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Short Review

Machine learning for expediting next-generation of fire-retardant polymer composites

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ABSTRACT

Machine learning algorithms have emerged as an effective and popular decision-making tool for solving complicated engineering problems and challenges. Although introducing these algorithms can accelerate the optimization of fire retardants for polymeric materials by replacing traditional tedious and time-consuming trial-and-error methods, this tool remains at the elementary stage of designing fire retardants for polymeric materials, and thus to date there is a lack of insightful yet review on this topic. Herein, we review the most practical and accurate algorithms used to predict flame retardancy features, such as limiting oxygen index (LOI) and cone calorimetry results, of their polymeric materials. We highlight the merits of some current algorithms, including artificial neural network (ANN), Lasso, Ridge, ANN (L-ANN), and extreme gradient boosting (XGB). Finally, key challenges with existing algorithms for predicting next-generation fire retardants, followed by some proposed solution and future directions. This review will help expedite the development of optimized fire retardants accelerated by machine learning.

1. Introduction

Polymeric materials have become incredibly prevalent in contemporary civilization ever since their initial identification. These versatile substances have permeated nearly every aspect of modern life, finding extensive application across numerous industries and sectors [1–3]. The Current advancement in polymeric materials reaps many benefits to communities nowadays such as being widely employed in applications like manufacturing, construction, healthcare, electronics, commodities, transportation, and building [4–8]. Polymeric materials, however, can pose significant safety risks when utilized in applications that necessitate strong flame resistance, primarily due to their flammability [9–12]. New heat-resistant polymer materials must possess excellent thermal stability and significant processability [13], but high thermal resistance in polymers can lead to undesirable, weaker processing properties [14]. Developing flame-retardant polymers having high standards has always been a challenge due to the time-consuming traditional methods established on experiential intuition and trial-and-error screenings [15, 16].

In recent times, there has been a growing interest in the exploration of new materials using Machine Learning (ML) models. This approach has gained attention for its practical application in enhancing the design of material properties, leveraging the advancements in computing power and related algorithms [17–21]. ML regression algorithms, with feature engineering and large datasets, predict material properties for quality fabrication and practical applications. By training on available data, researchers save time and effort in experimentation. ML algorithms optimize and discover functional materials in thermoelectric, photovoltaic, catalytic, and optical fields [22–30].

In the area of polymer science, ML has found significant applications in recent years and still is evolving. Zhu et al. [31] developed an ML algorithm to rationally design polymer nanocomposites. Sahu et al. [32] used an informatics method to predict electrical conductivity for designing conducting polymers. Kim et al. [33] combined a genetic algorithm with ML models to design polymers with their preferred properties. Wei et al. [34] systematically explored an ML algorithm to categorize different states of polymer configurations. Yaseen et al. [35] used extreme learning machines, which is a fast and efficient form of ML,

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to optimize the design and predict the compressive strengths of foamed concrete materials. A number of researchers started using available algorithms such as ANNs to predict the temperature-related characteristics of different materials such as composite, steel, concrete, and timber [35].

In this review, we investigate recent progress in applying ML methods to predict fire retardants used for polymer materials. Based on our review study, there appear to be several algorithms that researchers have employed to train their experimental datasets and optimize the design of their final products. However, not all of them possess high accuracy and enough efficiency to be considered robust research outcomes. Therefore, we have adopted the algorithms that had relatively high accuracy and introduce them to the practical application field of next generation advanced fire retardants. In accordance with our findings, the selected ML algorithms are ANN [36], L-ANN, Ridge model with the recursive feature elimination (RFE) [37], XGB regression [38] and the sure independence screening and sparsifying operator (SISSO) method [39]. In this review paper, we explain the basic foundations of ML, followed by a full introduction of the carefully screened algorithms and their methods of operation. The review also includes a comparison of ML methods, assessing their performance, strengths, and limitations. Conclusions are drawn, highlighting current challenges and prospects for further development and application of ML models in the optimal design of advanced fire retardants.

