Flame retardant properties of metal hydroxide-based polymer composites: A machine learning approach

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Abstract

With increasing the practical applications of polymeric materials, surging demands for the high-performance flame-retardant polymer composites are obvious. Accurately predicting the performance of flame-retardant materials is critical for expediting technology development. Here, we develop machine learning models based on Random Forest to create standard paradigms based on a self-generated comprehensive dataset consisting of 219 experimental data from the literature. integrated by plenty of randomly combined decision trees, the Random Forest algorithm is well known for its accurate predictability and easy interpretability. We predict the important flame-retardancy-evaluating parameters including time to ignition (TTI), peak heat release rate (pHRR), total heat release (THR) and flame retardancy index (FRI) of different polymer composites containing metal hydroxides as the main fire-retardant additive. Our optimized models achieve high accuracy with R-squared value of 0.81 for regression and over 0.85 for classification; mean absolute error is below 0.3 for all 4 models. The analysis of important features reveals that mass fraction of MH takes always the first place, and the influence of feature groups on target properties is usually multi-dimensional and complicated.

Keywords: *Flame retardancy; Polymer composites; machine learning; Data-driven prediction*

1. Introduction

Functional polymers are deployed as structural units and shell materials [1], temperature sensor [2], conducting substances [3,4], and eco-compatible materials [5,6] in advanced human society [7]. But major concern of the flammability of these polymeric materials at high temperatures persists [8,9]. The traditional trail-and-test method to improve the flame retardancy of commercial products is time-consuming and cost-ineffective. Today, machine learning (ML) techniques have been highly developed, which are well-aligned with materials research in mechanical analysis [10,11], image segmentation [12,13], and intrinsic properties prediction of polymers [14,15], and have been demonstrated to be a promising approach to predicting material properties [16,17]. Accurate predictions of flame retardant parameters are imperative to decipher new directions in production and optimization of fire-proof materials. However, this task is still challenging owing to nonlinear degradation in flame retardancy properties during their practical operation.

In general, various flame retardant (FR) additives are incorporated into the polymers to inhibit flame propagation through either physical processes or chemical mechanisms. Since 1980 [18,19], metal hydroxides (MHs) are considered a good choice attributed to its smoke-suppression [20], nontoxicity [21], and low cost [22,23]. Besides, the comprehensive understanding of its underlying FR mechanism enables data-driven prediction of the FR properties with proper features. In fact, an increasing tendency of utilizing ML algorithms appears in the research field of flame retardant materials: combustion states of fuels [24] and residential room fires [25] were successfully predicted via image-detecting ML method; Chen F. et al. Used ML tools to explore the relationship between limiting oxygen index (LOI) and components of fire-resistant [26]; Zhang Z. et al. investigated the optimization of flame retardancy index (FRI) with various ML algorithms [27].

In situations mentioned above, the supervised models perform well in accuracy and feasibility. Among those ML algorithms, Random Forest (RF) [28] is simple to use and qualified for plenty of tasks. RF is constructed with a large number of decision trees (DT) into a set, in which the prediction is made as an aggregation of those trees (see top right corner in **Fig. 1**). A single DT represents a series

of conjuncted features arranged in a top-to-bottom tree-like structure. The object propagates through the tree to obtain its final prediction result according to its features and tree structures. Randomness induced into RF ensure high generalization in unseen data and better performance. [29]

In this study, we plan to build separate models to predict the cone calorimeter test (CCT) characteristics of polymer composites. We have selected 9 polymer composites blended with MHs as main flame retardants from the literatures [30–51] to integrate with computational technique. Dataset was structured with selected features based on generality, representativity, and comprehensibility. Robust ML models validated with experimental results, serve as analytical tools. Finally, the assessed models are desired to pre-estimate the CCT values of formulations without real burning tests. Meanwhile, oriented optimization should be achievable through the importance analysis of selected features.

2. Materials and methodology

2.1 Preparation and characterisation of polymer composites

The used materials, preparation and characterization of polymer composites are presented in supporting information **S1-S3** with details. For simplicity, 5 different polymer composites were prepared using magnesium di-hydroxide (MDH) as main FR additive, together with other synergists like metal-organic framework [52]. Cone calorimeter results were collected to support the further usage.

