ESTIMATION OF LIQUIDUS TEMPERATURES OF STEEL USING ARTIFICIAL NEURAL NETWORK APPROACH

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Abstract

Presented works investigates a possibility of using modeling based on artificial neural network for prediction of liquidus temperatures of low-alloyed steels. Paper describes the methodology of creating such model by tools incorporated in commercial software MATLAB. Neural network is trained, validated and tested and previously unseen data measured by DTA method are used as new input data. Results are then compared to those measured and calculated by commonly used software for such applications like IDS and Thermo-Calc. Performance of these three modeling approaches is discussed.

Keywords: Artificial neural networks, liquidus temperature of steel, MATLAB, Thermo-Calc, IDS

1. INTRODUCTION

Advanced computer simulation technology is a powerful tool which can be used to model critical phenomena of heat transfer and fluid flow and their relationships to processes occurring during metallurgical manufacturing operations like casting, forging or heat treatment [1]. Computational models enable the design and production of more economical and higher quality castings. In order to obtain reliable and accurate results from a simulation of the usually complex processes accurate and realistic values of thermophysical properties are necessary but reliable data for many materials of industrial interests are limited. Experimental determinations of these are difficult and often expensive also.

Accurate knowledge of liquidus temperature is necessary for setting of optimum casting temperature in casting processes. The data for specific steel grades are often difficult to obtain. They are not available or inaccurate [2]. Best case scenario is represented by aqcuisition of values from measurement by some thermal analysis method, e.g. differential thermal analysis.

There are many empirical equations derived using regression analysis to estimate the liquidus temperature (T_L) of steels [3]. Comparing of various equations prediction capability and validity is difficult as they are usually closely related to the studied alloys [4]. So there is no equation covering the whole variety of steel compositions from low-alloyed to high-alloyed steels, eg. stainless steels. The main problem lies in the simple form of the equations - they are usually linear functions of compositions. So there is an assumption of factor independence and linear additivity [5]. In parametric predictive systems like that, the variable to be predicted (T_L) is considered as a function of predictor variables (element content) that are assumed to have independent effects on T_L. This would maybe accurately describe the behavior of two-component systems, e.g. Fe-Si but in reality effect of Si content in real multicomponent steels on T_L is not so clear as shown in **Figure 1**.

There are also software packages which allow to compute phase transformation temperatures and values of thermophysical properties dependent on composition and temperature. For example IDS (Inter Dendritic Solidification) is based on thermodynamic approach, more specifically on phase-field method [6]. Another thermodynamic approach is represented by CALPHAD method [7]. This method is used by software Thermo-

Calc. There are also other software packages based on these methods but they were not included into this paper.

