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XGBOOST-BASED MODEL FOR PREDICTION OF HEAT TRANSFER COEFFICIENTS IN LIQUID COLD PLATES

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ABSTRACT

Extreme gradient boosting (XGBoost) algorithm is a newly developed machine learning (ML) technique with demonstrated excellent accuracy and performance in modelling complex processes in science and engineering. In the present study, an XGBoost-based model is developed to predict heat transfer coefficients in liquid cold plates (CPs) subjected to surface roughness. The CPs operate in turbulent flow over a wide range of Reynolds numbers. Roughness sizes range from zero (smooth surface) to 0.5 mm. The input dataset for training the XGBoost model is prepared using a computational fluid dynamics (CFD) approach and by solving three-dimensional fluid flow and heat transfer inside the CPs. It was found that the model exhibits excellent accuracy such that 63% and 90% of heat transfer coefficients are predicted within $\pm 10\%$ and $\pm 20\%$ of true values, respectively. The present finding suggests XGBoost as an effective modelling tool for performance analysis of thermal management solutions, specifically when there is limited performance data available in literature.

KEY WORDS: Machine learning, XGBoost, Heat transfer coefficient prediction, Surface roughness, CFD.

1. INTRODUCTION

Accurate prediction of the hydrothermal performance of thermal management solutions (TMSs) using machine learning (ML) allows an economical strategy to design TMSs by overcoming the challenges of conducting expensive experiments and/or simulation analysis [1-3]. ML, as a subset of artificial intelligence, has been demonstrated as a powerful approach to investigate complex physics in science and engineering applications. Supervised learning is one of the ML categories that is applied for solving regression and classification problems. In a supervised learning, a set of data including the inputs and outputs is used to train the ML model; then, the model uses the learned pattern to generate new outputs based on new inputs. Although a large dataset results in a more accurate ML model, it is very likely that only limited numbers of data are available in literature for specific applications. As a result, predicting new outputs using limited numbers of datasets requires adopting an effective ML algorithm with a high accuracy. The requirement for using an effective ML technique becomes more crucial if the limited number of data are scattered as well [3]. As a result, it is necessary to evaluate the prediction capability of different ML techniques to identify the models with high accuracy in comparison with other ML algorithms.

The extreme gradient boosting (XGBoost) algorithm is an advanced ML technique that enhances the prediction accuracy and computational efficiency of the computer, as well as reduces the possibility of overfitting [4]. Moreover, XGBoost needs less training time, and supports various objective functions such as classification and regression [5]. Fig. 1 illustrates the structure of XGBoost. For the n number of independent variables of x_i across i observations, the XGBoost calculates the predictive value ($\hat{y}_i$) using a regression tree ensemble model consisting of K number of trees, as follows [5-7]:

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$$\hat{y}_i = \sum_{k=1}^{K} f_k(x_i) \tag{1}$$

where f represents a specific tree structure. When the loss function is calculated, the objective function (L) is obtained as described below [8]:

$$L = \sum_{i=1}^{I} l(\hat{y}_i, y_i) + \sum_{k=1}^{K} \Omega(f_k) \tag{2}$$

where l is the loss function, I is the total number of observations, and y_i is the true value. Also, Ω is the regularization term to penalize the model complexity and avoiding overfitting [5, 9, 10]:

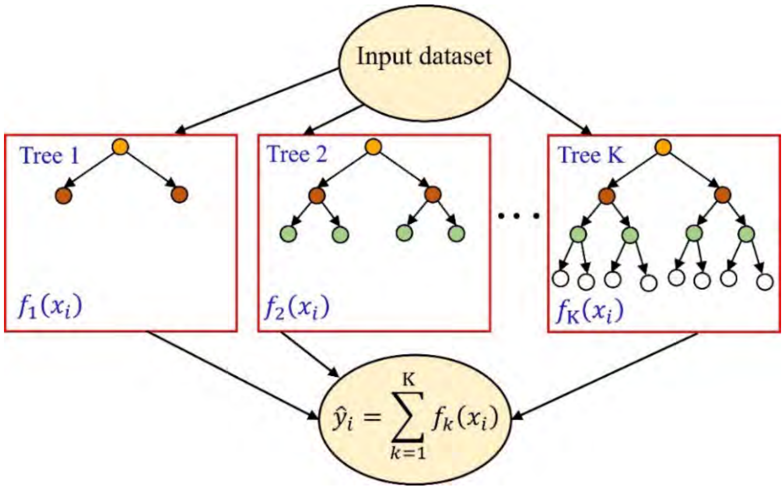

Fig. 1 The structure of XGBoost algorithm.

