Neural Network Model for Thermal Conductivity of Steels

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Introduction

Thermal conductivity is an important parameter in the heat treatment and use of steels. Temperature gradients during cooling can lead to microstructural gradients and to residual stresses in steel components. Thermal transients can influence the development of stresses reducing service life and safety.

The impetus for the development of our model was to provide thermal conductivity values for the design of a steel quenching probe. The critical dimensions of which scale linearly with the thermal conductivity, therefore a probe made from steel has to be proportionally smaller than commonly used standard probes made from silver or aluminium. Having a model for thermal conductivity would allow us to investigate the heat transfer coefficient of any steel, rather than being limited to only those with available data.

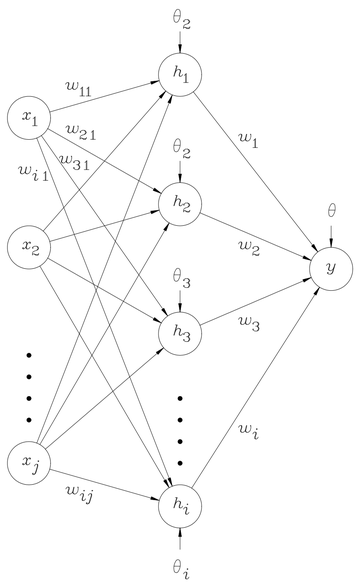
Previous work on the thermal conductivity of steel shows that there is a wide variation in the thermal conductivity as a function of composition. Presumably due to the complexity, there is very little fundamental research on the effect of alloying elements and temperature upon the thermal conductivity. There is a large amount of relatively low-quality data available which gives the thermal conductivity for particular grades of steel. This data is produced by steel suppliers for steel selection purpose, each steel grade in reality represents a range of compositions, and very few details of the microstructure at each temperature tested are available.

Due to the complexity of the composition dependence and the lack of any existing physical model, it is appropriate to proceed by developing a neural network model.

Bayesian Neural Networks

To enable the modelling of thermal conductivity for steels of arbitrary composition, a database was collated of 223 steels with compositions including 15 different elements.

The neural network was used as a general form of regression, as previously applied to many problems in materials science [1, 2]. The neural network used has been developed in a statistical framework, it is able to automatically infer the appropriate complexity of the model [3]. This helps avoid the problems of over-fitting the very flexible equations used in neural network models.



Structure of the three layer neural network

The output variable is expressed as a linear summation of activation functions, h_i, with weights w_i and the bias θ.

$$y = \sum_i w_i h_i + \theta \tag{1}$$

with the activation function for a neuron i in the hidden layer given by,

$$h_i = \tanh\left(\sum_j w_{ij} x_j + \theta_i\right) \tag{2}$$

with weights w_{ij} and biases θ_i. The weightings are simplified by normalising the data within the range ± 0.5 using the normalisation function, $x_j = x - x_{\min}/x_{\max} - x_{\min}$ - 0.5, where x is the value of the input and x_j is normalised value.

In the Bayesian neural network [3] 'training' is achieved by altering the parameters by back-propagation [4] to optimise an objective function which combines an error term (E_D) to assess how good the fitting is and regularisation term (E_W) to penalise large weights,

$$\mathrm{M}(w) = \beta\left(\frac{1}{2}\sum_i (t^{(i)} - y^{(i)})^2\right) + \alpha\left(\frac{1}{2}\sum_i w_i^2\right) \tag{3}$$

where β and α are complexity parameters which greatly influence the complexity of the model, $t^{(i)}$ and $y^{(i)}$ are the target and corresponding output values for one example input from the training data $x^{(i)}$.

This automatically infers over–complex and under–regularised models to be less probable, even though the flexibility of equation 1 allows them to fit the data better. Assuming that the uncertainty about the output y has a Gaussian distribution, the size of the error bars σ_u^2 can be calculated from the Hessian of the parameters by,

$$\sigma_u^2 = \mathrm{G}_{(u)}^{\mathrm{T}} \mathrm{A}^{-1} \mathrm{g}_{(u)} \tag{4}$$

where $\mathrm{g}_{(u)}$ is $\partial y/\partial \mathrm{w}$ evaluated at $\mathrm{x}^{(u)}$ [5].

Other modelling procedures also help to produce a robust model, such as the use of training and testing sets, and the formation of a committee of sub-models each converging from different positions in parameter space. After training the models can than be assessed by testing if the trends in the predictions are as expected, and more objectively by the prediction of unseen data. A major advantage of the approach is that is allows the calculation of error-bars which vary in size depending on the position in the input-space and indicating the confidence in the predictions.

