Thermal Conductivity Prediction of Composite Materials Based on Machine Learning Method

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Abstract—In this paper, a method based on machine learning and neural network to predict the effective thermal conductivity of composite materials is proposed and compared with the existing models and experimental results.For simple particle uniform distribution, this method rediscovers and verifies the existing theoretical results.The comparison between the predicted results and the experimental results shows that the predicted results are in good agreement with the experimental results.By training the thermal conductivity of different composites, our model can effectively predict the influence of different particle shapes, sizes and distributions on the thermal conductivity.

1. Introduction

Composite material refers to the material composed of two or more different substances combined in different ways. It can give play to the advantages of various materials, overcome the defects of a single material, and expand the application range of materials. The development of modern high technology cannot be separated from the development of composite materials. The research and application of composite materials and the speed and scale of its production development have become one of the important indicators to measure the advanced level of a country's science and technology. In many fields such as aerospace, auto mobile industry and chemical industry, they have played a great role in replacing many traditional materials. The form of composite materials has different properties according to the proportion, shape and distribution of the two mixed materials. Every year, many new composite materials are synthesized artificially. How to quickly deciding their properties is becoming a big problem. Thermal conductivity is one of the important properties that affects the application of certain materials. The existing approaches to estimate the thermal conductivity involve either complicated mathematical derivation or massive finite element computation.

These years, with the increasingly profound influence of artificial intelligence to the research of thermal dynamics and composite material, more and more researches start seeking opportunities from machine learning to provide more convenient approach to estimate the thermal conductivity.

In this paper, we present an machine learning approach to estimate the thermal conductivity of composite material. Different from the other existing attempts that use machine learning for the similar purpose, our work focuses on the influence of particle shape, so as to enhance the accuracy of estimation. By applying non-linear regression on the collected data, we verified it is possible to use artificial neural network to estimate the thermal conductivity.

Moreover, to study the effect of particle shape on the thermal conductivity and further include the particle shape in the model, we introduced an novel shape factor to characterize the shape of particles. By including this shape factor in the training process, we can generalize the model to be applicable for all particle shapes. In other words, the model trained from the data of one particular particle shape is applicable for the other particle shapes by properly choosing the shape factor. We also show that the shape factor can be estimated through another neural network model from the common parameters, such as volume and surface area etc.

Thus, all in all, the contributions in this paper may be summarized as follows.

- We verify that the non-linear regression of multi-layer neural network is capably of estimating the effective thermal conductivity of certain material.
- We introduce the novel generalized shape factor to characterize the particle shape. And propose a machine learning approach to estimate this shape factor.
- We build a semi-analytical system to quickly estimate the thermal conductivity of composite material, with particle shape considered. Also, we evaluate the system with several different particle shapes and compare results with existing analytical method and finite element simulation.

2. Background

In this section, we present some background knowledge related to the content of this paper for the purpose of making this paper self-contained.

2.1. Effective Medium Theory

Effective medium theory (EMT) or effective medium approximations (EMA) is an analytical approach to estimate the thermal conductivity of composite materials. There are many different kinds of EMT, each of them includes various factors and performs more or less accurate in different applications. Almost all of the EMTs include three primary factors: K_m, the thermal conductivity of the matrix phase; K_p, the thermal conductivity of the particle (dispersed phase) and f, the volume fraction of the dispersed phase in the composite material. These three factors has the primary effect to the overall thermal conductivity of the material. In this work, we study the effect of particle shape to the conductivity. Thus, the EMT model including the shape factor is derived and adopted.

For simplicity, we build our work on the basis the following assumptions: a) inclusion particles are of equal size and uniformly dispersed in the matrix; b) orientations of particles are completely random;

On the basis of above assumptions, we consider the multiple-scattering approach following Nan [?]. The multiple-scattering model suggests that the variation of thermal conductivity from point to point in a composite material can be expressed in the form: $K(r) = K^0 + K'(r)$, where K^0 is a constant part of homogeneous medium and $K'(r)$ denotes the fluctuating part. By applying the Green function G for the homogeneous medium and the transition matrix T for the entire composite medium, the resulting effective thermal conductivity K^* of the composite material is expressed as

$$K^* = K^0 + \langle T \rangle (I + \langle GT \rangle)^{-1}, \tag{1}$$

where I is the unit tensor and $\langle\rangle$ denotes spatial averaging. The matrix, T, is approximated by the sum of the T matrices of n particles. i.e. neglect the interaction between particles.