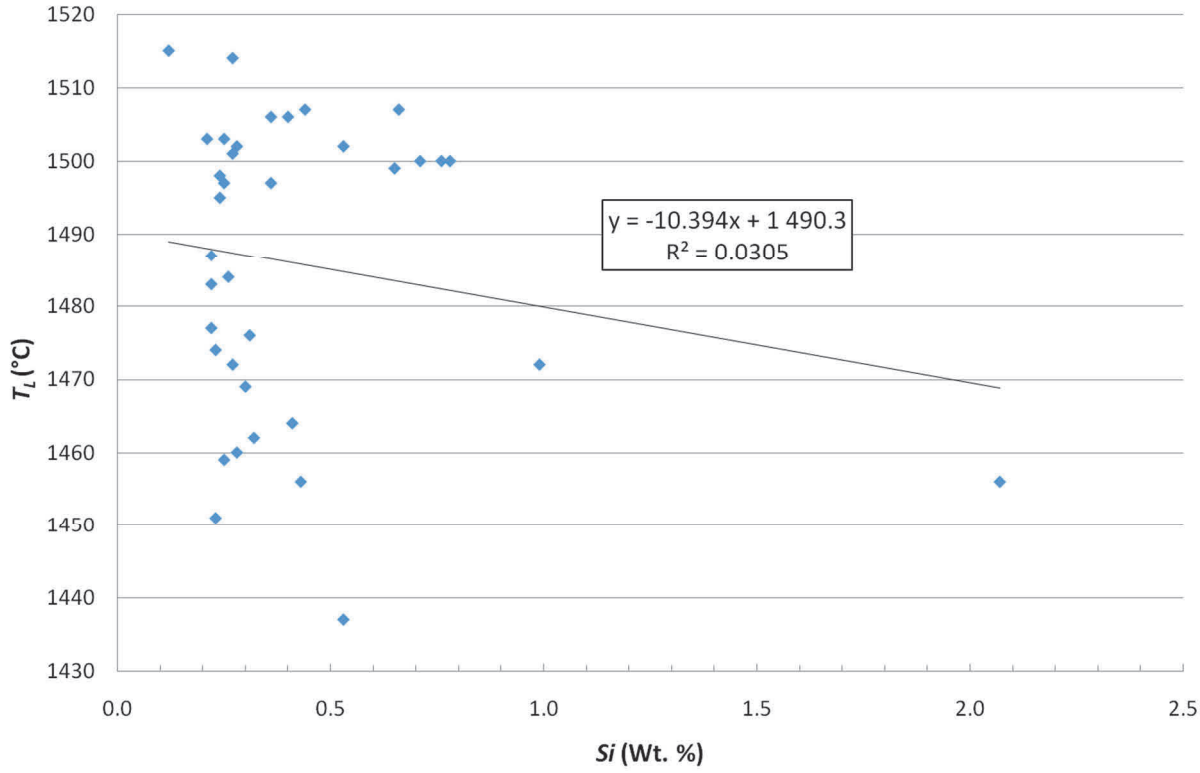

Figure 1 Effect of Si content on a liquidus temperature [own]

Paper presents a preliminary work aimed on prediction of liquidus temperature from steel grade composition by using an artificial neural network method (ANN). Using of methods based on ANN in the material engineering became a promising way for predicting a wide variety of steel properties like thermal conductivity [8-10], specific heat capacity [9], electrical conductivity [11], coefficient of thermal expansion [12] or phase transition temperatures [13]. It is even possible to propose a new alloy composition based on demanded material properties [14].

2. ARTFICIAL NEURAL NETWORK APPROACH

Neural network has the advantage of being fast, flexible efficient and accurate tool to predict and model highly nonlinear multidimensional relationships. Due to the flexible modeling and learning capabilities of ANN, it is possible to solve complex problems without any mathematical relationships between inputs and outputs. This method also reduces the need for experimenal work and time-consuming regression analyses.

2.1. Artificial neural networks

An ANN has non-linear basic processing units called neurons. The neuron model and architecture of a neural network describe how a network transforms its inputs into outputs. The neural network architecture consists of multiple layers of neurons which have a summing up junction and a transfer function. A single neuron (**Figure 2**) transmits an input *p* through the connection that multiplies its strength by the weight *w* to form a product *wp*. A bias *b* is then applied - it is much like a weight with constant value of 1 but can be omitted. The transfer function then produces the neuron output Y using the product *wp* and bias. There are various transfer

functions, most commonly used are sigmoid and linear. The central idea of an ANN is to adjust weights and biases or the network itself adjusts these parameters to achieve accurate results - desired output values.

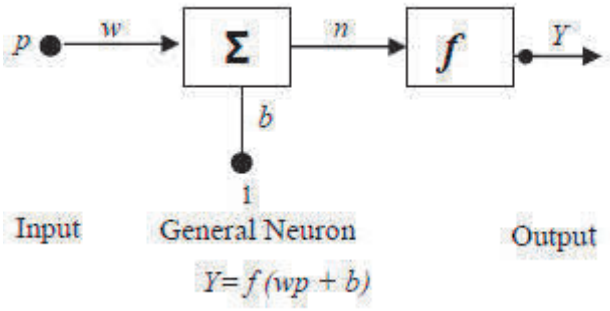

Figure 2 Simple neuron

The most commonly used neural network architecture is given in **Figure 3**:

