ARTIFICIAL NEURAL NETWORK USAGE FOR DETERMINING SOLIDUS TEMPERATURE OF STEELS

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Abstract

The potential use of artificial neural networks to determine the solidus temperature for steel based on composition has been investigated. Input data consist of solidus composition and temperatures both from literature and both from measurements. The primary performance testing of the model was then performed for steel grades measured. Several types of network topologies have been designed and trained and the best model selected. Testing was done on previously unseen data measured by differential thermal analysis method as on new input data. The used method is described. Obtained results are then compared to those measured and calculated by commonly used software among the academic and commercial community like IDS and Thermo-Calc. Performance of these three modelling approaches is discussed by means of selected statistic tools.

Keywords: Steel, solidus temperature, artificial neural networks, Matlab, DTA

1. INTRODUCTION

The general demand for increasing the quality of the cast steel with decreasing operational costs requires the correct setting of the boundary conditions, including the phase change temperatures like the temperature of liquidus or solidus [1]. Temperatures of liquidus and solidus characterise the basic thermophysical properties of the material in terms of solidification and primary metal structure formation [2]. Determining the solidus temperature is not a simple task. Experimental determination by methods of thermal analysis is very time and financially demanding [3]. One of the methods of determining phase transformation temperatures is the differential thermal analysis method based on accurate measurement of the temperature difference of the reference and reference samples during heating or cooling [4].

Empirical models are still an alternative to calculating phase transformation temperatures that have been used for decades. These are empirically derived computational relationships (analytical equations) obtained by regression analysis of experimentally measured phase transformation temperatures. These equations can be used to derive, for example, the liquidus temperature (T_L), and solidus temperature (T_S), etc., based on the chemical composition of the steel. Several analytical equations can be found to calculate in particular the liquidus temperature. Analytical equations for solidus temperature calculation are already considered as less available and reliable [5].

Therefore, calculations based on thermodynamic databases and methods like CALPHAD [6] or phase-field [7] are beginning to be promoted much more often to identify the liquidus temperature, where also other thermodynamic properties can be obtained based on the definition of chemical composition, which can be implemented, eg in the setting of numerical models used for the processes taking place during casting and solidification of steel [8].

Paper deals with potential use of an artificial neural networks for determination of T_S based on chemical composition, describes used methodology and compares obtained results with data from measurement and calculations by commonly used software.

2. ARTIFICIAL NEURAL NETWORK USAGE

Artificial neural networks (ANN) represents an information processing method which is inspired by the models of biological neural networks [9]. As an adaptive system changing its structure or internal information that flows through the network during the training phase, ANN is widely used in many areas of science because of its strong capacity of nonlinear mapping, high accuracy for learning, and robustness.

Algorithms and methods based on artificial neural networks are incorporated in commercially available software packages like Matlab, Statistica or can be implemented by scripting programming languages like R or Python. Those two languages has an advantage of being a free software with plenty of documentation, support forums and even prebuild "toolboxes" like DeepPy, DeepLearningKit or PyTorch.

Usage of artificial neural network in material science has been proofed by several studies on mechanical properties [9-14], on thermophysical properties [15-19], designing new alloys [21-22] or phase change temperatures [23,24].

2.1. Architecture of artificial neural networks

ANN can be divided into feedforward and feedback network. Backpropagation network and radial basis function network are the examples of the feedforward network, and Elman network is an example of a feedback network. The feedback has a profound impact on the learning capacity and its performance in modelling nonlinear phenomena [10].

Illustration of the simplest one type of ANN - single layer perceptron - with few inputs and one output is in **Figure 1**. The left side represents the common linear regression method. The inputs (concentrations of alloying elements) define the inputs, Bs the output node. Each input is multiplied by a random weight w_i, and the products are summed together with a constant θ (called also bias) give the output. The summation is an operation which is hidden at the hidden node.

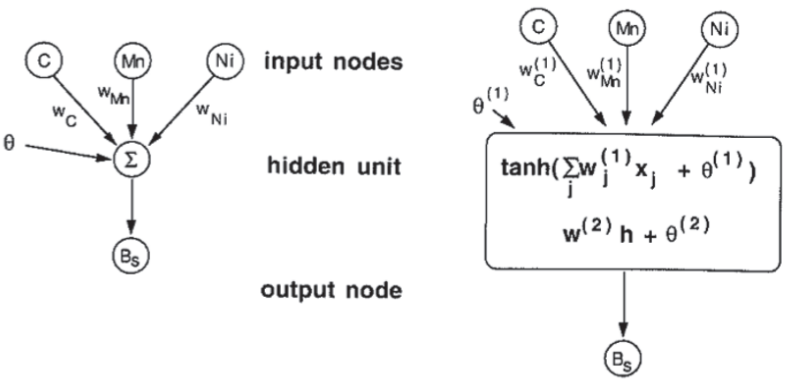

Figure 1 ANN representation of linear regression and non-linear network [13]

Since the weights and the constant θ were chosen at random, the value of the output will not match with experimental data. The weights are systematically changing until a best fit of the output is obtained as a function of the inputs; this operation is known as training the network. Right side of **Figure 1** shows non-linear network - the summation of inputs multiplied by weights and constant θ is an argument of transfer function - hyperbolic tangent. Resulting h is than multiplied with weight and summed with another constant θ which makes an output [13]. There are, also other transfer function like logistic, etc. which can be combined in one network [25].

