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Neural network modeling of thin carbon layer

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This paper presents the possibility of using neural networks model for designing a thin carbon layer obtained after carbonizing process in fluidized bed. The carbonizing process in fluidized bed is very complicated and difficult. Very often the structure of the materials is non-homogeneous. This fact and the lack of mathematical algorithms describing carbonizing process makes modeling properties of drive elements by traditional numerical methods difficult or even impossible. In this case, it is possible to try using another nonconventional numerical method such as, *e.g.*, neural network. Using neural networks for modeling carbonizing process in fluidized bed is caused by several nets' features: non-linear character, ability to generalize the results of calculations for data out of the training set, no need for mathematical algorithms describing the influence of changes of input parameters on the modeling properties of materials. This paper presents the manner of designing and preparing neural network structure, choosing input parameters, the way of formatting data in input database and preparing learning and testing. It also presents the method of learning and testing neural networks, the way of limiting nets structure and minimizing learning and testing error. The specially prepared neural networks model very often is helpful for engineering decisions and may be used in designing carbonizing process in fluidized bed as well as in controlling changes of this process.

Keywords: neural network, thin layer, process modeling, materials engineering.

1. Introduction

The carbonizing process in fluidized bed is very complicated and a multi-parameter one [1, 2], because changes of parameters during this process have non-linear characteristic, as shown in Fig. 1. The next problem is the lack of mathematical algorithms that describe it. Using neural networks for modeling carbonizing in fluidized bed is caused by several nets' features:

– non-linear character,

– ability to generalize the results of calculations for data out of the training set and no need for mathematical algorithms describing the influence of changes of input parameters on hardness,

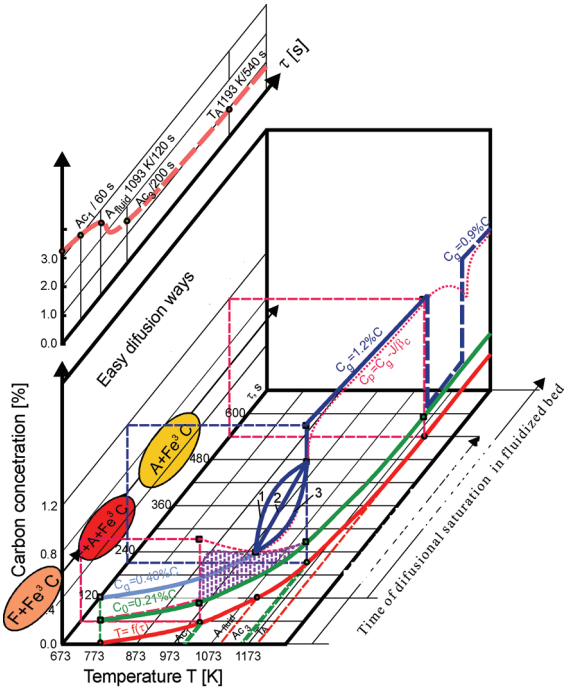

Fig. 1. Carbonizing process in fluidized bed [1].

– no need for mathematical algorithms describing the influence of changes of input parameters on the modeling properties of materials [3–7].

The research is divided into eight stages: choosing the modeling properties of materials, choosing heat treatment parameters to prepare data input vector, using special computer system to obtain training data set, designing and building neural network structure, minimizing model structure and learning error, minimizing testing error, using neural network model for prediction of carbon layer thickness of material after heat treatment in fluidized bed, practical verification of modeling results.

At present, different carbonizing techniques are used in the thermo-chemical treatment. One of these is carbonizing in fluidized bed. It is characterized by high coefficient of heat and mass transfer. These techniques are very often used in research institutes and small industrial plants [1, 8–11].

2. Research methodology

2.1. Methodology of design of neural network structure

Modeling the process with the use of neural networks should be started with designing the structure of the network. The characteristic features of neural nets are: the number of layers, the number of neurons in each layer and kinds of neural connections. The number of neurons in input layer and the number of input parameters are usually equal, *e.g.*, for carbonizing steel process in fluidized bed $n = 13$. Particular neural

network inputs are described by particular variables data inputs, such as: x_0 – kind of carbonizing process (in this example – in fluidized bed), x_1 – heating time, x_2 – austenitizing time, x_3 – cooling time, x_4 – tempering time, x_5 – temperature of batch, x_6 – austenitizing temperature, x_7 – cooling temperature, x_8 – tempering temperature, x_9 – kind of atmosphere, x_{10} – air excess ratio, x_{11} – kind of cooling, x_{12} – length of batch, x_{13} – width of batch.