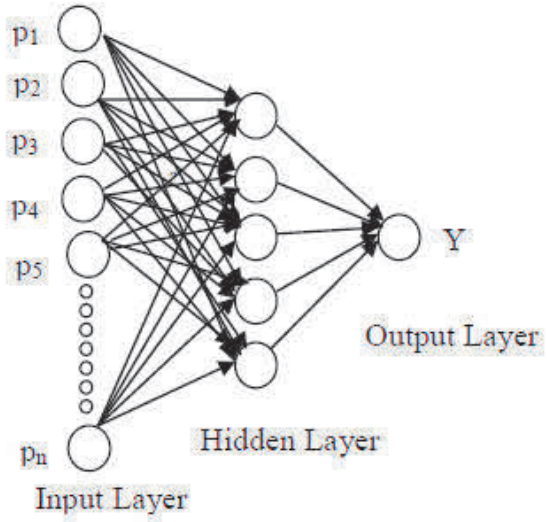

Figure 3 Neural network architecture

It consists of one input layer, one output layer, and one hidden layer. The added hidden layer contains intermediary parameters that are automatically generated by the model; the hidden layer is necessary in case of complex non-linear relationships between the inputs *p* and the output Y. One or multiple neurons connect the input to the hidden layer. Similarly, one or multiple neurons connect the hidden layer and the output layer.

2.2. Used method

Thirty-seven low-alloyed steel grades were used for training, validating a nad testing of ANN. These element contents represent inputs to the model. Output of model is a value of T_L. The chemical composition of the steels used in modeling is summarized in **Table 1**. Source of these data is [4].

Table 1 The composition of steels used for the creation of the ANN [own]

Content (wt%)	C	Mn	Si	P	S	Cu	Ni	Cr	N	Mo	V	Fe
minimum	0.01	0.02	0.12	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	bal.
maximum	1.20	1.63	2.07	0.04	0.04	0.2	3.30	5.00	0.02	0.99	0.14	bal.
mean	0.46	0.72	0.43	0.01	0.01	0.04	0.54	0.92	0.01	0.16	0.01	bal.

The MATLAB Neural Network Toolbox is used for the optimization of the ANN architecture. To avoid over-fitting inputs and targets are subdivided into three subsets - training (70 %), validation (15 %) and testing (15 %) subset randomly. Over-fitting leads to inability of the network to provide accurate predictions for new sets of inputs but it can only accurate correlate the given inputs.

Training subset (only) is used to develop the model. The validation subset is used to limit over-fitting - preventing the model from memorizing only a given data set and inability to model a new data set with unknown values of targets. The test subset is used for checking the generalization capacity of the network - ability to provide accurate prediction of unknown T_L for new composition of steel and temperature.

Several ANN were build, for further work ANN with lowest mean absolute error in prediction was chosen. Neural network consisted of multilayer perceptron (MLP) with 12 input neuron for element contents 6 hidden neurons in hidden layer and 1 output neuron with tanh activation function between inputs and hidden layer and exponential transformation function prior to output neuron was used. It has to be stated that there is no certain relationship between number of hidden neurons and performance of ANN. It can be ilustrated in **Figure 4** where coeffiecient of determination R^2 for predictions (test subset) is plotted against number of hidden neurons.

