.2
MLP-1HL, AFS, CW: 0.1, NI: 40 000, LR: 0.07	4A	541	549	−1.5
	4B	497	503	−1.2
	1C	572	570	0.3
	9A	538	523	2.8
	9B	558	536	4.2
MLP-1HL, AFL, CW: 0.1, NI: 20 000, LR: 0.07	4A	533	549	−2.9
	4B	502	503	−0.3
	1C	562	570	−1.3
MLP-2HL, AFL, CW: 0.1, NI: 20 000 LR: 0.03	4A	566	549	3.2
	4B	532	503	5.8
	1C	548	570	−3.7
	9A	555	523	6.2
	9B	570	536	6.4

The results of all the trained ANNs on the validation set are summarized in Table 6, by giving the predicted value of ultimate strength, the actual value and the percentile difference. Due to the large number of network topologies and conditions investigated, only selected values are represented here, those effectively pertinent to the discussion.

In some cases, to improve the predictive capability of the network the training set has been enlarged with the addition of samples taken from the validation set. In these cases the validation set is reduced, as evidenced in Table 6.

4. Discussion

The SLP network topologies gave maximum percentile errors in the range 6–15%, which is quite high, in view of the limited variation range of ultimate strength. The best result (MSE=4.2%, Δ_{max}=5.7%) was found by using sigmoidal activation function, initial weights below 1.0 and 20 000 iterations. A greater number of iterations always led to a decrease in the predictive capability.

The MLP network topology with one hidden layer improved prediction accuracy, especially by using sigmoidal activation functions. Good results were found with 20 000 iterations (MSE=2.4%, Δ_{max}=2.9%) and 40 000 iterations (MSE=2%, Δ_{max}=4.2%). Greater number of iterations always led to a decrease in both the MSE and maximum error.

The learning rate parameter was found to be very effective on prediction accuracy, the value 0.07 giving the best results.

Attempts were made to improve network performance by enlarging the training set with samples taken from the validation set (and thus reducing it). As an example, samples 9A–9B were added to the training set and samples 4A–4B–1C were the residual validation set. In this case (the fifth in Table 6), the maximum error is approximately 2.95%, thus unchanged with respect to the previous network considered. This means that the couple 9A–9B is not helpful in order to better describe the behaviour of the system. Similar considerations come from other attempts. Consequently, it can be stated that the actual training set is quite meaningful and better performances of the network can be achieved only if many other samples are added to it.

The MLP network topology with two hidden layers showed lower prediction accuracy, with maximum percentile errors in the range 6.5–12%. The best result (MSE=5.6%, Δ_{max}=6.4%) was obtained by using linear activation function on both the hidden layers and the output neuron, 20 000 iterations, a learning rate of 0.03 and random weights below 0.1.

The sensitivity of the system to the time to mould parameter is very good. In fact, by considering the predicted and actual values of strength in the 4A–4B and 9A–9B samples (identical in melt and diameter but with different times to mould), it becomes evident that the network ever predicts the right variation, even if this does not have the same direction.

In order to keep the effectiveness of prediction within the limited number of specimens considered, the variation range in tensile strength has been kept below 100 MPa. The extent of this range could be enlarged by increasing the size of the training set.

Attempts were also made to predict the elongation of the specimens by means of the ANN system. These experiments are not reported here because they failed to be effective, with errors even beyond 100% in some cases. This behaviour can be related to the considerable range of variation in elongation measurements, depending not only on the accuracy of the measurement, which is quite high [9], but also on the high variance of the variable itself. Consequently, the ANN system considers these random variations as if they were representative of real correlations and assigns wrong weights to the neurons. Only statistical processing of the variable could perhaps improve the results of the network, but this would be unfeasible for reasons of economy and simplicity.

In order to overcome this difficulty, attempts can be made to develop ANN systems with modified input patterns, provided by both process variables and micrographic results.

5. Conclusions

- This study has shown the capability of an ANN-based system to predict the tensile strength in spheroidal cast iron products. Input values to the network were: chemical composition of the melt, inoculation temperature, time before casting and diameter of the castings.
- Several ANN structures have been tested, the MLP with one hidden layer giving the best results.
- The maximum errors on the validation sets varied from 3 to 4% in different conditions of learning rates and initial random weights when the number of iterations was kept below 40 000.
- Due to the limited number of specimens considered, the variation range of tensile strength must be kept below 100 MPa to ensure effectiveness of the prediction.

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