Prediction of CADI Chemical Composition and Heat Treatment Parameters using a BPNN Optimized with the Genetic Algorithm

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Abstract. Due to the increasing application of the Carbide Austempered Ductile Iron (CADI) with carbides, it is of great significance to predict the CADI chemical composition and heat treatment parameters to meet the requirements of process prediction in the complete design process of CADI parts. This study combines a backpropagation neural network (BPNN) and the genetic algorithm (GA). Based on the domestic production data, six key influencing parameters are selected to establish the BPNN prediction model. The prediction results of the non-optimized BPNN and the BPNN optimized using the genetic algorithm (GA-BP) are compared with the real industrial data. The results show that the optimized prediction model can meet the design requirements for the accuracy and stability.

1. Introduction

The Austempered Ductile Iron (ADI) was developed by M. Johansson in Finland in 1977. In order to further improve the wear resistance of an ADI, American scientists manufactured a high performance cast iron material based on an ADI in 1992 which was named the Carbide Austempered Ductile Iron (CADI). The CADI has many advantages including the high hardness, high wear resistance, toughness, and many others. Due to its advantages, it is widely used in the agricultural machinery, mining metallurgy, railway and automobile industry and so on [1-2]. The field of CADI application is still widening with its performances optimization.

The presence of carbides in a CADI microstructure can increase hardness and wear resistance, but an excessive number of carbides will reduce the toughness. To get the balance between the wear resistance and toughness, many experiments were conducted [3-8], and it was concluded the following.
First, the number of graphitized elements (especially silicon) should be reduced to advance the precipitation of carbides during the solidification. Second, a chill in the molds can promote high undercooling. Third, a CADI should be alloyed with the carbide stabilizing elements such as chromium (Cr), molybdenum (Mo), and vanadium (V). Fourth, a high-temperature pretreatment should be performed. At present, the types of carbides in a CADI mainly depend on alloying elements such as chromium, which promote the formation of carbides in the solidification process. Professor Dhanapal [9] improved the composition and properties of a CADI using the Taguchi method. Their results showed that the hardness and the impact property of a CADI with the Cr content of 0.6% were the best, while the wear resistance was better at the Cr content of 1%. The results also showed that the hardness and impact properties of a CADI with the Cr content under 0.6% were superior, and the wear resistance of the CADI was better when the content is less than 1.0%. Moreover, the experimental results of Cheng Haiqiang et al. [10], who work at Beijing University of Technology, showed that with the increase in Cr content, the volume fraction of graphite and the spheroidizing rate of cast ductile iron gradually decreased, but the content of carbide increased and the diameter of graphite gradually decreased after a certain diameter of graphite was reached. Besides, when the sample was subjected to the austenitizing for 100 min at 900 ℃ and isothermal quenching for 100 min at 300 ℃, the hardness and wear resistance of a CADI reached the maximum at the Cr content of 1.42%. Considering the change in toughness, when the content of Cr was 0.96%, the comprehensive mechanical properties were the best. Zhang Qifei and Liu Jiansheng et al. [11,12], who all work at HeFei University of Technology, studied the influence of the high-temperature pretreatment on a CADI microstructure and properties, and it was found that with the increase in the temperature of the high-temperature pretreatment and the prolongation of the heat preservation time, the number of carbides in the sample tissues decreased and the hardness decreased slightly, and the impact toughness was significantly improved.

In addition, the related researches show that the austempering temperature has a great influence on the microstructure and properties of the CADI matrix [13,14]. Namely, it was reported in [15-20] that a lower isothermal quenching temperature produced a large-volume fraction of acicular ferrite and stable austenite, which led to higher strength and lower ductility. Moreover, with the increase in the isothermal quenching temperature, the acicular ferrite became thicker and larger, the hardness was reduced, and the impact toughness was increased. Harris D.A. et al. [21] stated that the transition temperature ranges of the upper bainite and lower bainite were from 330℃ to 500℃ and from 330℃ to Ms, respectively. Besides, the time of isothermal quenching affected the CADI microstructure and properties. The related studies reported that an isothermal quenching time had the influence on the mechanical properties of a CADI containing the copper, nickel (Ni), boron (B), and other elements [22-24]. The general austempering time was between an hour and 1.5 hours, depending on the wall thickness of the CADI parts.