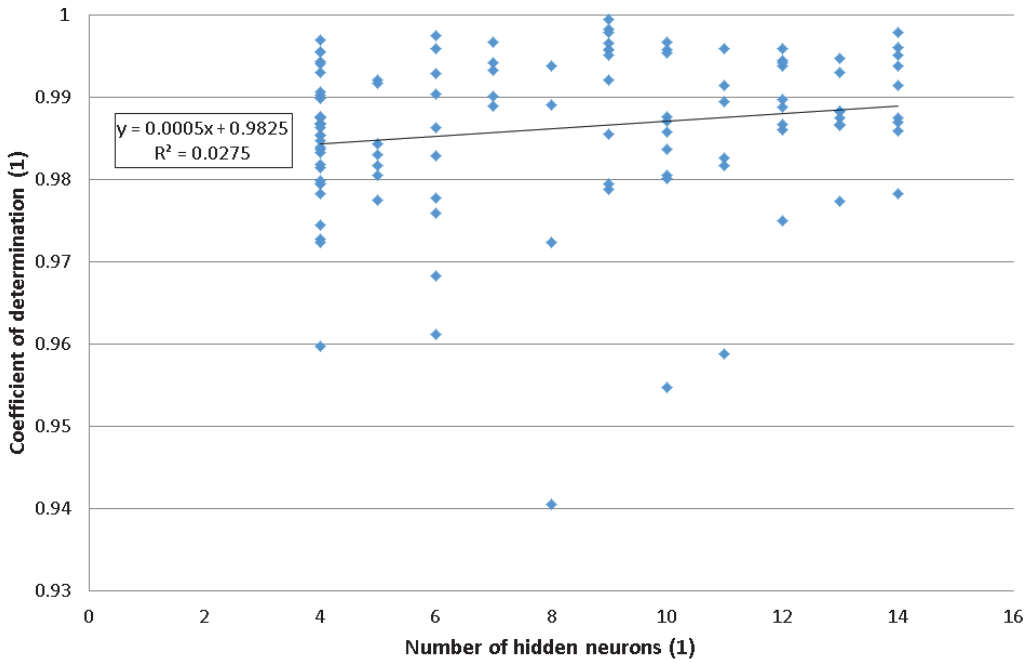

Figure 4 Number of hidden neurons vs. R^2 (test subset)

3. RESULTS

Liquidus temperatures of another thirty-three real steel grades were then modeled using the selected ANN. The composition range of these grades is in **Table 2**.

Table 2 The composition of steels used for evaluating of the ANN model [own]

Content (wt%)	C	Mn	Si	P	S	Cu	Ni	Cr	N	Mo	V	Fe
minimum	0.07	0.32	0.17	0.01	0.00	0.03	0.01	0.03	0.00	0.00	0.00	bal.
maximum	1.03	1.43	0.94	0.02	0.01	0.15	2.34	5.00	0.01	1.22	0.92	bal.
mean	0.35	0.85	0.32	0.01	0.00	0.08	0.22	0.93	0.01	0.18	0.09	bal.

Results were compared with measured values by DTA method. Also comparison of the ANN performance with results obtained from IDS and Thermo-Calc has been done.

The selected ANN based on the MLP12-6-1 architecture performed like this: the maximal absolute error in prediction was 10 °C, mean absolute error 0.9 °C with a coefficient of correlation R=0.92. Correlation between predicted and measured values is plotted in **Figure 5**, histogram of deviations from measured values is **in Figure 6**.