Then, consider an ellipsoidal particle in the matrix. The equivalent thermal conductivity along each symmetric axis is K_{ii} $(i = 1, 2, 3)$ equal to K_p, since we neglect the inter-facial thermal resistance. Thus, from Eq. 1, by taking $K^0 = K_m$, we obtain the effective thermal conductivity of the composite material as

$$K^*_{11} = K^*_{22} = K_m \frac{2 + f[\beta_{11}(1 - L_{11})(1 + \langle\cos^2\theta\rangle) + \beta_{33}(1 - L_{33})(1 - \langle\cos^2\theta\rangle)]}{2 - f[\beta_{11}L_{11}(1 + \langle\cos^2\theta\rangle) + \beta_{33}L_{33}(1 - \langle\cos^2\theta\rangle)]}, \tag{2}$$

$$K^*_{33} = K_m \frac{1 + f[\beta_{11}(1 - L_{11})(1 - \langle\cos^2\theta\rangle) + \beta_{33}(1 - L_{33})\langle\cos^2\theta\rangle]}{1 - f[\beta_{11}L_{11}(1 - \langle\cos^2\theta\rangle) + \beta_{33}L_{33}\langle\cos^2\theta\rangle]}, \tag{3}$$

with

$$\beta_{ii} = \frac{K_p - K_m}{K_m + L_{ii}(K_p - K_m)}, \tag{4}$$

and

$$\langle\cos^2\theta\rangle = \frac{\int \rho(\theta)\cos^2\theta \sin\theta d\theta}{\int \rho(\theta)\sin\theta d\theta}, \tag{5}$$

In Eq. (2) and (3), L_{ii} are geometrical factors depend on particle shapes and given by,

$$\begin{aligned} L_{11} &= L_{22} \\ &= \begin{cases} \frac{p^2}{2(p^2-1)} - \frac{p}{2(p^2-1)^{3/2}}\cosh^{-1}p, & for\ p > 1, \\ \frac{p^2}{2(p^2-1)} + \frac{p}{2(1-p^2)^{3/2}}\cos^{-1}p, & for\ p < 1, \end{cases} \\ L_{33} &= 1 - 2L_{11}, \end{aligned} \tag{6}$$

where p is defined as aspect ratio of the ellipsoid.

$$p = a_3/a_1$$

θ is the angle between the materials axis and the local particle symmetric axis, $\rho(\theta)$ is a distribution function describing ellipsoidal particle orientation, and f is the volume fraction of particles.

Note that the geometrical factor L_{ii} only depends on the aspect ratio p, which inspires us that p is the ultimate parameter that characterizes the effect of particle shape to the thermal conductivity.

In the case of completely misoriented ellipsoidal particles, $\langle\cos^2\theta\rangle = \frac{1}{3}$ the above formula can be simplified to

$$K^* = K_m \frac{3 + f[2\beta_{11}(1 - L_{11}) + \beta_{33}(1 - L_{33})]}{3 - f[2\beta_{11}L_{11} + \beta_{33}L_{33}]} \tag{7}$$

On the basis of this formula, we generate data as training set for the neural network.

2.2. Artificial Neural Network

Artificial Neural Network (ANN) is widely applied today as an effective approach for Machine Learning, which emulate the architecture of human brain to perform tasks that conventional algorithms had little success with. Intuitively, ANN is a directed, weighted graph, as shown in Figure 1. Neurons (Nodes) are connected to each other in various patterns, to allow the output of some neurons to become the input of others. The neurons are weighted by the parameters attached to it in the computation. The training process refers to adjusting these parameters to minimize the error between the predictive result and the real value. The application of ANN can be classified into two categories: classification and regression. Classification problem refers to identifying to which of the category the new observation belongs. Given the input data, the ANN will calculate the possibility of the observation belonging to each category, and select the most confidential

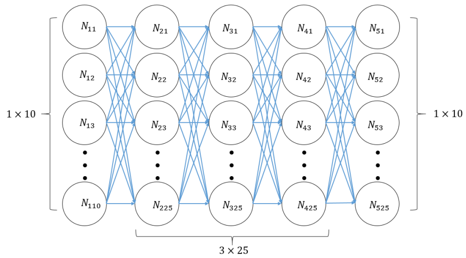

Figure 1. Graphic model of artificial neural network (hidden layers).