The alloy elements play an important role in improving the heat treatment ability of a CADI by helping to retard the transformation of austenite [25] because most CADI assemblies should be subjected to the austenitic isothermal quenching successfully [26,27]. In the isothermal quenching process, some austenite may turn into unnecessary pearlite during the cooling process if there is not enough austenite. Therefore, it is necessary to add from 0.2 to 5% of Cu, Ni, Mo, and other elements to a CADI to improve its heat treatment [28,29]. Besides, the addition of Mo and Ni will also increase the hardenability, which makes the light-weight and heavy profiles obtain a uniform hardening thickness of more than 40 mm. An economic alloying element V will increase the hardenability [30,31] when its content in a CADI is less than 0.30%. Peng Yuncheng and Liu Jinhai et al. [32], who all work at Hebei University of Technology, confirmed that traces of element B could improve CADI hardenability, but a higher content of B would decrease the hardenability and toughness of a CADI. On the other hand, Wang You et al., who work at Harbin Institute of Technology, carried out the research of using the nano rare earth (ceria oxide) to modify a CADI [33]. Their results showed that nano modification could effectively improve the CADI microstructure and increase its comprehensive
properties. However, only a little amount of nano cerium oxide was effective. The improvement in CADI performance was not obvious when a too high amount of the nanoscale cerium oxide was added.

A CADI can be an ideal substitute for the traditional metal wear-resistant materials. Therefore, making the CADI wear resistance and toughness to be as possible as possible is an important challenge in the CADI design. In order to get the best balance between the wear resistance and toughness in the CADI design, the process data of the 40-year-long CADI development and production are combined to optimize the chemical composition and heat treatment parameters to meet the design requirements for performance and cost. At present, there are a few domestic and foreign reports on the combined use of the neural network and genetic algorithm in the CADI materials design. The technology proposed in this work not only meets the needs of the CADI design but also reduce the amount of technological test research and the production cost of a CADI, which has high practical value.

In this paper, we will talk about the theory of neural network in the second chapter; in the third chapter, we will introduce how to use genetic algorithm to optimize neural network; the fourth part is our experiment; the fifth part is the summary of the whole paper. We will thank all those who helped finish this article in the last paragraph.

2. The Neural Network
The backpropagation neural network (BPNN) which represents a multilayer feedforward neural network based on the error backpropagation algorithm is used in this work. The learningtraining process of the BPNN consists of two parts: the forward propagation of a signal, and the backward propagation of an error. If the neural network (NN) output value is not in accordance with the desired NN output, the corresponding error value is sent backward to adjust the NN weights and thresholds, which represents the training process of an NN. The weights and thresholds of an NN are adjusted via the training process until a wanted output value is achieved. The flowchart of the training process of a BPNN is presented in Fig. 1.

Figure 1. The flowchart of the training process of a BPNN.
As the BP algorithm is a gradient-based maximum descent method, there are unavoidable defects: a slow convergence, a lack of the theoretical support for the selection of the number of hidden neurons, network training can easily fall into a local minimum, and the network generalization ability cannot be guaranteed.

3. Optimization of BPNN using genetic algorithm

3.1. Genetic algorithm based optimization methods

In view of the disadvantages of a BPNN regarding the low prediction precision and long calculation time, we propose the BPNN optimization using the genetic algorithm (GA). The main advantages of the GA are a strong global search ability, fast convergence, and high accuracy. At present, the genetic algorithm is widely used for BPNNs optimization, and there are four main optimization methods. (1) The genetic algorithm is used to optimize the initial weights and bias of a BPNN. The genetic algorithm is imitating the survival of the fittest in nature, searching for the global optimal solution of a network through a series of operations such as selection, crossover, and mutation, and then optimizing the initial weights and biases value of a BPNN according to the predefined optimal error value. (2) The GA optimizes the network topology. There is no doubt that the network topology has the greatest impact on the network processing ability, and redundant connection weights and neurons would greatly reduce the network processing capacity and decrease the training efficiency. In the specific application, the neural network structure is usually determined by means of trial and exploration because there is no unified theoretical guidance for the determination of a proper NN structure; thus, the genetic algorithm is used to solve this problem successfully. (3) The genetic algorithm is used to optimize the network training rules. (3) The combination of the above three methods is used to improve the NN performances.

