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Artificial Neural Networks to Predict of Liquidus Temperature in Hypoeutectic Al-Si Cast Alloys

[1]S. Farahany, [2]M. Erfani, [2]A. Karamoozian, [1]A. Ourdjini and [1]M. Hasbullah Idris
[1]Department of Materials Engineering, Faculty of Mechanical Engineering, UTM, Malaysia
[2]Faculty of Computer Science and Information Systems, UTM, Malaysia

Abstract: Determining the liquidus temperature of cast alloys is an important factor in considering the superheating temperature and melt treatment of aluminium-silicon cast alloys. In addition to experimental calculation, the liquidus temperature can also be determined using simulation software for more reliable results. In this study, Artificial Neural Network (ANN) with hyperbolic tangent was selected to predict the liquidus temperature of Al-Si alloys as a function of chemical composition. The neural network was trained with seven input parameters (Si, Fe, Cu, Mn, Mg, Zn and Ti) and one output parameter (liquidus temperature). Training and testing dataset has been chosen from different published works, any casting software and aluminium binary phase diagrams. The accuracy of neural network was verified using values reported in literatures. The result of this investigation has shown that the backpropagation feed forward neural network is accurate enough to predict liquidus temperature.

Key words: Liquidus temperature, Al-Si, cast alloys, Artificial neural network

INTRODUCTION

Aluminum-silicon cast alloys are prominent group among Al alloys and widely used in automotive and aerospace applications to produce critical components, because of good fluidity and castability, higher strength to weight ratio, good surface finish and better wear resistance in comparison with other aluminum cast alloys (Venkaltaramani *et al*., 1995; Prasada-Rao *et al*., 2004).

Alloys with 3-5% silicon are utilized in rotors, vessels, valve bodies and large fan blade fittings. Eutectic alloys containing between 11-13% Si are used for pistons, cylinders, blocks and heads of engines in automobile and aeronautical industries (Hegde and Prabhu, 2008). Alloy elements such as Fe, Cu, Mg and Mn are added Al-Si to achieve the desired properties.

It is common practice in the foundry industries to cast molten metal 100°C above the liquidus temperature which defined as superheat temperature to provide better molten metal fluidity and obtain desired microstructure.

Regarding to this issue, the knowledge of reliable liquidus temperature of alloys is necessary to estimate their corresponding superheat temperature. Since, the data about binary and tertiary phase diagrams of aluminium with other alloying elements are not sufficient, correct determine of liquidus temperature in multi component Al-Si alloys is essential to increase the efficiency of melt treatment and produce high quality components.

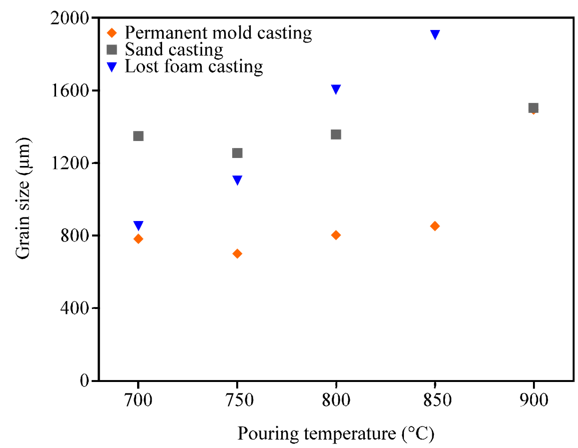

Fig. 1: Variation of grain size with pouring temperature

Grain size: The solidification microstructure of the alloy is dependent on the superheat temperature, as well as the cooling rate during solidification (Zhong-wei *et al*., 2005). It has been reported that grain refined structure achieved by controlling casting parameters such as superheat temperature, casting temperature and cooling rate (Conley *et al*., 2000). Figure 1 shows the relationship between grain size and superheat temperature in permanent mold casting, sand casting and lost foam casting for Al-7%Si. It can be see that grain size of the alloy increases with increasing the superheat temperature from 700 to 900°C (Venkaltaramani *et al*., 1995).