The size of output layer is equal to the number of process parameters. In an example case, neurons in output layer are divided into four sections shown in Fig. 2. The three sections which describe microhardness in chosen areas of Fig. 3 are presented in the Table.

The fourth section in the output layer is built of tree neurons which describe carbon layer thickness after carbonizing process in chosen places (shown in Fig. 3): y_{25} – carbon layer thickness in place 1, y_{26} – carbon layer thickness in place 2, y_{27} – carbon layer thickness in place 3.

After fixing the input and the output layer structure the next step is designing the inside layers of the model. Since mathematical algorithms describing correlations

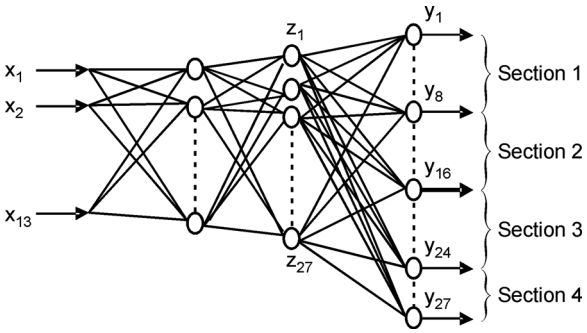

Fig. 2. Structure of neural network for modeling thickness in accordance with Kolmogorov statement.

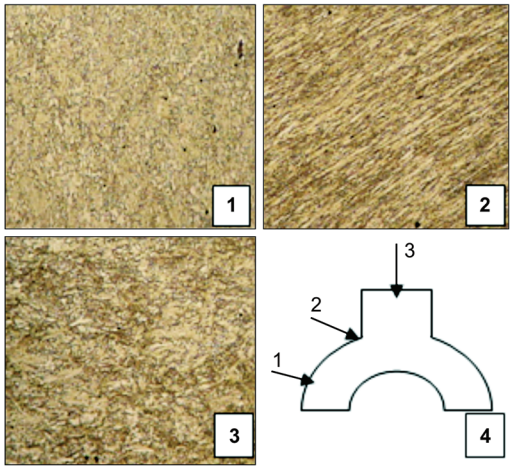

Fig. 3. Microstructure cross-section etched with nital at a scale 1:50.

T a b l e. Three sections of output layer of neural network.

Example distance from surface [μm]	Particular neurons in output layer of neural network describing microhardness for corresponding depth		
	Section 1	Section 2	Section 3
10	y_1	y_9	y_{17}
50	y_2	y_{10}	y_{18}
100	y_3	y_{11}	y_{19}
150	y_4	y_{12}	y_{20}
200	y_5	y_{13}	y_{21}
250	y_6	y_{14}	y_{22}
300	y_7	y_{15}	y_{23}
350	y_8	y_{16}	y_{24}

between vectors x_n and y_k are not known it is necessary to use an unconventional way of building the neural nets. It is based on information about output and input.

Theoretically, the problem of choosing neural structure is restricted to approximation of multi-variable function for a given vector x_n [3]. The case discussed in this paper concerns multi-dimensional input vector and continuous activation function. Building that kind of neural network model is defined by Kolmogorov statement [12]. He proved that in order to obtain k-dimensional output vector y_k for n-dimensional input vector x_n and continuous activation function, using one hidden layer neural network built of $2n + 1$ neurons is sufficient. It is shown in Fig. 2.

2.2. Example of material for research

Example materials for this research were provided by Visteon Industrial plant. The main problem during designing the parameters of surface layer is a non-homogeneous metallographic microstructure. This fact is presented in the cross-section of materials in Fig. 3.

The non-homogeneous metallographic structure in different areas of research materials was the cause of difficulty in designing carbonizing process, because it is very hart to obtain the same thickness of carbonizing layer in all parts of the material.

2.3. Learning and testing data

In order to use the designed neural network in practice it should be taught by learning data set. The size of learning data set depends on the expected generalization degree, which is the correct answer of the model to the input data different from the data of learning set. The better generalize qualities is obtain by using learning set far bigger than the number of adapted parameters of the neural network. If those proportions are disturbed, the network has reproduction abilities. In order to obtain the best approximation qualities for a designed model it is necessary to minimize the number

of adapted parameters of network and, in consequence, to minimize the generalization error $E_G(w)$:

$$E_G(w) \leq E_L(w) + \varepsilon\left(\frac{p}{h}, E_L\right) \tag{1}$$

where: E_L – learning error, ε – range of trust, h – the number of all synaptic weights,

$$E_L(w) = \sum_{k=1}^{p} E\left(y_k(w), d_k\right) \tag{2}$$

When the generalization error increases, the model becomes an interpolator for which all input signals different from those of the training set are rejected as a measure background. In order to avoid this it is necessary to minimize the generalization error by means of either building a bigger training set or limiting the network structure. Some time excessive limiting of the network structure is cause of increase of generalization error. Before it reaches minimum $E_G(w)$ starts behaving in the other way (it increases in contrast to decreasing $E_L(w)$). This quality can be used in searching for minimum $E_G(w)$, because it could make the selection of network structure faster. Direct observation of $E_G(w)$ is very time-consuming, because searching for its