In this work, the first method is used to optimize the BPNN. The ability of the genetic algorithm to search for the optimal solution is used to optimize the original BPNN model by using the selection, cross, mutation, and other optimization operations. Specifically, the initial weights and threshold value of a BPNN are optimized, so as to avoid the problem of network falling into a local minimum and speed up the network training. The flowchart of the GA-based optimization of the initial weights and thresholds of a BPNN is shown in Figure 2.
Figure 2. The flowchart of the neural network model based on genetic algorithm optimization.

3.2. Optimization of CADI chemical composition and heat treatment parameters using BPNN

The main GA parameters are the genetic coding, fitness function, and operators. The operators include three types of operators, namely, the selection operators, crossover operators, and mutation operators. In the specific applications, the appropriate population size, selection probability, crossover probability, and mutation probability are selected according to the application requirements. The basic steps of the algorithm are as follows:

1) Population initialization.
   In this work, the binary coding is used to encode the individuals, where an individual is a single binary string, which is composed of four parts: the weights of the input and hidden layers, the hidden layer thresholds, the associated weights between the hidden layer and output layer, and the output layer thresholds. All thresholds and weights are encoded together to form an individual code.

2) Fitness function.
   The initial weights and thresholds of a BPNN before optimization are obtained from individual. The output of a BPNN is calculated for the training data, and the sum of all absolute values of differences between the predicted output and the expected output is taken as the individual fitness value and labeled as $F$. The calculation formula is as follows:

$$ F = \sum_{i=1}^{n} |y_i - o_i| $$  \hspace{1cm} (1)
In (1), \( n \) is the number of network output neurons, \( Y_i \) is the expected output of the \( i^{th} \) neuron of a BPNN, and \( O_i \) is the predicted output of the \( i^{th} \) neuron.

3) Selection operator.

Here, the roulette wheel method is chosen as a selection operator of the genetic algorithm, and the probability \( P_i \) is defined as follows:

\[
f_i = \frac{1}{F_i}
\]

\[
p_i = \frac{f_i}{\sum_{j=1}^{N} f_j}
\]

where \( F_i \) is the fitness value of individual \( i \); as the fitness value is smaller, the better, the fitness value is obtained before the individual selection. \( N \) is the number of individual population.

4) Crossover operator.

Individuals are coded as follows: the crossover between \( a_k \) of \( i \) chromosome and \( a_l \) of chromosome \( K \) at level \( j \) is calculated by:

\[
a_{ij} = a_{ij}(1 - b) + a_{ij}b
\]

\[
a_{ij} = a_{ij}(1 - b) + a_{ij}b
\]

where \( b \) is a random number in the interval \([0, 1]\).

5) Mutation operator.

The \( j \) gene of individual \( i \) \((a_{ij})\) is mutated, and the variation formula is:

\[
a_{ij} = \begin{cases} a_{ij} + (a_{ij} + a_{max}) \times f(g), & r \geq 0.5 \\
& a_{ij} + (a_{min} - a_{ij}) \times f(g), & r < 0.5 
\end{cases}
\]

\[
f(g) = r_2(1 - g/G_{max})
\]

Where \( a_{max} \) is the upper bound of gene \( a_{ij} \), \( a_{min} \) is the lower bound of gene \( a_{ij} \), \( r \) is a random number between \([0, 1]\), \( r_2 \) is also a random number, \( g \) is the number of current iteration, \( G_{max} \) is the maximum number of evolutionary times.