2.2 Machine learning modelling

As shown in **Fig. 1**, the entire dataset was divided into two key parts: modelling set and validation set. In the modelling part, 85% of data were used to train the models (hereafter as ‘training set’), and the rest of the data was used as the ‘test set’ to perform a real-time evaluation of the models on unknown samples. The data for validation was consisting of 5 different formulations prepared as last section, which was excluded in the modelling set.

The to be predicted CCT characteristics are time to ignition (TTI), peak heat release rate (pHRR), total heat release (THR) and flame retardant index (FRI). The first three properties are directly

measured, whereas FRI is derived from them as a dimensionless ratio calculated by equation (1) [53]. In consequence of the size of dataset and feature structures, TTI, pHRR, THR and FRI were converted to corresponding target properties (see supporting information **S4**). Due to the complex nature of combustion processes as well as the great diversity of chemicals in FR composites, all the features in our dataset are preliminarily defined from the viewpoint of simplicity and universality as $\vec{X}$ in equation (2). (see **Table S2**).

$$FRI = \frac{\left[THR \times \frac{pHRR}{TTI}\right]_{polymer\_matrix}}{\left[THR \times \frac{pHRR}{TTI}\right]_{composite}} \quad (1)$$

$$y = f(\vec{X}_{polymer\_matrix}, \vec{X}_{loading\_of\_MH}, \vec{X}_{synergists\_besides\_MH}, \vec{X}_{process\_parameters}) \quad (2)$$

The pre-processing and feature selection were conducted as in support information **S5**. Finally, dataset with optimised size and feature structure was generated to train, test and validate the ML models.

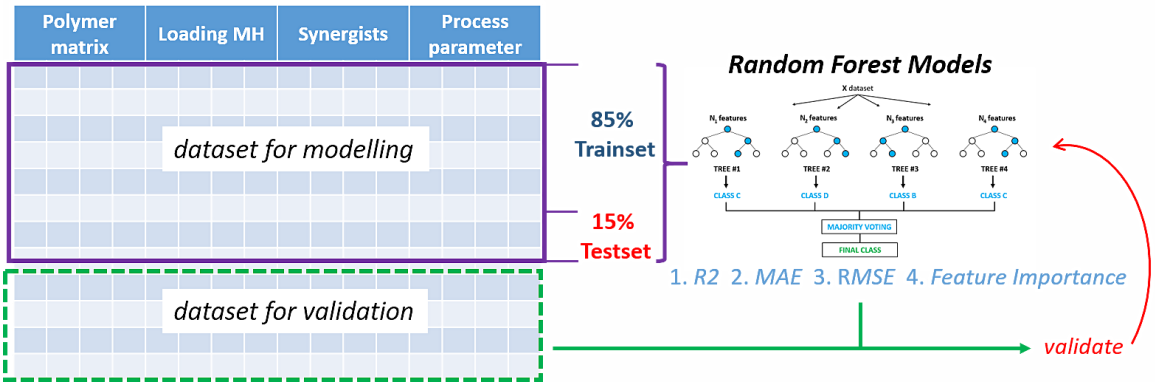

Fig. 1 Dataset used to build machine learning models and validate their accuracies.

3. Results and discussion

3.1 Experimental flame retardancy of MH-blended polymer composites

The generated dataset consisting of 219 records was used as input in our ML approach. Each formulation was unique due to the combination of the polymer matrix, FR additives, and processing parameters. From the graphic illustration in **Fig. 2**(a), decreasing D-pHRR with increasing amount of FR additives was found, corroborating the empirical rules. Interestingly, with increasing the FR loading over 50 wt%, the D-pHRR value is estimated to be significantly lower. It should also be noted

that the high amount of FR additives significantly enhances the TTI of the polymers from **Fig. 2**(b). Similar decreasing trends in D-THR and FRI in **Fig. 2**(c) and (d) are observed as the behaviour of D-pHRR. However, high filling of inorganic compounds (such as metal hydroxides) lowers the content of flammable polymers as well as provides a cooling function additionally and thereby effectively reduces heat generation [54].

Although MHs as the key FR components are effective to prolong the TTI and lower the D-pHRR, D-THR and FRI, the influence of other factors including synergists and polymer matrix cannot be ignored. Furthermore, no distinct correlation is observed between the CCT characteristics and the other affecting parameters in the input dataset. Despite the fact that these additional affecting parameters have a certain impact on the combustion process of polymer composites, however, their effects are not as significant as the effect of MHs.

