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Design of medium carbon steels by computational intelligence techniques

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ABSTRACT

Steel design with the targeted properties is a challenging task due to the involvement of many variables and their complex interactions. Artificial neural networks (ANN) recognized for representing the complex relationships and genetic algorithms (GA) are successful for optimization of many real world problems. ANN has been used to identify the relative importance of variables those control the mechanical properties of medium carbon steels. We propose the combination of ANN and GA to optimize composition and heat treatment parameters for the desired mechanical properties. The trained ANN model was used as a fitness function and also as a predictive model. The predicted properties were realistic and higher for the model suggested with the optimum combination of composition and heat treatment variables. The proposed framework is expected to be useful in reducing the experiments required for designing new steels.

1. Introduction

The design of alloy steels with the desired properties is a challenging task as it involves a multi-objective optimization of various problems [1,2]. For example, it is hard to design a material that combines high strength and ductility, which are the two most key mechanical characteristics of metals [3]. There are excellent facilities to measure the composition, microstructure, and properties. However, it is difficult to predict reliable mechanical properties with the comprehensive description of the chemical composition, processing parameters and structure of steels. The microstructure in steels determine the mechanical properties and the typical metallurgical approach for the prediction of properties through structure-properties relationships follows the hierarchy of composition and processing conditions → microstructure → mechanical properties.

Developing models for the analysis of complex multicomponent steel properties is a difficult task as a quantitative treatment is necessary. Physical models are not capable of predicting the mechanical properties of steels. The conventional linear regression is not sufficient to describe the relationships; hence the biologically inspired artificial neural networks (ANNs) have been identified as appropriate tools. ANN models are well-known for function approximation and feature extraction of the highly complex nonlinear relationships from the data [4,5]. In the present approach, both the compositions and heat treatment variables which determine the microstructure are related directly to the mechanical properties. Hence, it is appropriate to attempt these techniques to enable the quantitative expression and understanding of the complicated nonlinear problem [6–9].

ANN model is a combination of a mathematical function and associated weights between the inputs, hidden units and outputs. Experimental data are presented to the network in the form of input and output parameters, and optimized nonlinear relationship is found by minimizing mean square error. The error adjustment step takes place once the data is presented to the input layer and forward propagation is finished. Every processing element in the output layer estimates an output and compared with the actual output specified in the data set. An error value for every unit is calculated based on the difference. The weights of these units are adjusted based on the error for all of the interconnections established with the output layer. After this, the subsequent sets of weights are adjusted for the interconnections coming into the hidden layer located just beneath the output layer. Upon each presentation, the weights are adjusted to decrease the error between the network's output and the actual output. This process is continued

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until all the weights of the network are adjusted [10,11]. ANN model captures complex interactions involving the input and output variables, which are difficult to visualize from an assessment of the weights. These optimized weights are stored in a matrix form in the model. The model is ready to make rapid predictions with the new data using the optimized weights, to plot the predictions, and to examine the metallurgical significance of the results. The back-propagation neural network is more commonly used for modelling many complex systems effectively [11]. The application of ANNs in material science for evaluation of various phenomena has been reported earlier in many research reports [12–16].

Genetic algorithms (GA) are based on the concepts from population genetics and aimed at global optimization [17]. GA combines persistence of the fittest between string structures with organized information exchange to form a search algorithm with the flair of human problem solving. GA ensures the production of optimum solutions while exploring new solutions by means of a systematic data exchange that uses probability factors. This allows GA to exploit the available information to find different solutions in the search space with better performance [18,19]. GA in numerous systems has been applied to many scientific and manufacturing problems [17,20,21] and a wide variety of optimization tasks [22,23]. Use of GA is growing and a comprehensive analysis of the GA applications in materials science can be evolved further [24–26].

Since, the ANNs and GA are the computational models of learning and evolution process of natural intelligent system, the proposed framework is referred as computational intelligence. The computational intelligence models have been used to identify the quantitative relationships between the composition, heat treatment parameters and properties and to design the medium carbon steels for the desired mechanical properties.