6) Optimal individual of GA.

The initial weights and threshold values of a BPNN model are obtained, and the optimal solution is finally exported.

In the experiment, Matlab R2015a was used to build a BPNN model. The BPNN algorithm program was written in the Matlab programming language. The error of the experiment was characterized by the relative error and root mean square error (RMSE) which were defined by:

\[
E_r = \left[ (x_i - y_i)/x_i \right] \times 100\%
\]

\[
RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left[ (x_i - y_i)/x_i \right]^2}
\]
4. CADI chemical composition and heat treatment parameters

4.1. BPNN training and testing

The factors affecting the CADI performance include its chemical composition and heat treatment parameters. Further, the heat treatment parameters include the austenitizing temperature, austenitizing time, austempering temperature, and austempering time. The chemical constituents of a CADI include the content of various elements such as carbon (C), silicon, manganese (Mn), phosphorus (P), sulfur (S), copper, molybdenum, and many others. Therefore, it is of great significance to select a reasonable ductile iron composition to promote the formation of carbide to improve the comprehensive properties of a CADI. Moreover, sulfur and phosphorus are harmful elements, which are strictly controlled in the scope of production, while vanadium (V) and boron (B) are less added and less reported in the application of the CADIs. Consequently, in a BPNN, they are not used as the input and output values.

The addition of molybdenum, manganese, and other alloys can increase the hardenability of a CADI material. The CADI tissues contain carbides whose content should be controlled and kept within a certain range, so the content of silicon cannot be too high. When the CADI composition is designed, the carbide forming elements (such as Cr, Mo, etc.) should be added. Generally, copper and molybdenum are used together in a CADI to adjust the chemical composition, such that different mechanical properties can be obtained. Therefore, when the neural network model is established, the contents of Mn (wt%), Cu (wt%), Mo (wt%), and Cr (wt%) are selected as the network input, the CADI properties were selected as hardness (HRC), impact toughness (αk) input, C (wt%) content, Si (wt%) content, austenitizing temperature (℃), austenitizing time (h), isothermal quenching temperature (℃) and the output of isothermal quenching time (h). In this study, a three-layer BPNN is adopted. By using (10), after verification, 5 hidden layers are selected, and the BP network structure is 6-5-6, which means that BP NN has six neurons in the input layer, five neurons in the hidden layer, and six neurons in the output layer.

\[ H = \sqrt{m + n + L} \quad (1 \leq L \leq 10) \]  \hspace{1cm} (10)

In (10), m is the number of neurons in the input layer, and n is the number of neurons in the output layer.

In the experiment, 38 groups of data were selected from the domestic and foreign literature containing the research results of the tempered ductile iron with the carbide \([8,33-37]\), of which 33 were used for training, and the remaining 5 were used for network testing, as shown in Table 1.