3.2 Statistical machine learning models of fire properties

To evaluate the accuracy of RF models, three common used statistical indices (R2, MAE and RMSE) [55] are calculated in **Table 1**. The R2 scores meet the requirement for precise predictions in test sets: R2 values of 0.81 for prediction of D-pHRR and over 0.85 were achieved for classification of Lv-TTI, Lv-THR and Lv-FRI, respectively. The MAE and RMSE in test sets for all target properties were comparable, relatively small.

Table 1: Model indices in training and test sets in predicting D-pHRR, Lv-TTI, Lv-THR and Lv-FRI

	D-pHRR		**Lv-TTI**		**Lv-THR**		**Lv-FRI**	
Indices	**training set**	**test set**	**training set**	**test set**	**training set**	**test set**	**training set**	**test set**
R2	0.97	0.81	1.0	0.9	1.0	0.84	0.99	0.88
MAE	0.02	0.06	0	0.3	0	0.16	0.02	0.14
RMSE	0.04	0.09	0	1.43	0	0.4	0.16	0.42

The predictions are plotted against truly measured values in **Fig. 2**(e) to (h)**Fig. 2**. Blue dots stand for samples in training sets and red stars are from test sets. In all plots, blue points of training sets are

distributed along the green lines closely, indicating the high equivalence between measured and predicted values. Red marks in testsets spread themselves along the diagonal line but with relatively wider range than the blue dots. Some red stars can be noticed located far away from the green line which are unseen/untrained formulations to the models that lead to high error in predictions. For example **Fig. 2**(e), 2 samples in testset (22wt% synergist without MH and 1.8wt% MH with 7wt% synergist) locate to the left side due to these rare combinations. These "outliers" can be classified as the minorities in the dataset. [56]

In addition, we prepared the validation samples to evaluate the predictive performance of our models. The red bars in histograms in **Fig. 2**(i) to (l) stand for the measured values in to the same format as target properties, and the blue bars are the predictions made by our assembled models correspondingly. In summary, the predictions match the measurements well. Higher accuracy is found in predicting D-pHRR, Lv-THR and Lv-FRI, where their MAE values remain as low as 0.06, 0.16 and 0.24, respectively. The model for Lv-TTI showed inferior performance for some samples, the predicted TTI values are much different from the experimentally measured values. In EVA01 and EVA02 samples, unseen synergists were introduced with varied ratios, which strongly influenced the ignition properties. Bad performance on HDPE01 sample is attributed to the minority of data featured with HDPE as polymer matrix. Even so, the predictions and measured values are still comparable in most cases. This indicates that the models can be promoted by feeding rare formulations to compensate the inhomogeneity of dataset.

The prime reason for the overfitting can be attributed to the construction of the input dataset. Since most data come from researches with high MH-loading to achieve good performance, and published results have commonly similar formulations. Consequently, the predictive performance of such models is inferior for low MHs loading and rare composites. However, the disadvantages during the data collection cannot be ignored. Due to a lack of comprehensive databases on FR polymer composites, our input dataset is constrained in size and feature structure. The information that was retrieved is selective and unable to account for every conceivable type of additive and process. On the other hand,

certain errors in characterization are inevitable due to the differences in device conditions, operation skills, and the standard of experimental instruments in labs.