Corresponding Author: Saeed Farahany, FKM, UTM, 81310, Malaysia

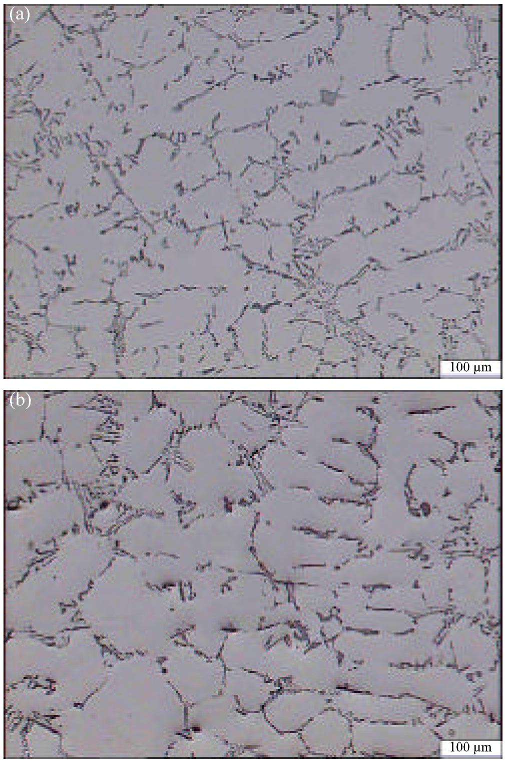

Fig. 2: Microstructure of Al-7Si-0.4Mg alloy at two different pouring temperatures: (a) 680°C and (b) 710°C

Srinivasan *et al.* (2006) also obtained same results in sand cast Al-7Si-0.3 Mg. Figure 2a and b show the effect of pouring temperature on microstructure of Al-7%Si in two different pouring temperatures. It is clear that DAS increases with increasing pouring temperature and in turn reduces the mechanical properties (Srinivasan *et al.*, 2006).

Moreover, increasing pouring temperature causes to increase fluidity length of molten metal as shown in Fig. 3 (Rzychon and Kielbus, 2007).

Calculation and Prediction of liquidus temperature: Differential thermal analysis (DTA) (Wu and Perepezko, 2000) and Differential Scanning Calorimeter (DSC) (Dong and Brooks 2005) are used to determination of liquidus temperatures, the result even for binary alloys was variable. Also, thermal analysis is applied for calculation of liquidus temperature based on cooling curve of molten metal. In this condition the result is dependent to cooling rate and geometry of the mould sample.

Drossel (1981) Eq. 1 to predict the liquidus temperature of Al-Si cast alloy.

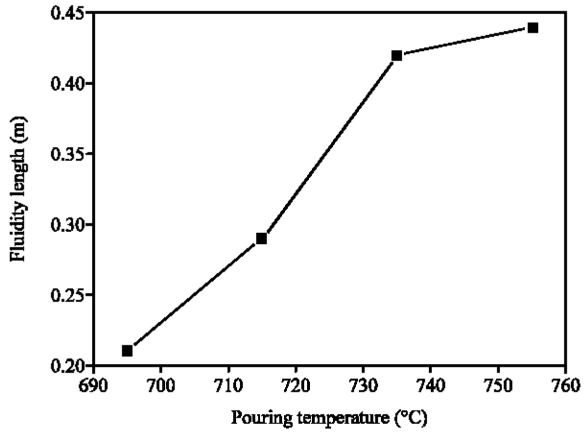

Fig. 3: The effect of pouring temperature on the fluidity length

$$TL_{IQ(°C)} = 661\text{-}4.97Si\text{-}0.15\,(Si)^2 \\ \text{-}6.13Cu\text{-}17.4Mg+2.72Zn + 5.08CuMg \qquad (1)$$

However, the range of chemical composition is limited for application. Besides, Eq. 2 has been proposed (Vijayaraghavan *et al.*, 1996) based on the ternary phase diagram:

$$T_{LIQ(°C)} = 664\text{-}6.9Si\text{-}2.5Cu\ (°C) \qquad (2)$$

This equation can be used just for Al-Si-Cu alloys. Another relationship developed based on silicon equivalent by Djurdjevic *et al.* (1998):

$$T_{LIQ(°C)} = 660.452\text{-}6.110Si_{EQ}\text{-}0.057\,Si^2_{EQ} \qquad (3)$$

The result is more accurate compared with Eq. 1 and 2. However, all of the major alloying elements must have eutectic or peritectic reaction with Al.

Due to chemical composition limitation and their assumption to validate above equations, forecast of liquidus temperature based on Artificial Neural Network has drawn attention.

The aim of this study is to use artificial neural network method for the prediction of the liquidus temperature of multi-component hypoeutectic Al-Si alloys, based on their chemical compositions.

Modeling with artificial neural network: Artificial neural network has been widely used in solving material science problems that involve the manipulation of several parameters and non-linear interpolation and therefore not easily amenable to conventional theoretical (Sha and Edwards, 2007) and experimental approaches.