| N  | L  | CJ | Mn  | Mo  | Cr  | Cu  | OT | OTi | T  | Ti  | C  | Si |
|----|----|----|-----|-----|-----|-----|----|-----|----|-----|----|----|
| 1  | 53 | 9.8| 0.4 | 0.4 | 0.8 | 0.125| 900| 1.5 | 250| 1   | 3.6| 2.3|
| 2  | 50.9|32.72|0.27 |0.32 |0.53 |0.79 |920 |1.5 |280 |2   |3.63|2.63|
| 3  | 38.3|56.03|0.27 |0.32 |0.53 |0.79 |920 |1.5 |320 |2   |3.63|2.63|
| 4  | 54  | 7.59| 0.4 | 0.4 | 0.8 | 0.125| 900| 1.5 | 230| 1   | 3.6| 2.3|
| 5  | 50  | 11.4| 0.4 | 0.4 | 0.8 | 0.125| 900| 1.5 | 270| 1   | 3.6| 2.3|
| 6  | 49  | 11.5| 0.4 | 0.4 | 0.8 | 0.125| 900| 1.5 | 290| 1   | 3.6| 2.3|
| 7  | 53.8| 9.8 | 1.54| 0.26| 0.56| 0.67 | 900| 1.5 | 250| 1.5 | 3.88|2.74|
| 8  | 55.3| 7.9 | 2.04| 0.26| 0.53| 0.61 | 900| 1.5 | 250| 1.5 | 3.7 |2.65|
| 9  | 55.4| 7.6 | 2.32| 0.28| 0.59| 0.68 | 900| 1.5 | 250| 1.5 | 3.69|2.82|
| 10 | 57.1| 8   | 1.8 | 0.28| 0.55| 0.63 | 900| 1.5 | 220| 1.5 | 3.84|2.66|
| 11 | 55  | 9.2 | 1.8 | 0.28| 0.55| 0.63 | 900| 1.5 | 250| 1.5 | 3.84|2.66|
| 12 | 52  | 12  | 1.8 | 0.28| 0.55| 0.63 | 900| 1.5 | 280| 1.5 | 3.84|2.66|
| 13 | 50.38|12.8 |1.273|0   |0.608|0.561|900 |1.5 |270 |1.5 |3.61|2.74|
In the experiment, the training rate of the BPNN was 0.05, and the target error was set to $10^{-4}$. According to the size of the training samples, the maximum number of training epochs was set to 10,000. If the training lasted 10,000 epochs, but the network did not converge to the target error, the training would stop, and the final output would be the average value of the outputs of 20 cycles. The training samples were normalized between 0 and 1 to decrease the data range, with the aim to achieve a better generalization ability of the network. After the samples normalization, the network was trained using 33 sets of data, and after the training, the network was tested using the remaining 5 sets of data. The test errors were calculated using (8) and (9).

The test parameters are given in Table 2. The comparison of the data predicted by the BPNN and the real data is given in Table 3, and the relative error between the values predicted by the BPNN and the real values is given in Table 4. The average error on five test samples was 28.16%, which was a large error, so the network optimization was needed.

### Table 2. The test parameters

| N  | L     | CJ    | Mn | Mo  | Cr   | Cu   | O   | T  | OTi | T   | Ti | C   | Si  |
|----|-------|-------|----|-----|------|------|-----|----|-----|-----|----|-----|-----|
| 1  | 53.7  | 17.37 | 0.27 | 0.32 | 0.53 | 0.79 | 920 | 1.5 | 270 | 1.5 | 3.72 | 2.94 |
| 2  | 55    | 9.2   | 1.8  | 0.28 | 0.55 | 0.63 | 900 | 1.5 | 250 | 1.5 | 3.84 | 2.66 |
| 3  | 52.74 | 16.9  | 1.255 | 0.416 | 0.617 | 0.57 | 900 | 1.5 | 270 | 1.5 | 3.58 | 2.79 |
| 4  | 52.6  | 10.8  | 1.44 | 0   | 0.53 | 0.63 | 900 | 1.5 | 250 | 1.5 | 3.79 | 2.7 |
| 5  | 54.7  | 8.8   | 2.25 | 0.32 | 0.5  | 0.69 | 900 | 1.5 | 260 | 1.5 | 3.63 | 2.77 |

Table notes: $N$ number, $L$ Rockwell hardness, $CJ$ impact toughness, $O$ austenitizing temperature, $OTi$ austenitizing time, $T$ isothermal temperature, $Ti$ isothermal time.
Table 3. The comparison of the values predicted by the BPNN and real values

| N | OT | OTi | T   | Ti  | C   | Si | OT | OTi | T   | Ti  | C   | Si |
|---|----|-----|-----|-----|-----|----|----|-----|-----|-----|-----|----|
| 1 | 920| 1.5 | 240 | 2   | 3.63| 2.63| 899.708 | 1.5009 | 255.77 | 1.508 | 3.5686 | 5.8 |
| 2 | 900| 1.5 | 250 | 1.5 | 3.84| 2.66| 899.558 | 1.5009 | 287.66 | 1.5129 | 3.5544 | 5.8 |
| 3 | 900| 1.5 | 270 | 1.5 | 3.58| 2.79| 840.696 | 1.0043 | 250.00 | 0.5341 | 3.4057 | 2.3 |
| 4 | 900| 1.5 | 250 | 1.5 | 3.79| 2.7 | 870.473 | 1.4712 | 295.00 | 1.012 | 3.5994 | 2.6 |
| 5 | 900| 1.5 | 260 | 1.5 | 3.63| 2.77| 899.986 | 1.9857 | 339.87 | 1.4844 | 3.7998 | 2.8 |

