NEURAL NETWORK-ASSISTED SENSITIVITY ANALYSIS ON THE CONDUCTIVITY OF MULTIFUNCTIONAL CEMENTITIOUS COMPOSITES

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ABSTRACT

Incorporating graphene derivatives (GDs), as a reinforcing filler, into cementitious composites can enhance their mechanical properties, durability, and conductivity. Thermally conductive cementitious composites can be employed in multiple applications. Accordingly, cementitious composites reinforced by graphene derivatives (CCRGDs) have attracted much attention due to their multifunctional capabilities. For these multifunctional applications, comprehending the impact of different parameters, such as component properties, on the thermal conductivity of CCRGDs is essential.

This study develops a nonparametric method called neural network (NN) to investigate the thermal conductivity of CCRGDs. To provide the required data set for the learning process of the NN model, a micromechanics model is developed using the concept of the representative volume element. In fact, this study uses a hybrid modelling framework through synergistically coupling data-based (NN) and knowledge-based (micromechanics) methods to investigate the thermal conductivity of CCRGDs at an optimized computational cost and complexity while maintaining high accuracy.

Finally, a sensitivity analysis is conducted using the NN model. The sensitivity analysis clarifies how the parameters, including the volume fraction of GDs, the aspect ratio of GDs, and the conductivity of the cementitious matrix to GDs ratio affect the thermal conductivity of CCRGDs.

1 INTRODUCTION

Cementitious composites play an influential role in the global construction industry, serving as the most extensively utilized man-made material [1]. To meet the evolving needs of modern infrastructure, it is essential for the construction industry to embrace more innovative and sustainable cementitious composites [1, 2]. Accordingly, the single function of traditional cementitious composite has not been able to respond to the requirements of multifunctional infrastructures [3, 4]. As a result, there is a global focus on developing multifunctional cementitious composites [2, 5, 6].

Much research has focused on the application of conductive nanomaterials to provide cementitious composites with multifunctional capabilities [7, 8]. Among these, graphene derivatives (GDs) have shown great potential to enhance the characteristics of cementitious composites from atomic to macro scale [9-11]. Graphene is a single layer of carbon-carbon hexagonal plane [12]. GDs are obtained by modifying or functionalizing graphene. Even though graphene itself possesses remarkable physical and functional properties, GDs have altered properties compared to pristine graphene [12]. The most commonly used graphene derivative in the cementitious composites industry includes graphene oxide (GO), graphene nanoplatelet (GNP) and reduced graphene oxide (rGO) [11, 13]. GDs exhibit unique mechanical properties, conductivity (both electrical and thermal), and piezo resistivity [14]. The thermal conductivity of GDs can reach 5000 W/mK [15, 16]. This makes them a promising option for manufacturing thermally conductive cementitious composites. Consequently, cementitious composites reinforced by graphene derivatives (CCRGDs) with enhanced thermal conductivity, mechanical properties and durability can be potentially applied in the construction industry for multiple applications [15, 17-19], as shown in Figure 1.

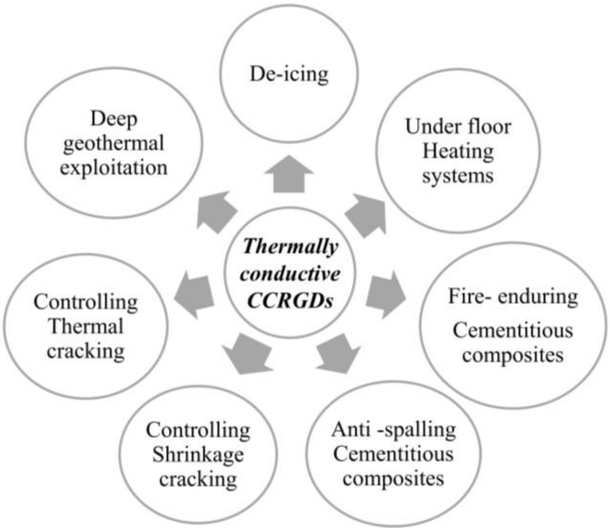

Figure 1: Applications of thermally conductive CCRGDs

Understanding the impact of various parameters, such as the properties of the components, on the thermal conductivity of CCRGDs is crucial for certain applications. Even though a comprehensive micromechanics model can precisely investigate the conductivity of GDs-reinforced composites [20], it is associated with considerable computational costs and complexity [21]. Alternatively, the NN model can offer an efficient way to predict the thermal conductivity of CCRGDs, reducing both the computational cost and complexity compared to micromechanics models [22, 23]. However, NNs necessitate a comprehensive dataset to ensure trustworthy predictions.