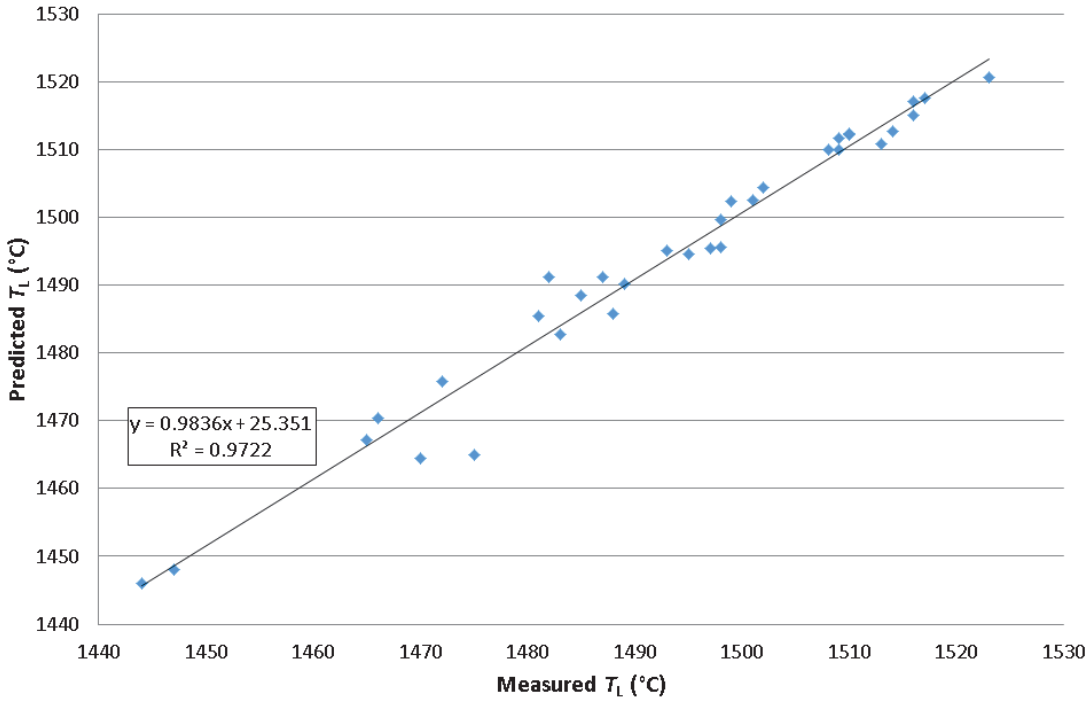

Figure 5 Measured vs. predicted values by ANN

Table 3 contains performance results for ANN, IDS and Thermo-Calc calculations for mutual comparison. It can be seen that difference between results from ANN and IDS is generally small and almost negligible but IDS seem to be slightly more reliable as values of R^2 indicates.

Nevertheless approach based on ANN showed significantly better accordance between predictions and measured values than computations with Thermo-Calc software. One of the possible reasons of this should be in fact that not all of the elements from steel composition were used in calculations but this was also the case of IDS and ANN calculations.

Table 3 Comparison of results obtained by different modeling approaches [own]

	ANN	IDS	Thermo-Calc
maximum of absolute error (°C)	10.0	10.0	28.0
mean absolute error (°C)	0.9	4.3	6.7
maximum relative error (%)	0.68	0.68	1.88
mean relative error (%)	0.18	0.29	0.45
correlation coefficient R	0.986	0.99	0.94
coefficient of determination R2	0.920	0.982	0.883

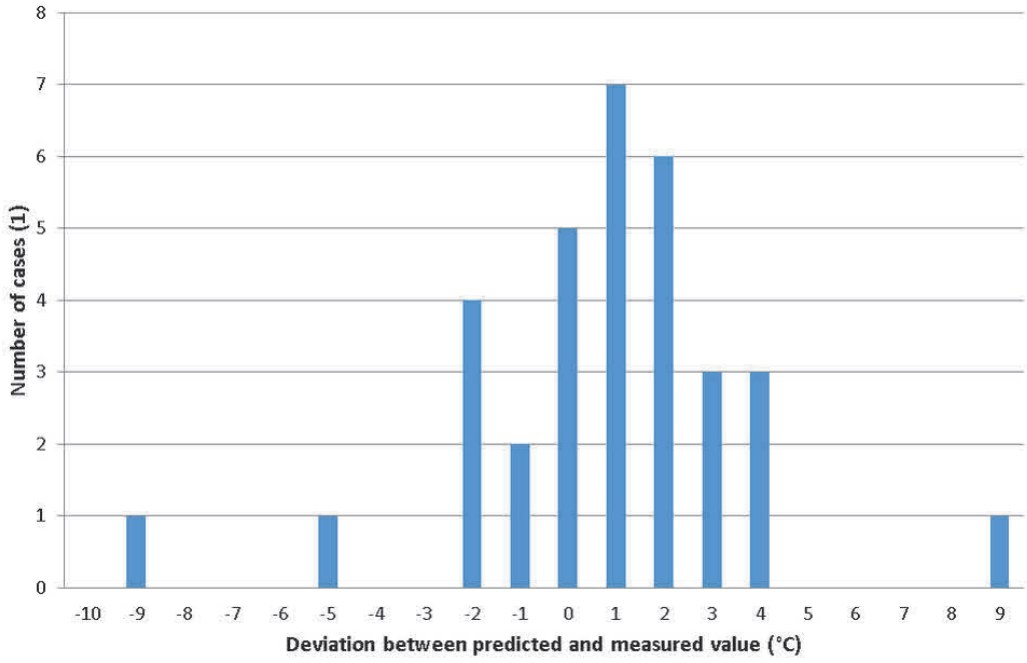

Figure 6 Histogram of errors

4. CONCLUSION

Neural network predictions of liquidus temperatures brought promising results in comparison with commonly used software tools like IDS (Inter Dendritic Software) and Thermo-Calc.

Maximal absolute error in prediction was 10 °C, mean absolute error 0.9 °C with a coefficient of correlation R=0.986. These values are at least comparable with those from IDS calculations where a maximal absolute error was the same 10 °C, mean absolute error was higher - 4.3 °C and value of R=0.99. Predictions based on Thermo-Calc calculations with TCFE8 database came as such: maximal absolute error 28 °C, mean absolute error 6.7 °C and value of R=0.94.