Table 4. The relative error between predicted and real values on five test samples

| N | OT  | OTi | T   | Ti  | C   | Si |
|---|-----|-----|-----|-----|-----|----|
| 1 | -2.56 | 0.06 | 6.17 | -32.62 | -1.72 | 54.66 |
| 2 | -0.05 | 0.06 | 13.09 | 0.85 | -8.04 | 54.14 |
| 3 | -7.05 | -49.36 | -8.00 | -180.85 | -5.12 | -21.30 |
| 4 | -3.39 | -1.96 | 15.25 | -48.22 | -5.30 | -3.85 |
| 5 | -0.002 | 24.46 | 23.5 | -1.05 | 4.47 | 1.07 |

RMSE 3.68 24.65 14.55 84.97 5.33 35.75

Figure 3. The relative error of the values predicted by the BPNN.

4.2. Optimization of BPNN model

Since the BPNN had a slow convergence speed in the experiment, the thresholds and weights of the hidden neurons of the BPNN were used as input information of the genetic algorithm. Further, coding them into a chromosome, the selection operator, crossover operator, and mutation operator of the genetic algorithm were used to generate a new offspring used as an initial value of the BPNN; then, the BPNN was trained, and the corresponding error was calculated. This process was repeatedly run until the accuracy of the BPNN, i.e., the error, met the predefined value. Thus, the advantage of the genetic algorithm was used to optimize the original BPNN, and the optimized BPNN was established. The CADI chemical composition and heat treatment prediction was based on the established three-
level BPNN. The parameters of the network training were set as follows. We set the number of epochs to 20000, the goal mean squared error (mse) to 10^-4, the training rate to 0.05, the individual coding length of the genetic algorithm to 36, the size of the population to 50, the probability of mating and mutation to 0.8 and 0.2, and the number of evolitional times to 100. To eliminate the influence of a random parameter settings to the results, this experiment was repeated for 10 times, utilizing the presented simulation testbed and Matlab software. As it can be seen in Fig. 4, the training goal was met at the 37th epoch.

![Figure 4. The training performance of the BPNN optimized using the genetic algorithm](image)

When the optimization of the BPNN model was finished, the newly obtained model was tested using the same five datasets as in the previous test, and the predicted values and relative errors are given in Table 5 and Table 6, respectively, and graphically presented in Fig. 5.

| N  | OT | OTi | T  | Ti | C  | Si | OT | OTi | T  | Ti | C  | Si |
|----|----|-----|----|----|----|----|----|-----|----|----|----|----|
| 1  | 920| 1.5 | 240| 2  | 3.63| 2.63| 916.495| 1.497| 227.002| 1.9313| 3.410| 2.710|
| 2  | 900| 1.5 | 250| 1.5| 3.84| 2.66| 899.833| 1.499| 248.026| 1.4994| 3.846| 2.641|
| 3  | 900| 1.5 | 270| 1.5| 3.58| 2.79| 900.168| 1.500| 270.506| 1.5018| 3.580| 2.782|
| 4  | 900| 1.5 | 250| 1.5| 3.79| 2.7 | 900.142| 1.499| 256.962| 1.4991| 3.688| 2.750|
| 5  | 900| 1.5 | 260| 1.5| 3.63| 2.77| 899.886| 1.499| 260.706| 1.5018| 3.435| 4.297|

| N  | OT | OTi | T  | Ti | C  | Si |
|----|----|-----|----|----|----|----|
| 1  | -0.38| -0.2 | 13 | -3.56| -6.45| 2.95|
| 2  | -0.019| 0.07 | -0.8| -0.04| 0.16| -0.72|
| 3  | 0.019| 0.19 | 0.119| 0| -0.29|
| 4  | 0.016| 0.07 | 2.7 | -0.06| -2.77| 1.82|
| 5  | -0.013| 0.27 | 0.119| -5.37| 35.53|
| RMSE | 0.17| 0.12 | 5.69| 1.61| 3.02| 15.54|