This study employs a hybrid modelling approach by coupling a micromechanics model with a NN model to investigate the thermal conductivity of CCRGDs as multifunctional cementitious composites. Accordingly, a representative volume element (RVE) is developed to predict the thermal conductivity of CCRGDs using finite element methods. The developed RVE is validated against experimental data from previously published research. Subsequently, the validated RVE is utilized to generate the necessary dataset for training the NN model. The NN model is then employed to conduct a sensitivity analysis, investigating the impact of non-dimensional parameters such as the volume fraction of GDs (V_f), aspect ratio of GDs ($\frac{D}{t}$), and the cementitious matrix to GDs conductivity on the thermal conductivity of CCRGDs ($\frac{K_G}{K_C}$). Figure 2 summarizes the workflow of this study.

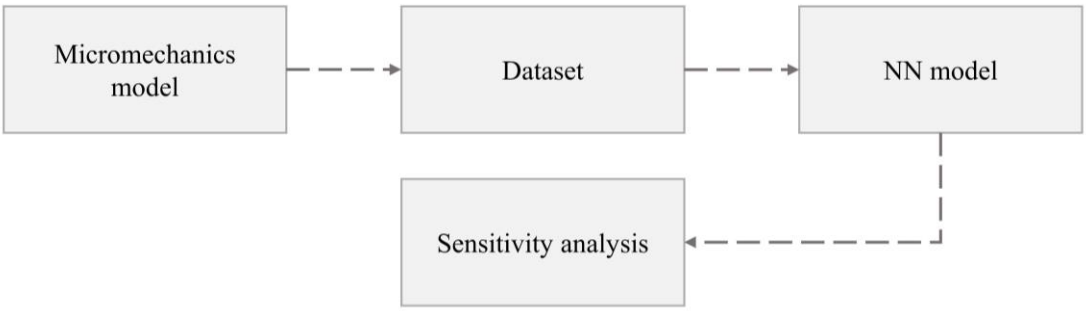

Figure 2: Workflow of hybrid modelling approach to implementing the sensitivity analysis.

2 HYBRID MODELING FRAMEWORK FEATURES

2.1 FEATURES OF MICROMECHANICS MODEL

A two-dimensional RVE was generated to reduce the complexity of the simulations. We used periodic boundary conditions and geometry periodicity in this study. Figure 3 displays the flowchart for the RVE creation.

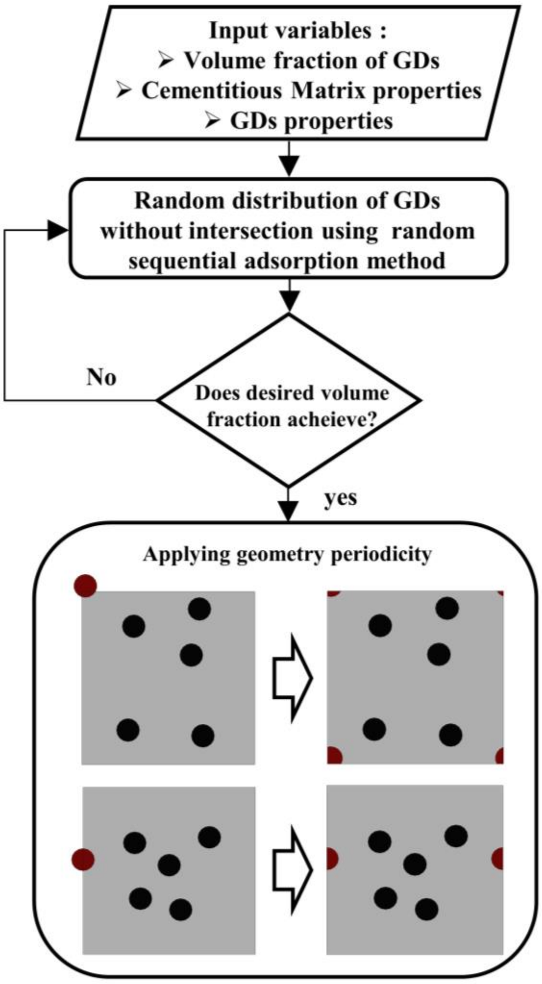

Figure 3: Flow chart of RVE generation.