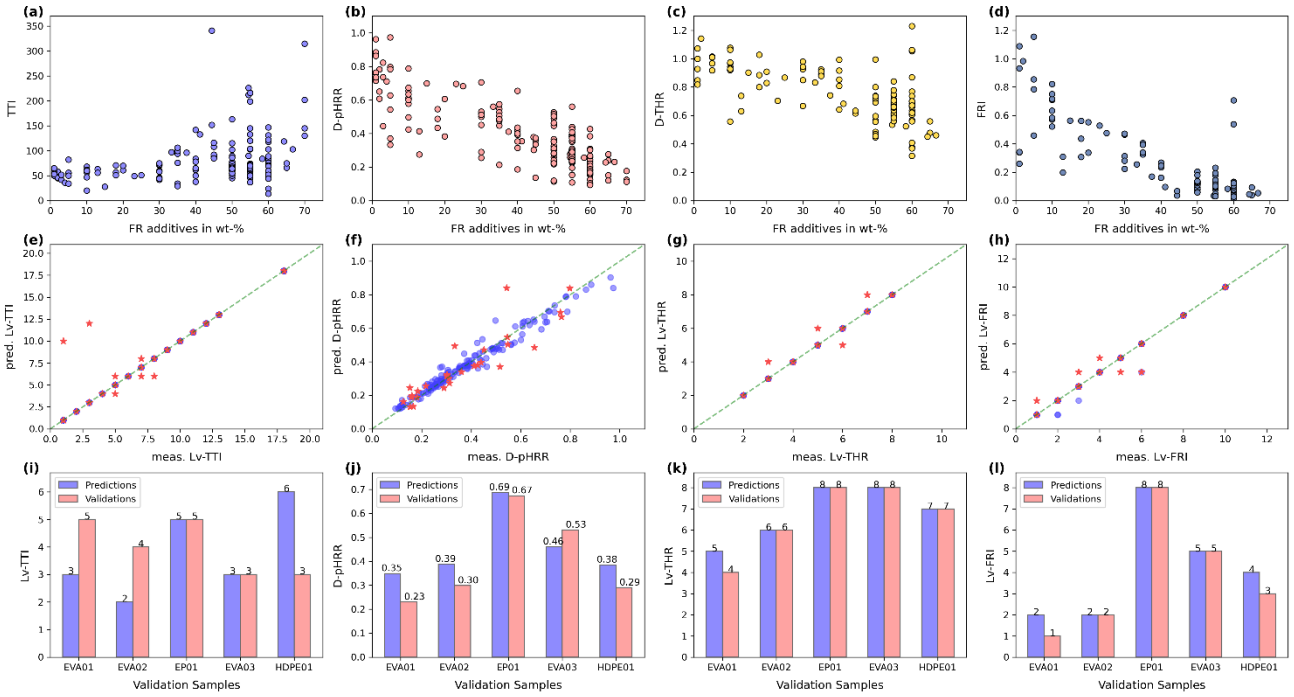

Fig. 2. Distribution of pHRR (a) and TTI (b) with respect to the mass fraction of flame-retardant additives, different colours stand for different polymer matrixes in the dataset. The size of the dots represents the mass fraction of flame-retardant additives; Predictions versus measurements: D-pHRR (c) and Lv-TTI (d) in train- and testsets; D-pHRR(e) and Lv-TTI (f) in validation set.

3.4 Feature importance analysis

RF algorithmic framework allows to calculate importance of every feature based on information gain, aiming to investigate its significance in deciding target properties in our predictive models. All features are coloured into 4 parent groups marked as subscripts in equation (2).

Unsurprisingly, all target properties are significantly affected by the mass fraction of MH shown in **Fig. 3**. The difference is that MH mass nearly dominates in deciding D-pHRR: MH related features take 57% feature importance in total. In other 3 models, features referring to polymer matrix, synergists and processing parameter still have significate impact. The influence of features in deciding Lv-TTI, Lv-THR and Lv-FRI is more multi-dimensional; and the size of feature structure increases with higher complexity of target properties: compared to Lv-TTI and D-pHRR, more features are needed to improve the accuracy in predicting Lv-THR and Lv-FRI.