Since, ANN has been established in the field of material science (Bhadeshia, 1999), researchers utilized this modeling technique in forecasting parameters in hot working Aluminium alloys (Chun *et al*., 1999), prediction of mechanical properties of automotive Al alloys (Emadi *et al*., 2001), prediction of porosity formation in Al-Si cast alloy (Shafyei *et al*., 2006), forecasting of tensile and density properties in Al metal matrix composite (Altinkok and Koker, 2006), modeling creep life behaviuor of aluminium composite (Gupta *et al*., 2007), grain size prediction of AA5754 (Lela *et al*., 2008), study surface roughness (Caydas and Hascalýk, 2008) and forecasting the tensile strength of welded A319 cast aluminium alloy (Jayaraman *et al*., 2009). This variety of applications demonstrates the capability of artificial neural network method in the prediction of physical and mechanical properties of aluminium alloys.

Artificial neural network theory: A neural network is a system composed of many simple processing elements operating in parallel whose function is determined by network structure, connection strengths and the processing performed at computing elements or nodes.

One of the prominent advantages of ANN is its ability to learn how to do tasks based on the set of data, called training set. There are several types of neural network such as feed forward neural network, Radial Basis Function (RBF) network, Kohonen self-organizing network and etc. As mentioned above, several neurons, which are highly connected to each other in different layers form an ANN.

One of the most frequent types of ANN is feed forward which consists of an input layer, one or more hidden layers and an output layer (Shafyei *et al*., 2006) that has been demonstrated schematically as a three-layer ANN in Fig. 4.

Each node is composed of four main elements which are input, weighted connection, activation function and output. Basically, the inputs are information received from the preceding layer which is of the form:

$$X_j = \sum_{i=1}^{n} W_{ij} X_i + b_j \quad (4)$$

where, X_j is the net input, X_i are inputs from the previous layer, W_{ij} are weights entered node j, which are values assigned to the connections between nodes and express the effect of an input set on the node, b_j is the bias associated with node j and n is the number of nodes. The bias neurons do not have any input. They just affect the neurons of the next layer by emitting a constant output value across the weighted connections. Details are shown in Fig. 5 for better understanding.

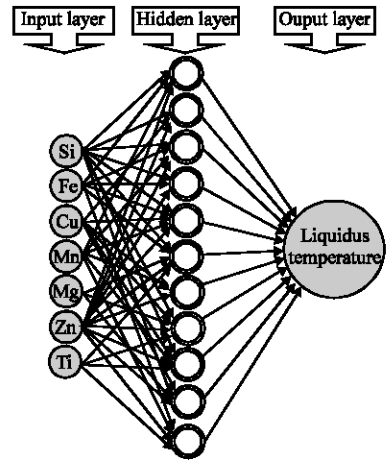

Fig. 4: Artificial neural network topology

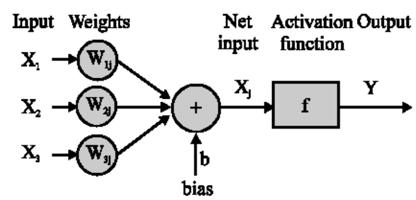

Fig. 5: A processing element (neuron) operation

To avoid the numerical overflows due to very large or very small values, normalization of the inputs is necessary which could be minmax function formulated as follows (Sola and Sevilla, 1997):

$$\text{Normalized value} = \frac{\text{Input value} - \text{Minimum value}}{\text{Maximum value} - \text{Minimum value}} \quad (5)$$

Normalization limits the range of the output values into [0, 1] where data can be retrieved by the reverse method of normalization.

Another element of a neuron is activation function which shows the internal activation level and the other one is output (Y) which is generally obtained as a function of inputs and determined as follows:

$$Y = f\left(\sum_{j=1}^{n} W_{ij} X_j + b_j\right) \quad (6)$$

A multilayer network, in general, learns much faster when the activation function is represented by a hyperbolic tangent. Hence, the activation function f in the hidden layer is selected as hyperbolic tangent sigmoid transfer function. The hyperbolic tangent can make the network non-linear whose strength is determined by the weight Wij. The output Y is therefore a non-linear function of Xj. The function usually chosen to be the hyperbolic tangent because of its flexibility and faster convergence (Bhadeshia 1999).

There are three types of learning in neural network which are supervised learning, unsupervised and reinforcement learning.