The finite element analysis was done in Abaqus software. The thermal conductivity of the RVE (k) was calculated using Fourier's law [24, 25],

$$k = \frac{q\Delta H}{\Delta T}\,. \tag{1}$$

Where q represents the imposed heat flux, ΔH expresses the height of the RVE and ΔT represents the temperature difference of the surface where the heat flux is applied.

Furthermore, the mesh convergence analysis and RVE size sensitivity analysis were conducted before validating the RVE prediction results against experimental values. Finally, the validated RVE was used to generate the required dataset to train the NN model.

2.2 Features of neural network model

Multi-layer perceptron was employed in this study as it is one of the most widely used types of NN in cementitious composites property prediction [26-28] . The developed multi-layer perceptron includes an input layer, and three hidden layers, each containing 80 neurons and one output layer. The backpropagation algorithm was used for the learning process. Input layer comprised the non-dimensional parameters, including the volume fraction of the graphene derivative, the aspect ratio of graphene derivatives, and the conductivity of the cementitious matrix to GDs. The thermal conductivity of GRCCs was the output layer. Furthermore, in the MLP model, the activation function and solver selected were Rectified Linear Unit (ReLU) and LBFGS (Limited-memory Broyden-Fletcher-Goldfarb-Shanno), respectively. The prediction performance of the MLP model was evaluated using the coefficient of determination (R^2) and root mean square error (RMSE) as evaluation metrics for the prediction performance of the model,

$$R^2 = 1 - \frac{\sum_{j=1}^{m}(k_o - k_p)^2}{\sum_{j=1}^{m}(k_o - k_o^m)^2}, \tag{2}$$

$$RMSE = \sqrt{\frac{1}{m}\sum_{j=1}^{m}(k_o - k_p)^2}\,. \tag{3}$$

where m represents the number of samples, k_o indicates the experimental thermal conductivity, k_p denotes the predicted thermal conductivity, and k_o^m is the average of the experimental thermal conductivity.

3 SENSITIVITY ANALYSIS

Using the NN model, a sensitivity analysis was conducted to evaluate the effect of parameters, including V_f , $\frac{K_G}{K_C}$ and $\frac{D}{t}$ on the thermal conductivity of GDRCCs. One of the parameters was kept constant at its average value, while the other parameters were changed over a certain domain to assess their impact on the thermal conductivity of GDRCCs.

4 RESULTS AND DISCUSSION

4.1 Hybrid modelling framework prediction performance

Figure 4 shows the prediction performance of the micromechanics model against experimental values from the literature.