2. Basic foundations of machine learning

2.1. Algorithms and their performance

The field of artificial intelligence, particularly machine learning (ML), has found extensive applications in various areas of scientific research [40]. Catalyst development [41], perovskite synthesis [42,43], 3D printing materials [44], studies on batteries [45,46], biomaterials [47,48] and other domains [49] have all benefited from the widespread adoption of AI techniques. Furthermore, several autonomous systems or ML-driven frameworks have been proposed to expedite the development of materials and simplify the process of achieving targeted performance [41,50,51]. The ML methods can create a model from analysis of linear or nonlinear complex relationships without regarding the essence of the relationships between the input and the output, illustrating benefits over conventional computational techniques. Unlike other conventional computing methods such as CFD [52] or FEM [53], which are usually time-consuming, ML algorithms are more efficient to predict any unknown data without any necessity for human interventions [54]. There are several steps to attain an ML model. These begin with a collection of data from reliable data sources, such as carefully performed single experiments or collating a large suite of datasets from comparable experiments where errors in datasets are a minimum. Choosing relevant descriptors for input data and splitting the dataset into the training and test sets are the next steps. Then, an ML algorithm should be selected to train the data, an evaluation process needs to be implemented to obtain relevant accuracy of the proposed model, and finally the model needs to be improved by increasing the accuracy of the predicted results. These steps are briefly shown in Fig. 1.

Constructing an ML model could be a significant challenge when creating a material dataset. For the input and output parameters, one should provide a reliable and well-defined dataset [36], which needs to come from carefully performed experiments or simulations. In research, datasets are commonly created using experimental results, databases, or existing literature. Descriptors are used to represent specific properties with numerical values, and they serve as input variables that describe the characteristics of materials. When training a dataset, researchers typically use the entire dataset to develop a machine learning (ML) model. However, to evaluate the reliability of the ML model, it is recommended to train it with unfamiliar data. This is done by dividing the dataset into two sets: the training set and the test set. In some cases, a validation set is also used to select the best model from multiple trained models. The test set, which represents future predictions, is used to