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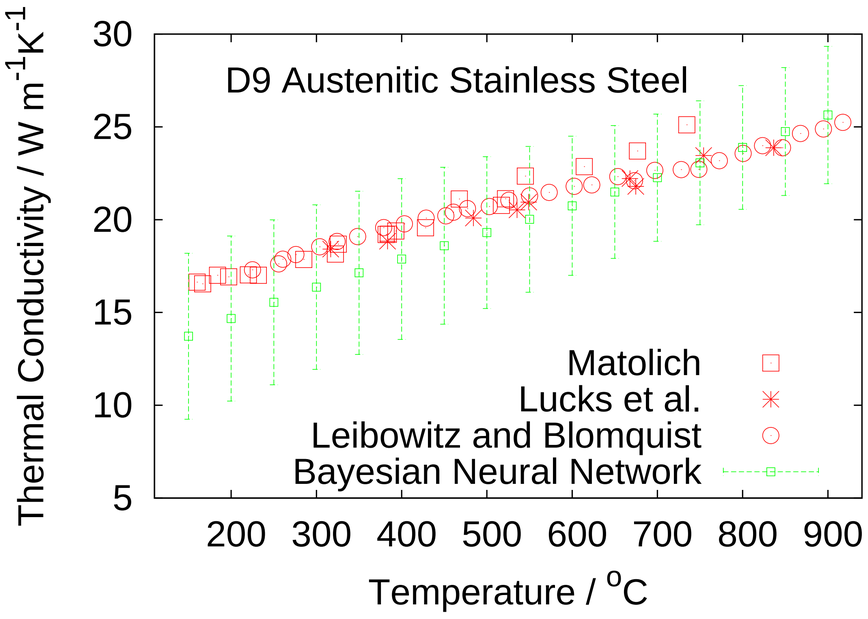
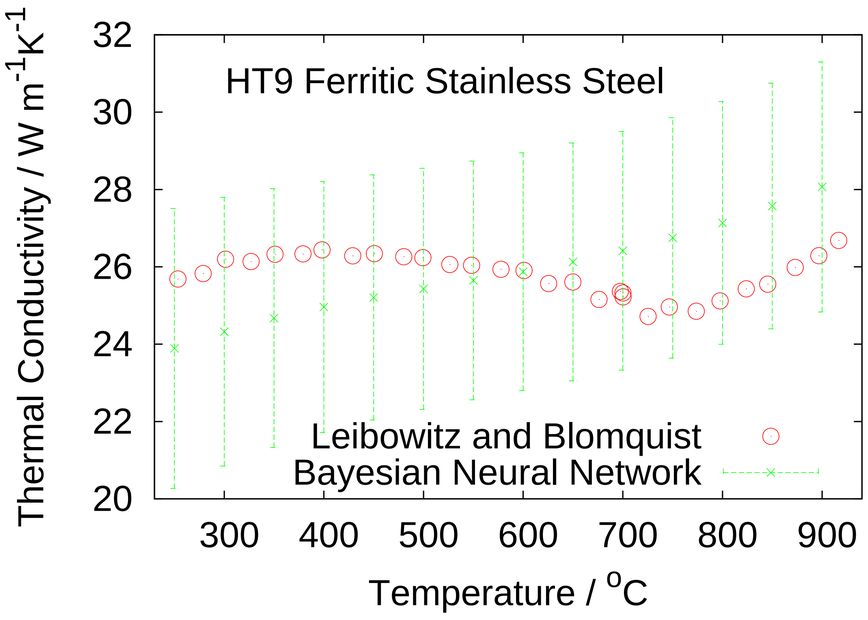
Predictive ability

The model is found to be able to generalise sufficiently to reproduce the general trends in the data, and be capable of making useful predictions of unseen compositions. Here we compare the predictions of the model against data for a ferritic steel and an austenitic stainless steel used in the nuclear industry [6]. In these cases it can be seen that the measured values lie completely within the error bars of the model, even though the exact variation as a function of temperature reported is not matched, particularly for the ferritic steel. The difference in the prediction for the ferritic steel is similar to the experimental differences reported in various papers.





Predictions for Sandvik alloys D9 (Fe-15.5Ni-13.5Cr-2Mn-2Mo-0.75Si-0.25Ti-0.04C Wt%) and HT9 (Fe-0.5Ni-12Cr-0.2Mn-1Mo-0.25Si-0.5W-0.5V-0.2C Wt%)

The general performance of the model can be tested by predicting on unseen data, these were grouped into those within the range of data used for training and those outside the range, this does not necessarily classify them as interpolation and extrapolation because they can have the elements in different combinations. As can be seen from the table, the perceived error (1 standard deviation) matched well with the root mean squared error.

Data set	Perceived Error	Root mean squared error
Unseen data within range of model	5.5	6.1
Data beyond range of model	82.3	50.8

Conclusions

A model has been developed which can predict the thermal conductivity of steels, along with meaningful estimate of the accuracy of the predictions. The model is publicly available online [7].

In future work it may be possible to improve the model by including calculation of physically meaningful parameters. For example the equilibrium volume fraction of austenite, cementite and ferrite could be included to attempt to distinguish the effect of the different components as they vary as a function of temperature.

It seems likely that any significant improvement to the model would require new experiments to be performed to measure the effect of microstructure, which would be required to model thermal conductivity changes as a function of time and temperature.

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