Additive manufacturing (AM) has been replacing traditional manufacturing processes in major engineering applications such as thermal management of electronic devices. Since surface roughness (ε) is an inevitable consequence of AM, it is necessary to investigate the impacts of surface roughness on the hydrothermal performances of additively manufactured TMSs. Liquid cold plates (CPs) are effective TMSs that have been widely used in broad applications due to their high cooling capacity and compactness. Fig. 2 illustrates the schematic of the CPs used in this study.

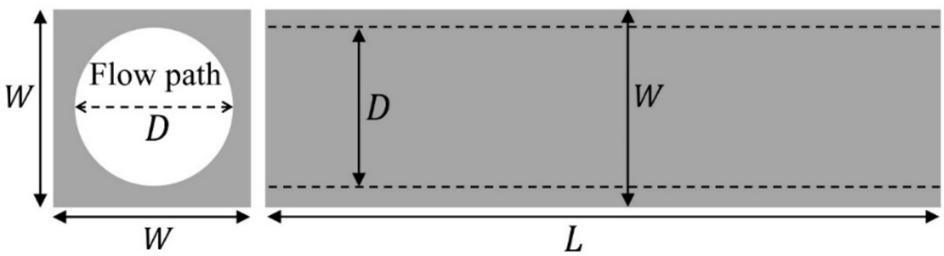

Fig. 2 Schematic of the cold plate. (Left): Cross-sectional view; (Right): side view.

The CPs consist of an aluminium plate with a square cross-sectional area. The flow path is a circular cross-sectional pipe implemented at the center of the cross section of CP. Water is used as the coolant. Five different CPs with different cross-sections and flow path diameters are considered in this study. Table 1 lists the geometrical information of the CPs as well as the range of Reynolds number (Re) and surface roughness at individual CPs.

Since ML is a data-driven technique, preparation of input data for training a ML-based model is a main step. In this study, the input data to train the XGboost algorithm is prepared through a CFD simulation process by solving three-dimensional steady state turbulent flow and heat transfer in CPs. The turbulent flow is simulated using the RNG $k - \varepsilon$ model. Detailed explanations about the governing equations and turbulent model were provided in [11] and are omitted here for brevity. A wide range of surface roughness is considered for the flow path at each diameter, as described in Table 1. Simulations are performed over a wide range of Re as specified in Table 1. Re is defined as $\mathrm{Re} = 4\dot{m}/\pi D\mu$, where $\dot{m}$ is the mass flow rate of water. At the inlet of the CP, water flow rate and temperature (20°C) are set. At the outlet of the CP, zero axial gradients for all variables are imposed. The remaining surfaces are walls with a no-slip boundary condition. A constant heat flux equivalent to 50 W is applied to one surface of the CP. The rest of the surfaces are adiabatic. Since the purpose of this study is not to verify the accuracy of CFD results, grid independence tests are not conducted, although the simulations are performed using sufficiently fine grid structures. Ansys Fluent is used to solve the governing equations. The height of surface roughness is set as the boundary condition at the interface of fluid and solid in Ansys Fluent.

Table 1 Information of the cold plates investigated in the present study.