To illustrate how a neural network works and to estimate how accurate a neural network is, the data set is divided into two categories:

- Training category which includes the weights associated with each interconnection
- Test category which verifies the network predictions for instances that are not learnt previously

The supervised learning method procedure is as follows: A training process starts by introducing an input vector to the input layer and distributing it throughout the network to the output layer. At each observation, the output vector, which is produced from the output nodes, is compared with the target vector and errors are calculated.

To minimize the error, the weights are recalculated according to the difference between output and target vector and the training process turns back to the previous layer to update the weights and train the network again with new values. This kind of training is called backpropagation training algorithm (Shafyei *et al*., 2006).

ANN structure and training: However, based on the definition of network structure and components, there are several ANN models trained and tested using training data sets. Here, in this study, we use feed forward neural network structure (Fig. 4). The ANN consists of element concentrations and liquidus temperature in the input and the output layers, respectively.

The number of hidden layers and neurons within each hidden layer can be varied based on the complexity of the problem and the dataset. In our study, only one hidden layer is used while the neurons within this layer varies from 2 to 12. The optimal configuration was based upon minimizing the difference between the neural network predicted values and the desired outputs. A total dataset of 156 samples were selected from AnyCast software, Binary phase diagram of aluminium and previous published works (Byczynski, 1997; Djurdjevic *et al*., 1998; McDonald *et al*., 2004; Robles-Hernandez *et al*., 2005) to train and test the network where 15 of them applied as the test set. Also, the range of input data used for prediction of liquidus temperature is shown in Table 1.

Table 1: Maximum and minimum of input parameters

Elements	Minimum concentration (wt %)	Maximum concentration (wt %)
Si	0.0	12.60
Fe	0.0	2.00
Cu	0.0	33.20
Mn	0.0	1.00
Mg	0.0	36.80
Zn	0.0	3.00
Ti	0.0	0.50

The data applied to the process of learning and testing have been normalized by means of the *minmax* function that transforms the domains of variables to range [0,1].

The hyperbolic tangent sigmoid transfer function which demonstrated in Eq. 7 was used as the activation function in the hidden layer and a linear transfer function was used in the output layer.

$$\tan\text{sig}(n) = \frac{2}{1+e^{-2n}} - 1 \qquad (7)$$

Furthermore, the learning algorithm used in the proposed methodology is Levenberg-Marquardt backpropagation.

RESULTS AND DISCUSSION

As explained before, number of neurons in each hidden layer varies according to the intricacy of the problem. Therefore, it should be selected in such a way to minimize the network performance function.

The network performance function is measured according to the Mean Square Error (MSE). The variation of network performance function with the number of hidden neurons is shown in Fig. 6. It illustrates that a hidden layer with 8 neurons results in minimum MSE. So, the ANN model trained by 7 neurons as input layer, 8 neurons in hidden layer and one neuron as the output. It was also implemented using feed forward backpropagation neural network.

The investigation is shown in Fig. 7 and 8 using a regression analysis. Regression is a method of determining relationships among different data in order to predict future behavior or results. The regression of training and test steps are shown. As the figures depict, the training and test step regression results are 0.99109 and 0.97981, respectively.

To compare the accuracy of the proposed methodology with the methods developed by Drossel, Vijayaraghavan and Djurdjevic for calculation of liquidus temperature in Al-Si cast alloy, Fig. 9 and 10 have been plotted.

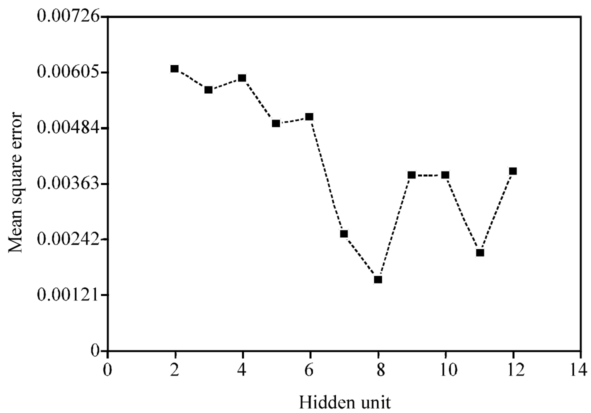

Fig. 6: Variation of network performance function with the number of hidden neurons