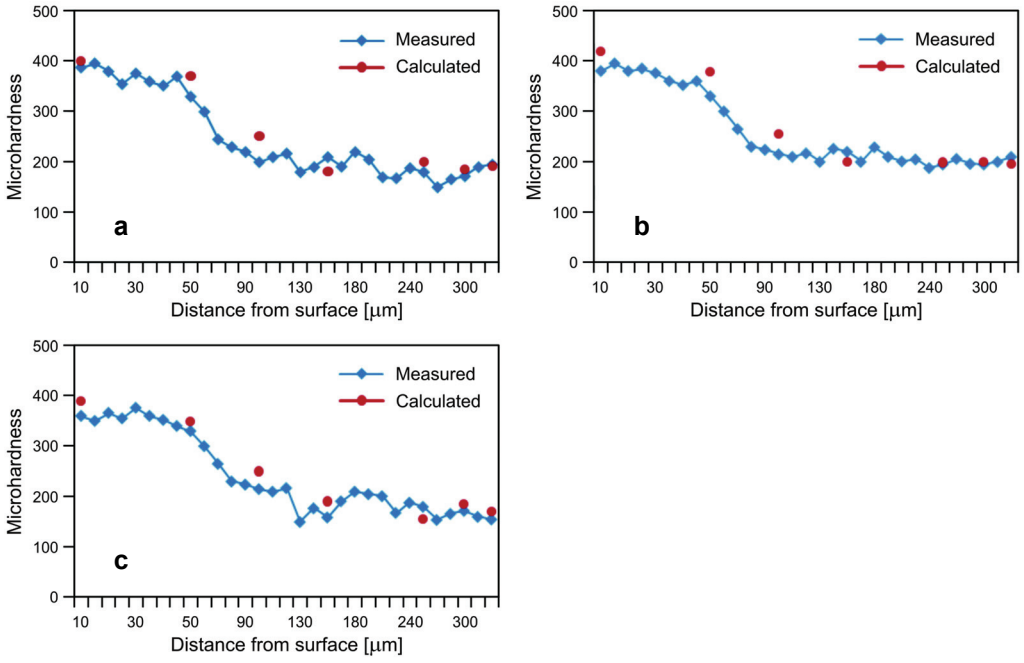

Fig. 4. Comparison of empirical and calculated curve of microhardness for area 1 (**a**) area 2 (**b**) and area 3 (**c**) shown in Fig. 3.

minimum needs checking error $E_G(w)$ for fully learned network each time. A better solution is observing error $E_L(w)$, whose changes can be observed continuously during teaching the network. In this case, the structure of networks could be corrected each time after stopping teaching process with the constant control value of learning set, because too big a learning set causes the re-increase of the generalization error.

2.4. Comparison of calculated and empirical results

The results of our investigation are presented in Fig. 4. Neural network can predict values of microhardness at a particular depth with average error in the range 4.5%–6.8%. This result makes it possible that the way neural network thus prepared can be used to design the assumed carbon layer thickness of materials carbonized in fluidized bed.

3. Conclusions

Neural network model MPL 13-13-55-27-27 designed and used in this research is able to predicted distribution of microhardness in surface layer after carbonizing process in fluidized bed in this case. In this way, data concerning the distribution of carbon layer thickness was obtained. The error of neural network prediction was determined after comparing the empirical and computed results.

The neural network model thus designed and built has the ability to calculate carbonizing parameters for different processes, kinds of materials, assumed parameters of carbonizing material (for example, for thin carbon layer). The real time of calculation of designed model is shorter than 1 min.

This research will be continued to solve this subject in a complex way and apply it in industrial plant. The final solution will be a special computer system, which will be connected in real time [13] with the heat medium and gas distribution station. This connection and special work application make it to possible to add new records in training and testing data. Connecting the neural network model whit a heat treatment control system offers the possibility of building a special system for on-line control running process [14, 15] and support of engineering decision in real time.

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