Cold plate design	D (mm)	W (mm)	L (mm)	ε/D	$\mathrm{Re} = 4\dot{m}/\pi D\mu$
1	1	1.5	50	0 – 0.5	3,167 – 11,404
2	2	2.5	50	0 – 0.25	3,270 – 11,510
3	3	3.5	50	0 – 0.167	3,027 – 11,123
4	4	4.5	50	0 – 0.125	3,220 – 10,560
5	5	5.5	50	0 – 0.08	3,379 – 11,193

The XGBoost modelling consists of three inputs, which are D, ε, and $\dot{m}$. The only output of the model is the heat transfer coefficient (h). Since the same amount of heat is applied to all CPs, the heat transfer coefficient is independent of the footprint area of the heating surface ($W \times L$); as a result, there is no need to consider W as an input. Among 232 prepared datapoints through CFD, 87% are used for training, and the remaining data is a testing dataset that is used to evaluate the accuracy of the XGBoost model. The XGBoost model is developed in Python using xgboost (version 1.6.1, https://github.com/dmlc/xgboost), scikit-learn. Table 2 lists the information of the XGBoost hyperparameters in this study.

Table 2 Range of XGBoost hyperparameters and the optimal values.

Hyperparameter	Lower limit	Upper limit	Optimized value
Alpha	0.001	10.0	8.1×10^{-3}
Col. sample by tree	0.3	1.0	1.0
Lambda	0.001	10.0	8.4×10^{-3}
Number of leaves	1	10	8
Learning rate	0.008	0.02	0.018
Max depth	5	17	5
Min child weight	1	300	2
Subsample	0.4	1.0	0.6

2. RESULTS

Fig. 3 illustrates the difference between the predicted h by the XGBoost model and true h obtained by the simulation that is calculated as $(h_p - h_t)/h_t \times 100$, which h_p and h_t correspond to the predicted h and true h, respectively. Using the developed XGBoost model in the present study, the heat transfer coefficients of 63% and 90% of the CPs are predicted within $\pm 10\%$ and $\pm 20\%$ of true values, respectively. Impressively, all heat transfer coefficients are predicted within $\pm 26\%$ of true values. Since the XGBoost model in this study was trained with a limited number of data, such high accuracy indicates the great performance of XGBoost algorithm to predict hydrothermal performances of engineering systems when limited performance data is available in literature.

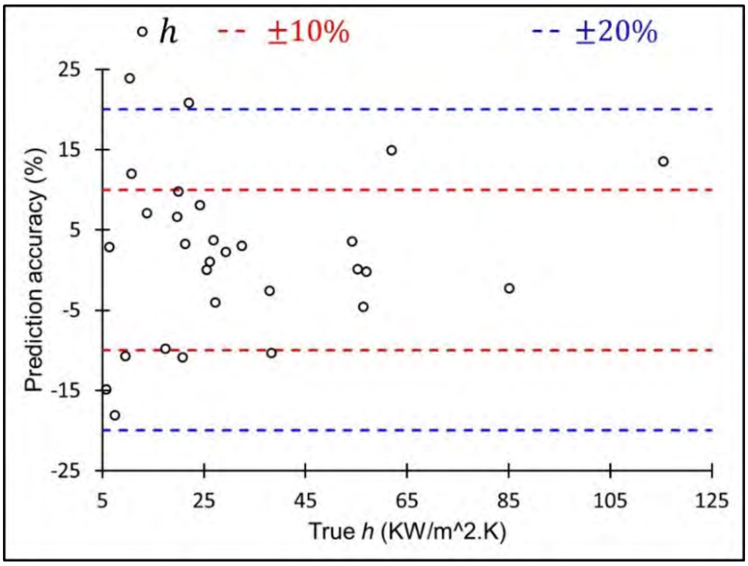

Fig. 3 Prediction accuracy of the developed XGBoost model in this study.

3. CONCLUSIONS

XGBoost algorithm was used to predict heat transfer coefficients of liquid CPs with surface roughness operating in turbulent flows. Since surface roughness is an inevitable consequence of the additive manufacturing process, the present study provides a practical insight on using XGBoost to predict thermal performances of additively manufactured thermal management solutions. The input dataset for training the model was prepared through solving three-dimensional fluid flow and heat transfer inside CPs using a CFD approach. Although limited datapoints were used for the training XGBoost model, excellent prediction accuracy was achieved such that 63% and 90% of the heat transfer coefficients were predicted within $\pm 10\%$ and $\pm 20\%$ of true values, respectively.

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