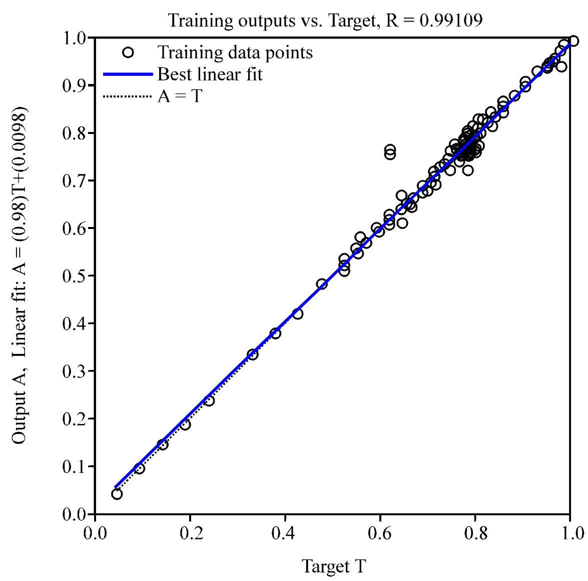

Fig. 7: Training step regression

As it can be figured out, the predicted values have more convergence to the real data compared to developed equations for input test data. Although, djurdjevic equation shows better prediction than other two equations, suggested ANN model is more efficient.

Not only reliable and accurate prediction of liquidus temperature helps to obtain desired microstructure result in improving mechanical properties of Al-Si cast alloy, but also, it assists to provide required viscosity and surface tension of molten metal for better fluidity to produce high quality Al-Si casting components.

As the results show, the proposed ANN gives satisfactory results to predict the liquidus temperature.

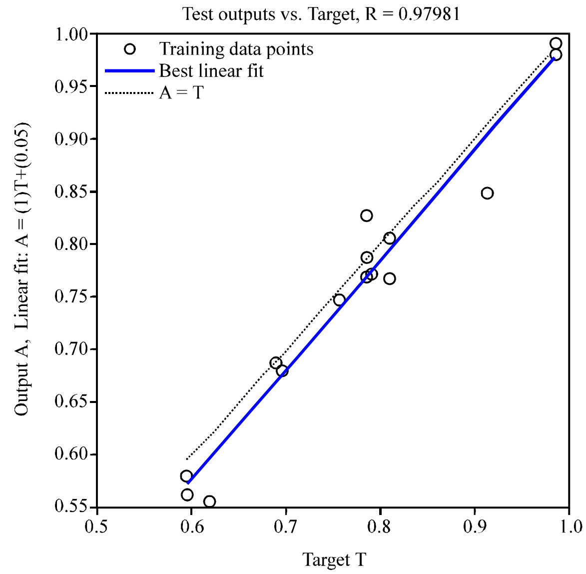

Fig. 8: Testing step regression

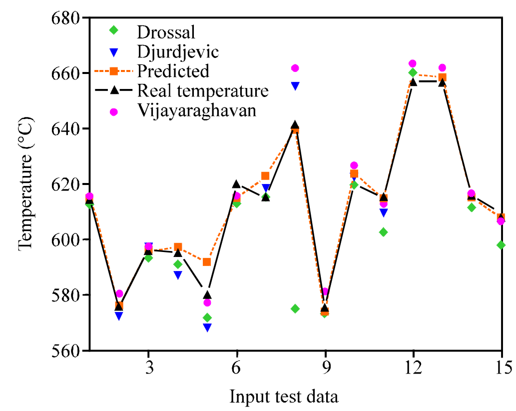

Fig. 9: Comparison of predicted values with drossel, vijayaraghavan and djurdjevic

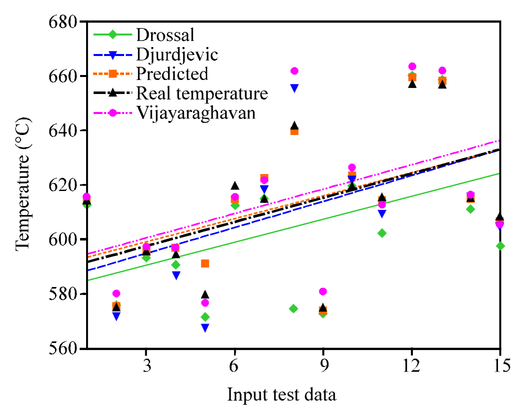

Fig. 10: Linear regression of predicted values compared with developed methods

CONCLUSION

It has been shown that the application of artificial neural networks is accurate to forecast different phenomena in material science. Hence, in this investigation, the ANN with one hidden layer and eight units in the hidden layer has been used to predict the liquidus temperature of Al-Si cast alloys. The research shows that ANN performs well in prediction of liquidus temperature when compared to the experimental measurements. Furthermore, the model obtained from ANN can be used in the modeling of the solidification behavior of aluminum-silicon alloys.

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