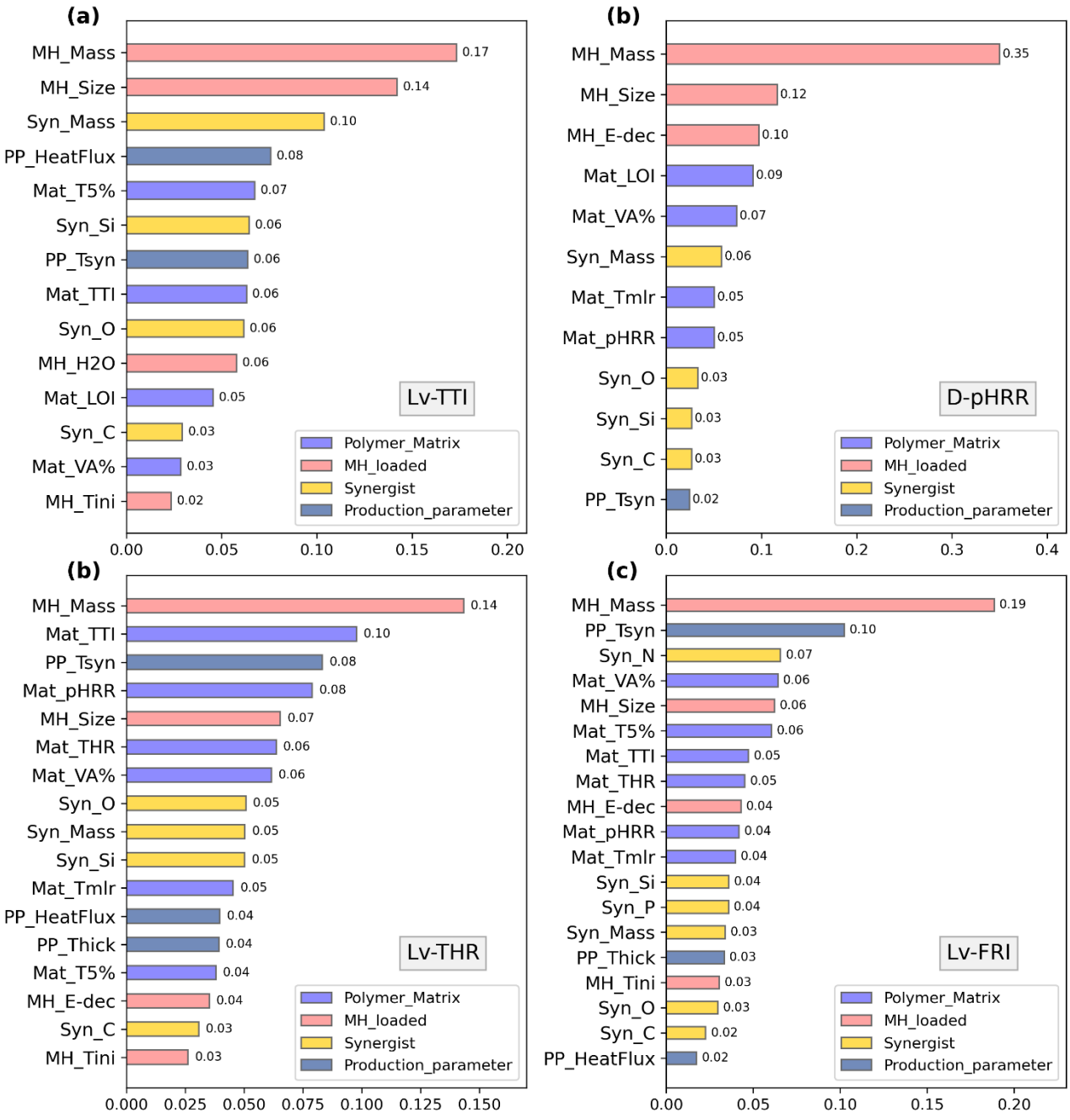

Fig. 3 Importance of all features selected to build the random forest models predicting Lv-TTI (a), D-pHRR (b), Lv-THR (c) and Lv-FRI (d); Coloured legends illustrate the parent groups of each feature.

In comparison to the most important feature group 'MH_loaded' of D-pHRR model, all feature groups mixed together ranking by decreased importance with little difference. Features related to additional synergists have similar impact on the composites' TTI as the polymer matrix; while THR is strongly influenced by the properties of neat polymer. As derived property, predicting FRI is more complicated with 19 features in order to achieve high accuracy.

3.5 Virtual dataset-based multi-objective optimization

To find the optimized formulations for flame retardant polymer composites, virtual datasets featured with the same structures from the original input dataset were generated computationally, in which values were automatically varied in corresponding ranges (4 grades of 0, 0.33, 0.67, and 1). Due to the limitation of computer performance, the virtual dataset was only imported into the constructed models to predict their D-pHRR and Lv-TTI. Points with D-pHRR < 0.4 and Lv-TTI > 8 are classified into high-performance samples as shown in equation (3).

$$y_{performance} = \begin{cases} high & \substack{D-pHRR<0.4 \\ Lv-TTI>8} \\ low & \substack{D-pHRR\geq 0.4 \\ Lv-TTI\leq 8} \end{cases} \quad (3)$$

As presented in **Fig. 4**, Y-axis represents the value range of each feature in the original dataset after label encoding. Each column depicts the individual histograms of feature listed below. Bars in red and blue with different lengths indicate the number of screened formulations with correspondingly low- and high-performance.

To achieve high performance, the suggested formulation should correspond to the values where the blue bars are relatively long. Along the green line, a large amount of MHs with moderate particle size and high enthalpy of decomposition is preferred. [57] The mass fraction of synergist should be low. The content (atomic percentage) of carbon, nitrogen and oxygen in the synergists should be as much as low, while silicon content is required to be high. Last but not the least, the process temperature required to prepare the samples should preferably be low.