Of course, one hidden unit in one hidden layer is not usually enough so ANN can be created with much more hidden layers, even thousands of them for deep learning tasks. There is, unfortunately, no general rule for estimating the needed number of hidden layers and hidden units. More or less, it is still a question of trial-error approach. The hidden neuron can influence the error on the nodes to which their output is connected. The stability of ANN is estimated by error. The minimal error reflects better stability, and higher error reflects worst stability. The excessive number of hidden neurons will cause overfitting; that is, the neural networks have overestimated the complexity of the target problem with significant degrading effect on the generalisation

capability which leads to a significant deviation in prediction. In this sense, determining the proper number of hidden neurons is critical in the prediction problem [26].

2.2. Source and preparation of input data

Creating and training of ANN predicting liquidus temperature in [24] was based on information about chemical composition and liquidus temperature found in literature. Because information about the temperature of solidus are quite rare and usually with unacceptable low information about composition, totally different approach was used. Based on composition of 308 heats of real steel grades equilibrium calculations with InterDendriticSolidification (IDS) software have been made and database of composition and corresponding Ts was prepared. **Table 1** sums up spread of chemical composition used for computations, i.e. for training, validating and testing of ANN. Ten alloying elements were chosen, Fe content is not involved into computation as it is dependent on the sum of the alloying elements.

Table 1 Chemical compositions of steel grades used as dataset [own]

wt.%	C	Mn	Si	P	S	Cr	Ni	Mo	V	Cu	Fe
Min	0.050	0.085	0.056	0.003	0.003	0.040	0.010	0.000	0.000	0.000	balance
Max	1.150	1.985	1.000	0.079	0.086	1.994	1.985	1.973	0.087	0.342	balance
Mean	0.426	0.921	0.383	0.018	0.014	0.571	0.523	0.491	0.005	0.090	balance

Even though theory does not require scaling of data for multilayer perceptron (MLP) ANN, it is usually recommended for better stability and faster convergence to required state of ANN [27]. As the distribution of input values (chemical composition) and output values is not normal, then it should not be standardised, but the data should be normalized according to equation (1).

$$y = \frac{x - min}{max - min} \tag{1}$$

where:

y - normalised value (1)
x - original value (wt.%)
min - minimum of the set (wt.%)
max - maximum of the set (wt.%)

2.3. Results

Matlab Neural Network Toolbox was used to create and train several MLP networks from which the one with best performance was chosen. Composition of 34 real steel grades which phase change temperatures were measured by DTA were used as new inputs for model. Resulting values of T_S were than compared with those from measurements - totally 102 measurements with results corrected to equilibrium conditions. Average absolute deviation was 8.5 °C, root mean square error (RMSE) 12.2 and coefficient of determination R^2 0.936. Plot of predicted against measured T_S is in **Figure 2**.

Comparison of ANN performance with IDS and Thermo-Calc (T-C) is in **Table 2**.

Table 2 Chemical compositions of steel grades used as dataset [own]

	Average absolute error	*RMSE*	R^2
ANN	8.5	12.2	0.94
IDS	9.6	12.3	0.93
T-C	14.0	22.0	0.82

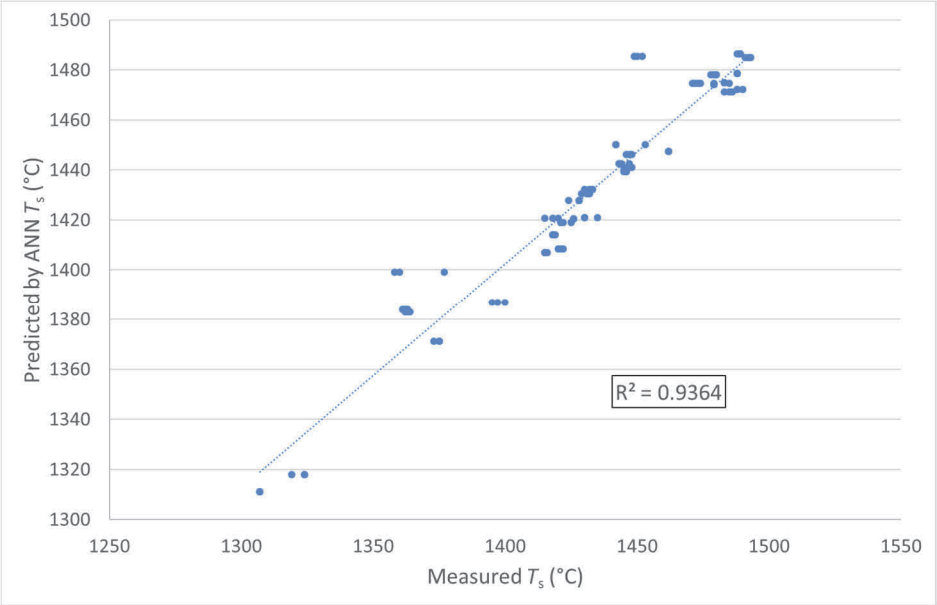

Figure 2 Predicted vs. measured T_S by ANN [own]

3. CONCLUSION

The ability of artificial neural networks to predict the temperature of solidus has been proofed by validation on a set of 102 measurements of 34 real steel grades. With slightly better performance than currently commonly used software like IDS or with significantly better performance in comparison with Thermo-Calc. Similar character of results between ANN and IDS is caused by fact that IDS computed data were used as primary learning data set. It should be noted that overperforming proofs the higher ability of generalization of ANN. Incorporating more data from actual measurement should improve the performance. Next logical step is to continue collect data for non-equilibrium computations with different cooling/heating rates and create an ANN based model predicting both liquidus and solidus temperatures from chemical composition and cooling rate.

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