category as the output. Other than classification, ANN is also suitable for non-linear regression. In the context of regression problem, ANN will try to fit the training data set by adjusting the weight on each neuron. When a new observation is given, the ANN can predict the result base on the fitted weight. In our case, we adopt the regression function of ANN. Specifically, we use the Multi-layer Perceptron regressor. This regressor fits the training data iteratively. The loss function is defined as the Mean Square Error (MSE) between the predicted value and the real value. At each time step the partial derivatives of the loss function with respect to the model parameters are computed to update the parameters.

Practically, we use the off-the-shelf $MLPRegressor$ from scikit-learn library of Python. Experiment results show that this function is sufficient for our purpose.

3. System Design

Given Eq.7 above, we made an assumption that the map from relevant factors K_p, K_m, f etc. to the effective thermal conductivity of the composite material is a non-linear relationship. While this relationship varies among different particle shapes, it can be generally captured by ANN as the weight parameters in the neurons. We assume that by generating data from a known particle shape, we can train the neural network to fit the data. As a result, the ANN model trained from a particular particle shape data can be used to replace the analytical formula that generate the data. The actual result is evaluated in the section below.

3.1. Generalized Shape Factor

On basis above, we want to extend the function of this ANN model by generalizing it to fit for other particle shapes. As in the misoriented ellipsoidal particle case shown in section 2.1, the shape of the ellipsoidal particle is characterized by its aspect ratio. By generalizing this definition, we expect to assign each particle shape with a particular number to characterize its shape, referred to as generalized shape factor (GSF). This GSF can be plugged into the analytical formula or the ANN model to predict the thermal conductivity.

To solve this generalization problem, we used another ANN model, with conventionally adopted parameters for particle shapes: volume, surface area and projection areas, as input and estimate the GSF as output.

3.2. Data generation

To obtain the training data, we use the Eq.7 above. Specifically, we randomly generate values for K_p, K_m, f and length of two axes of the ellipsoid a_1, a_3 (assume $a_2 = a_1$), then plug in Eq.6 to compute L_{ii}. The L_{ii} is plugged into Eq.4 to obtain β_{ii}. Finally, K_m, f, β_{ii} and L_{ii} are plugged in Eq.7 to compute K^*, the thermal conductivity of the composite material. For simplicity, we narrow the range of parameters as below.

- $K_p,\ K_m \in (0, 20]$;
- $f \in (0, 1]$;
- $a_1, a_3 \in \{0.1, 0.2, ..., 0.9, 1.0\}$

With the above restriction, we generate 100,000 entries of data as our training set. For each entry, the target conductivity value K^*, volume of the particle V, surface area of the particle S and Projection areas from three directions Pro_i $(i = 1, 2, 3)$ are computed and recorded.

3.3. K model

K model is the ANN model trained to predict the thermal conductivity of the composite material. The input values are K_p, K_m, f and p, and the output is the effective thermal conductivity K^*.

3.4. P model

P model is the ANN model trained to predict the GSF of the particular particle shape. The input values are V, S and Pro_i, and the output value is the predictive GSF for this particular shape.

The result of the P model can be plugged into Eq.4 6 and 7 for evaluating the analytical thermal conductivity. Or, it can be plugged into the K model to give a predictive value of the thermal conductivity. We will evaluate the result of each method in the follow sections.

4. Evaluation

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5. Limitation and discussion

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6. Conclusion

We present a machine learning model that can accurately predict the thermal conductivity of composite materials in this paper.As discussed above, it is feasible and reliable to use machine learning to predict the thermal conductivity of composite materials.The thermal conductivity predicted by our training model is very close to the real thermal conductivity, and is not limited to the prediction of elliptical particles.When we used the training model to predict other composite particle types, the prediction still provided acceptable error results.Our research work can still be further improved in the future to accurately predict the thermal conductivity of various new composite materials. When this problem is solved, the prediction model can also be extended to predict other similar property problems, such as conductivity.

References

[1] H. Kopka and P. W. Daly, A Guide to LaTeX, 3rd ed. Harlow, England: Addison-Wesley, 1999.