The recommended formulation is constructed according to our models. Consequently, restrictions related to our input dataset exist. For example, the requirement for high content of Si is partially attributed to the fact that all the Si-containing formulations in the dataset contain high mass fractions of MHs too, resulting in lower pHRR and longer TTI. Such data combination emphasizes a monotonic relationship between the atomic percentage of Si present in the samples and the target features. However, silicon additives have certainly a synergetic effect together with MHs, especially in the condensed phase to facilitate char formation [38].

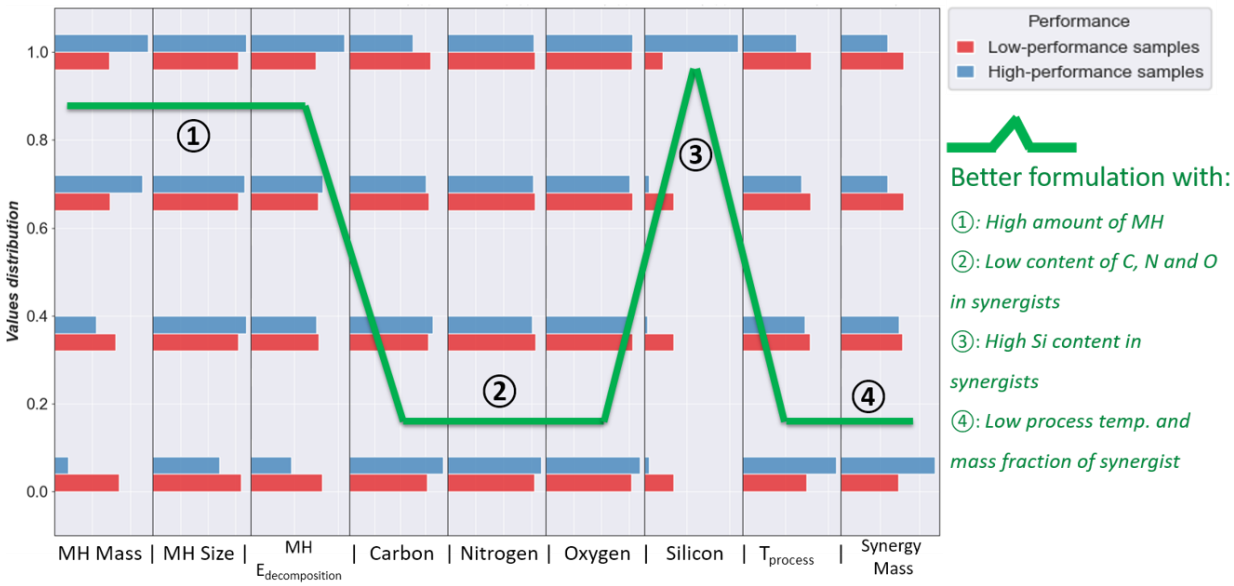

Fig. 4 Histograms of values distribution of each important feature, red bars refer to low-performance points and blue bars are high-performance ones; Green segments represent the recommended composition of polymer composites with high performance.

4. Conclusions

The machine learning approach is a promising route for materials investigation and development through predicting the optimized performance. We successfully develop predictive models for TTI, pHRR, THR and FRI using an experimental dataset generated from the literature on polymer composites with different mass fractions of MHs. The R-squared values for all models in training sets were close to 1 and those for in test sets were over 0.81(highest R2 of 0.9 for TTI prediction). This high level of prediction accuracy is achieved by implementing a supervised learning algorithm of Random Forest and generating a virtual dataset to reinforce the decision-making formulations. The analysis of feature importance reveals that the amount of MHs is a prime governing factor for deciding CCT properties, especially in pHRR prediction. Categorical classification models have relatively better performance due to oversampling of the small dataset. Feature screening provides the critical suggestion in constructing the formulations consisting of the high mass fractions of MHs, high content of silicon, low addition of synergists, and low processing temperature in sample preparation. However, there is still plenty of scope in improving the machine learning models to achieve higher accuracy in

predicting the flame retardancy properties of fire-resistance polymer composites. With the availability of additional experimental data from the literature, it is possible to predict heat release rate against time in CCT.

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