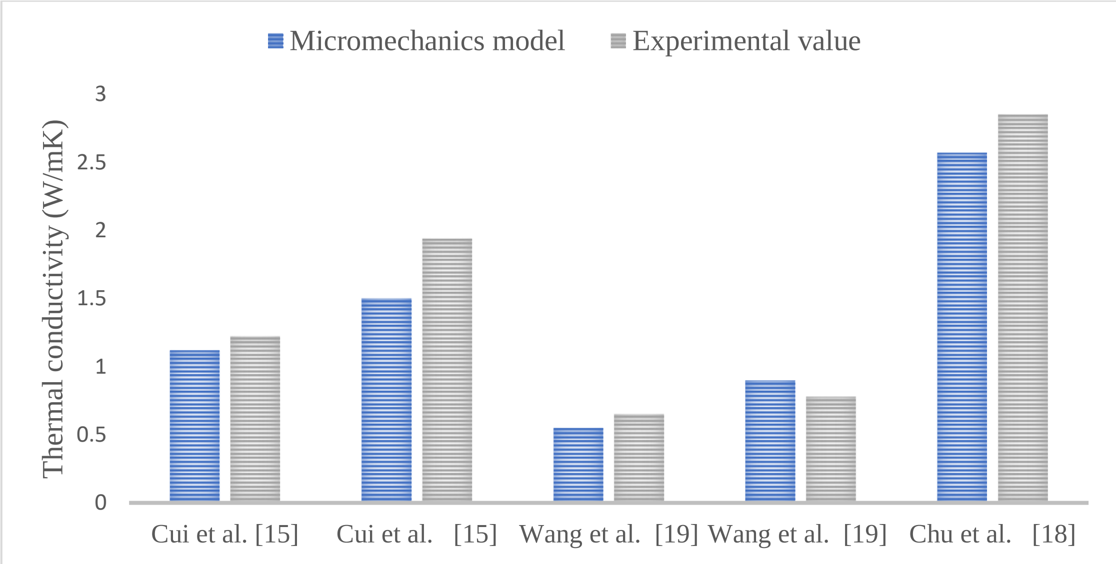

Figure 4: Prediction performance of the micromechanics model against the experimental value

Figure 4 shows an acceptable agreement between the micromechanics model prediction results and experimental values. Thus, the developed RVE was used to create the required dataset to train the NN model. The dataset includes 964 data points. The dataset was divided into training and testing sets with a training-to-testing ratio equal to 0.2. Table 1 indicates the prediction performance of the NN model in the training and testing process.

NN Model	Train		Test	
	R^2	RMSE	R^2	RMSE
	0.96	0.14	0.96	0.13

Table 1: prediction performance of the NN model.

Moreover, the prediction performance of the NN model was further evaluated using the experimental values from the literature, as depicted in Figure 5.

Figure 5 demonstrates a good degree of conformity between the prediction outcomes obtained from the NN model and the corresponding experimental values. This finding implies that the NN model can be employed directly to predict and investigate the thermal conductivity of GDRCCs with comparable accuracy and reliability as the micromechanics approach while exhibiting reduced computational cost and complexity.

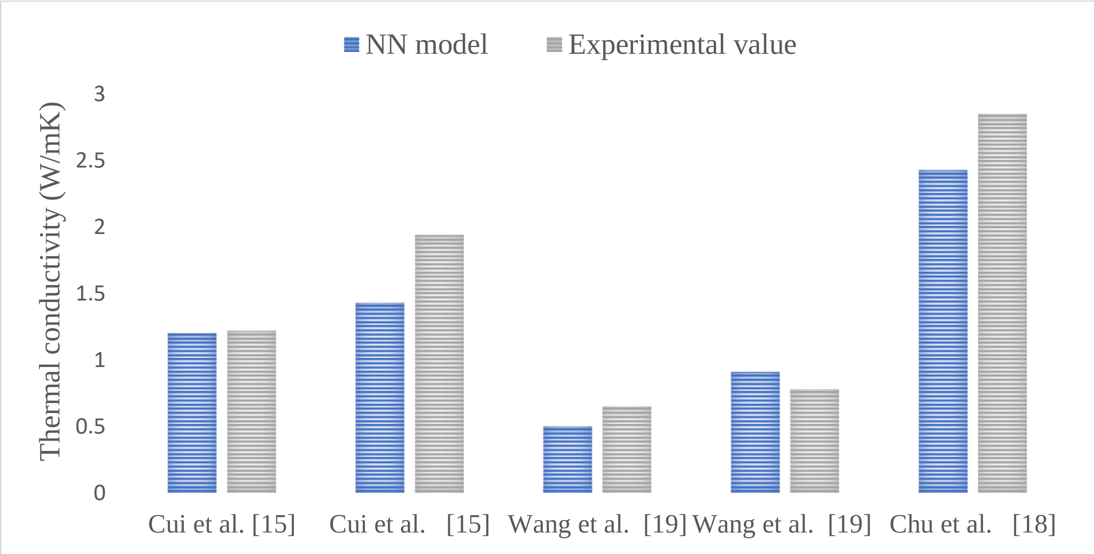

Figure 5: Prediction performance of the NN model against the experimental value.