2. Materials and methodology

2.1. The variables under consideration

The experimental data of medium carbon steels used in the present work has been collected from the EN Steels handbook [27]. The data contains the alloying elements (carbon, silicon, manganese, sulfur, phosphorous, nickel and chromium), section size, soaking temperature and nature of quenching. The Mn/S ratio was calculated and considered as an input due to its influence on mechanical properties of steels. The heat treatment processes applied are sub-critical annealing at 650–690 °C followed by oil quenching or air cooling. Hardening process at 830–860 °C was followed by oil quenching and tempering at 550–660 °C and by air cooling or oil quenching. Cooling rate (C.R) is very critical in determining the microstructure, hence the mechanical properties of the steels. Therefore, C.R has been estimated by developing cooling rate equations for different section sizes [28] based on the ASM handbook [29].

The input parameters considered for model development are C, Si, Mn, P, Ni, Cr, Mo, Mn/S ratio, cooling rate (C.R) and tempering temperature (T.T) and the outputs are mechanical properties. The properties are yield strength (YS), the ultimate tensile strength (UTS), % elongation (% EL), % reduction in area (% RA), and impact strength (IS). The minimum, maximum, mean and standard deviation values of all the input and output parameters of steels data are shown in Table 1. Entire data sets of the steels used in the present modelling are shown in supplementary material.

2.2. Methodology

In the present work, the approach of modelling medium carbon steels is taken as three fold.

- Development of ANN model for mapping relationships between the composition, heat treatment parameters and mechanical properties, and identification of important input parameters on different properties by calculating index of relative importance.
- Use of genetic algorithms to get the optimum combination of input parameters for the desired outputs.
- Predicting the properties of steels for the suggested composition and heat treatment parameters by the ANN model.

3. Theory

3.1. Artificial neural networks (ANN) model

ANN model consists of an input layer, one or two hidden layers and an output layer. The input layer has ten hidden neurons representing steels composition and heat treatment parameters and an output layer has five hidden nodes consisting of mechanical properties. The ANN model was trained with back propagation learning algorithm. A comprehensive explanation on algorithm used in the current study is reported in literature [4,11].

The training of the ANN model was conducted by using the tailor-made software and the complete details were reported in an earlier work [28,30]. The training involves optimization of hidden layers, hidden nodes, momentum term, learning rate, and number of iterations. Several ANN models were created using the data. The optimum ANN model was achieved with 10-22-22-5 structure with 0.65 momentum term and 0.55 learning rate by trial and error method.

The significance of inputs on output parameters over entire data set is reported in literature [6,31]. We propose a new method to calculate the instantaneous relative importance of inputs on the output parameters. The developed neural networks model was tested with zero offset inputs. After adding up the ±2.5% variation to the inputs, there are twenty combinations of input data created. The variation of ±2.5% was achieved from the relationship $(2.5 \times 2) \times$ (maximum value of input parameter – minimum value of input parameter)/100. The tempering temperature for steel sample 2, shown in Table 4, is 500 °C and the maximum and minimum temperatures in the entire database are 400 °C and 700 °C, respectively, with a difference of 300 °C. A band of 5% offset gives a value of 15 $[(300/100) * 5]$, and on further dividing the obtained result by 2 gives a value of 7.5. Thus, two temperatures obtained with -2.5% offset and $+2.5\%$ offset are $500 - 7.5 = 492.5$ °C and $500 + 7.5 = 507.5$ °C, respectively.

While the first input varied with -2.5% offset and $+2.5\%$ offset, the remaining nine input parameters were kept constant with no offset. These two rows of the matrix were supplied to the ANN model and the respective outputs were recorded. Thus, two values were obtained for each output parameter. The index of relative importance (I_{RI}) of input variables was calculated as follows: (predicted output for +2.5% offset) − (predicted output for −2.5% offset)/(maximum − minimum) value of the output parameter. This method was applied to all the inputs. The estimation of I_{RI} values for yield strength is presented in Table 2. The graphical user interface of the developed model is shown in Fig. 1. The magnitude and sign of I_{RI} values indicate the relative importance of input parameters on output properties and are represented in Fig. 2.

3.2. Development of genetic algorithm neural network (GANN) model

In GA there are three main features viz. objective, objective function, and n-dimensional search space. In the present work, the objective is to optimize the combination of alloy chemistry and heat treatment parameters for the desired properties. Objective function is ANN model which is described in the earlier section of this