Table 5. The comparison of the values predicted by the genetic algorithm and real values

Table 6. The relative error of the optimized BPNN model on five test dataset (%)
Figure 5. The relative error of the optimized BPNN model on five test dataset.

The comparison of the relative error of the BPNN model before and after the GA-based optimization is given shown in Table 7. The relative error of the optimized BPNN model was 4.35%; compared with the non-optimizes BPNN model, the prediction accuracy was higher and the computation time was shorter.

Table 7. The comparison of the relative error of the BPNN model before and after the GA-based optimization

|          | BP forecast data | Prediction data of BP neural network after optimization of genetic algorithm |
|----------|------------------|--------------------------------------------------------------------------------|
|          | N    | OT   | OTi  | T   | Ti   | C    | Si   | OT   | OTi  | T   | Ti   | C    | Si   |
| 1        | -2.56 | 0.06 | 6.17 | -32.62 | -1.72 | 54.66 | -0.38 | -0.2 | 13   | -3.56 | -6.45 | 2.95 |
| 2        | -0.05 | 0.06 | 13.09 | 0.85 | -8.04 | 54.14 | -0.019 | 0.07 | -0.8 | -0.04 | 0.16 | -0.72 |
| 3        | -7.05 | -49.36 | -8.00 | -180.85 | -5.12 | -21.30 | 0.019 | 0    | 0.19 | 0.119 | 0    | -0.29 |
| 4        | -3.39 | -1.96 | 15.25 | -48.22 | -5.30 | -3.85 | 0.016 | 0.07 | 2.70 | -0.06 | -2.77 | 1.82 |
| 5        | -0.002 | 24.46 | 23.5 | -1.05 | 4.47 | 1.07 | -0.013 | 0.07 | 0.27 | 0.119 | -5.37 | 35.53 |

4.3. Software interface and instance test

The man-machine conversation function in the BPNN-based prediction software was realized through the Matlab automatic graphical user interface (GUI). In Fig. 6, the GUI where a user could set six input parameters: hardness (HRC) of a CADI material (HRC), impact toughness (ak), Mn content (wt%), Cr content (wt%), Mo content (wt%), and Cu content (wt%), is presented. By clicking on the “Prediction Button” the predicted values would be presented on the right side, Fig. 7. The presented predicted values were calculated using the parameters that a user set using the GUI. The predicted values were: C content (wt%), Si (wt%) content, austenitizing temperature (C), austenitizing time (H), isothermal quenching temperature, and isothermal quenching time (H).
Figure 6. The GUI for prediction of the CADI chemical composition and heat treatment parameters.

Figure 7. The presentation of the predicted values.

5. Conclusion
In this paper, the BPNN model for prediction of the CADI chemical composition and heat treatment optimized using the genetic algorithm is presented. The graphical user interface is developed to allow a user to set the input parameters values easily. The realized man-machine conversation function is of great significance to the research and development of the CADI materials. The concrete contributions of this study are as follows.

1) A BPNN network was trained with a certain number of the CADI samples; the test error of the BPNN was large.
2) The error of the optimized BPNN was obviously smaller than that of the non-optimized BPNN; the final prediction error was below 5%. 
3) A graphical user interface was designed to form a complete software set for prediction of the CADI chemical composition and heat treatment parameters. Using the interface, a user could set six input parameters which the software used to calculate the values of output parameters.

4) By applying the software, the relative error of 4.5% was achieved, which was within the allowable range; thus, the presented software could meet the requirements of the complete design of a high-quality ductile iron of the isothermal quenching parts in the CADI production.

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