4.2 Sensitivity analysis

The outcomes of the sensitivity study are summarized in the following sections:

4.2.1 Combined effect of graphene derivatives diameter to thickness ratio $(\frac{D}{t})$ and volume fraction (V_f)

The $\frac{K_G}{K_C}$ was kept constant on its average value to determine the combined impact of V_f and $(\frac{D}{t})$ on the thermal conductivity of GDRCCs, as shown in Figure 6.

According to Figure 6, regardless of the $\frac{D}{t}$, increasing the volume fraction leads to a rise in thermal conductivity. However, the rate of increase becomes more pronounced beyond a volume fraction of 3%, possibly due to a lack of conductive paths below this threshold. Additionally, with constant V_f, increasing the $\frac{D}{t}$ values result in an increase in thermal conductivity. As the volume fraction increases, the impact of $\frac{D}{t}$ on the thermal conductivity of GDRCCs becomes more highlighted.

Moreover, according to Figure 6, the impact of the V_f on the thermal conductivity of GRCCs is more significant compared to the effect of $\frac{D}{t}$.

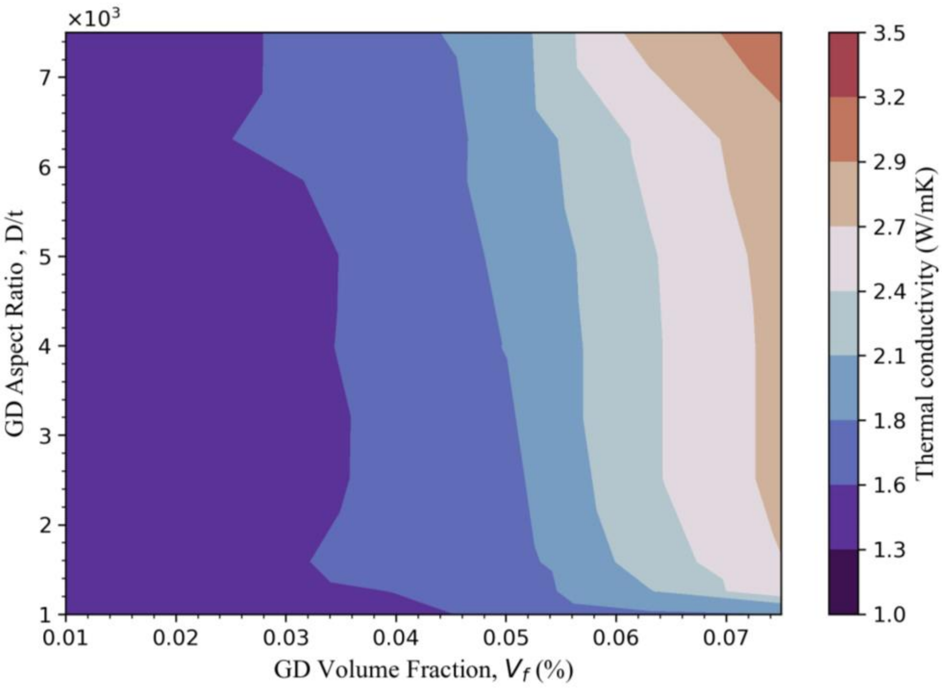

Figure 6: Combined effect of aspect ratio and volume fraction of DGs on thermal conductivity

4.2.2 Combined effect of graphene derivatives to cementitious matrix thermal conductivity ratio $(\frac{K_G}{K_C})$ and volume fraction (V_f)

The $\frac{D}{t}$ was kept constant on its average value to assess the combined effect of V_f and $\frac{K_G}{K_C}$ on the thermal conductivity of GDRCCs, as shown in Figure 7.

According to Figure 7, the influence of variations in V_f and $\frac{K_G}{K_C}$ on the thermal conductivity of GDRCCs is negligible when V_f is below 3%. This observation could be attributed to the lack of conductive pathways below the $V_f = 3\%$. However, beyond the 3% threshold, an increase in both the V_f and $\frac{K_G}{K_C}$ values, increases thermal conductivity. Nevertheless, it should be noted that the effect of V_f on thermal conductivity is more pronounced compared to that of $\frac{K_G}{K_C}$.