Approach based on ANN is a suitable solution for this specific case of liquidus of steel prediction, further work has to be done for other phase transition temperatures for which data are even less available in common literature (solidus temperature). It should be stated that presented model was created from data published in common literature so procedure can be repeated by almost everyone even with open-source software (Octave).

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REFERENCES

[1] VALENCIA, J. Thermophysical properties. In: VALENCIA, J., Quested, P., eds. *ASM Handbook,*. Materials Park: ASM International, 2008, Volume 1: Casting, pp. 468-481.

[2] DROZDOVÁ, Ľ., SMETANA, B., ZLÁ, S., NOVÁK, V., KAWULOKOVÁ, M., ROSYPALOVÁ, S., ŘEHÁČKOVÁ, L., MARTINÍK, O., DOSTÁL, P. Study of phase transformation temperatures of alloys based on Fe-C-Cr in high-temperature area. *Journal of Thermal Analysis and Calorimetry*. 2018; doi:10.1007/s10973-018-7012-6

[3] MILLS, K. C., YUCHU, S., ZUSHU, L., BROOKS, R. F. Equations for the Calculation of the Thermo-physical Properties of Stainless Steel. *ISIJ International*. 2007. ISSN 1347-5460. Available from: https://doi.org/10.2355/isijinternational.44.1661

[4] MIETTINEN, J., HOWE, A. Estimation of liquidus temperatures for steels using a thermodynamic approach. *Ironmaking and Steelmaking*. 2000, no. 27, p 212-227.

[5] NISBET, R., ELDER, J. F., MINER, G. *Handbook of statistical analysis and data mining applications*. Burlington: Elsevier/Academic Press, 2009. p. 824.

[6] MOELANS, N., BLANPAIN, B., WOLLANTS, P. An introduction to phase-field modeling of microstructure evolution. *CALPHAD.* 2008; doi: 10.1016/j.calphad.2007.11.003.

[7] ANDERSSON, J. O. et al. THERMO-CALC & DICTRA, Computational Tools For Materials Science. *Calphad*. 2002, vol. 26, no. 2, p 273-312.

[8] ŽMAK, I., FILETIN, T. Predicting thermal conductivity of steels using artificial neural networks. = Predicting thermal conductivity of steels using artificial neural networks. *Transactions of FAMENA*, 2010, vol. 34, no.3, p 11-20. ISSN 1333-1124.

[9] LÓPEZ-MARTÍNEZ, E. et al. Artificial Neural Networks to Estimate the Thermal Properties of an Experimental Micro-Alloyed Steel and Their Application to the Welding Thermal Analysis. *Strojniški vestnik - Journal of Mechanical Engineering*, [S.l.]. 2015, vol. 61, no. 12, p. 741-750. ISSN 0039-2480.

[10] Peet, M. J., Hasan, H. S., Bhadeshia, H. K. D. H. Prediction of thermal conductivity of steel, *International Journal of Heat and Mass Transfer*, 2011, vol. 54, no. 11-12, p. 2602-2608, ISSN 0017-9310.

[11] Koley, S., Ray, T., Mohanty, I., Chatterjee, S., Shome, M. Prediction of electrical resistivity of steel using artificial neural network. *Ironmaking & Steelmaking*. 2017; DOI: 10.1080/03019233.2017.1403109.

[12] BANO, N., NGANBE, M. Modeling of Thermal Expansion Coefficients of Ni-Based Superalloys Using Artificial Neural Network. *Journal of Materials Engineering and Performance*. 2012; doi: 22. 10.1007/s11665-012-0398-6.

[13] Wang, J., van der Wolk, P. J., van der Zwaag, S.. Determination of Martensite Start Temperature in Engineering Steels Part I. Empirical Relations Describing the Effect of Steel Chemistry, *Materials Transactions, JIM*, 2007; doi: https://doi.org/10.2320/matertrans1989.41.761.

[14] Conduit, B. D., Jones, N.G., Stone, H.J., Conduit, G.J, Design of a nickel-base superalloy using a neural network. *Materials & Design*. 2017, vol. 131, p. 358-365, ISSN 0264-1275, https://doi.org/10.1016/j.matdes.2017.06.007.