Generally, based on the observations from Figures 6 and 7, the influence of $\frac{K_G}{K_C}$ and $\frac{D}{t}$ on the thermal conductivity of GDRCCs is found to be dependent on the V_f. Notably, for V_f values below a specific threshold (3%), the impact of $\frac{K_G}{K_C}$ and $\frac{D}{t}$ is evidently marginal. However, as the V_f increases, the effects of $\frac{D}{t}$ and $\frac{K_G}{K_C}$ become more obvious.

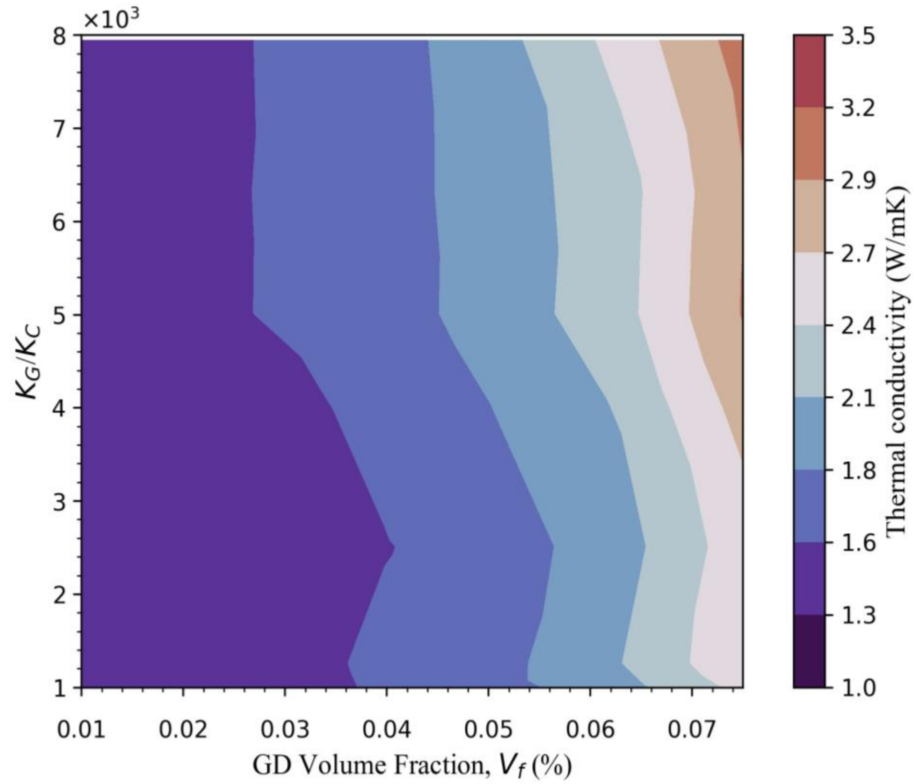

Figure 7: Combined effect of $\frac{K_G}{K_C}$ and volume fraction on thermal conductivity

5 CONCLUSIONS

This study combined a micromechanics model with a NN model to investigate the thermal conductivity of CCRGDs as multifunctional cementitious composites. Accordingly, a RVE was created using finite element methods to predict the thermal conductivity, and its prediction performance was confirmed using experimental data from the literature. The validated RVE was then used to generate a dataset for training the NN model. Finally, the NN model was employed to conduct a sensitivity analysis, exploring the influence of features on the thermal conductivity of CCRGDs.
The main conclusions can be summarized as follows:

I. The developed NN model (trained by the micromechanics model) could reliably predict the thermal conductivity of CCRGDs with lower computational costs compared to micromechanics model.

II. Increase in V_f and $\frac{D}{t}$ leading to an increase in the thermal conductivity of GRCCs. However, the magnitude of this effect is mainly dependent on the V_f.

III. Increase in V_f and $\frac{K_G}{K_C}$ leading to an increase in the thermal conductivity of GRCCs. However, the magnitude of this effect is mainly dependent on the V_f.

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