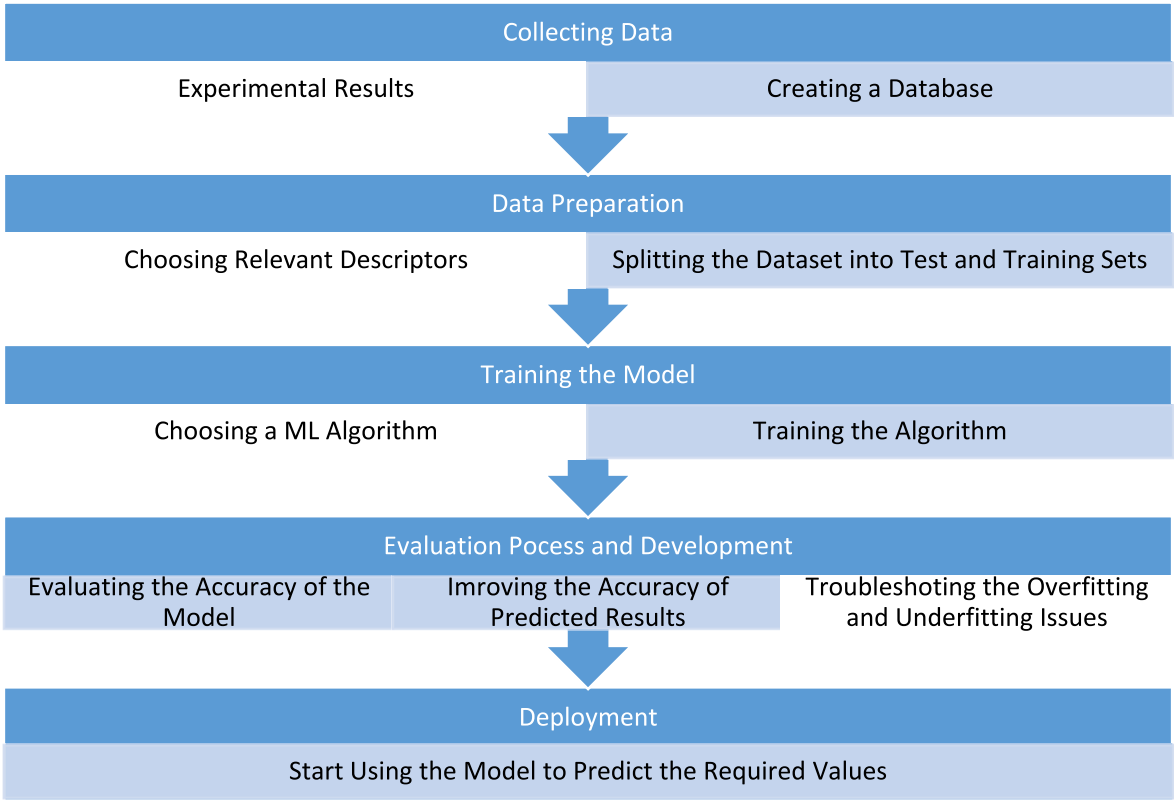

Fig. 1. Machine learning data driven design.

assess the predictability of the ML model, while the training set is used to identify patterns in the data and effectively train the proposed ML model. The selection of an algorithm for an ML model is crucial because no single algorithm can guarantee sufficient accuracy in terms of predictive performance.

Machine learning is generally divided into three sub-groups based on the structure of the training data: unsupervised, supervised, and semi-supervised [55]. In supervised ML, data are classified, and predictions are made using correctly labelled datasets whereas in unsupervised ML where labelled data are not available, researchers attempt to understand relationships within datasets. While supervised ML is much more resource-intensive because of the need for labelled data, it can lead to remarkable results if such training data are readily available. Decision trees, support vector machines (SVM), artificial neural networks, ensemble learning, and clustering are more popular rather other algorithms in designing and developing advanced materials [56].

2.2. Assessing the performance of ML models

To determine the accuracy of a machine learning model in its prediction, an assessment needs to be performed to demonstrate the difference between the actual and the predicted results. For regression problems, there are usually three statistical values to obtain the accuracy of machine-learning models, including the mean square root (MSR) or root-mean-square error (RMSE), average absolute error (AAE), and the coefficient of determination (R^2). These statistical values are demonstrated as follows:

$$R^2 = \frac{\sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{1}$$

$$AAE = \frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{n} \tag{2}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{n}} \tag{3}$$

In the above equations, n denotes the total number of data points, $\hat{y}_i$ is the predicted value for each point, y_i is the experimental value for each point, and $\bar{y}$ is the mean value of all experimental cases. The R^2 ranges from 0 to 1.0, and the closer it is to 1.0 for a model, the more accurate the model is.

3. Machine learning algorithms in developing fire retardants for polymer composites

In this section, most of the accurate and practical machine learning algorithms employed to predict fire retardant properties, such as limiting oxygen index (LOI) and cone calorimeter results, including the time to ignition (TTI), total heat release (THR), and peak heat release rate (pHRR), are introduced. The performance of these algorithms is explained and their accuracy in predicting the results is compared.

3.1. Artificial neural networks

Artificial neural networks, as one of the most well-established algorithms, are typically employed to tackle the issues that are challenging for algorithms to analyze, where there is a lack of complete or accurate data, or there is a nonlinear relationship between the parameters being researched [57]. An ANN imitates the neuronal structure of brain [55]. This structure has a minimum of three levels, each of which has a group of processing units referred to as neurons. The first level is defined as the input layer because input variables and features used to control a specific phenomenon are entered.

Subsequently, the first layer is linked to the second group of one or some layers, which might be called the hidden layers. Then, the hidden layer is connected to an output layer with the desired qualities that need to be predicted. Activation functions that are non-linear, such as Sigmoid, Step, Logistic, tangent hyperbolic and rectified linear unit (ReLu), are typically utilized to help link these layers [55]. With the use of these functions, an ANN model can provide an approximation form that facilitates gradient-based optimization.

In order to provide the best match to the input data, the parameters between each layer of the network are changed during the calculation process. Obviously, the scales of the values for various input descriptors are different. Therefore, before training the model, the data must be standardized to a range of 0–1, or -1 to 1 for all descriptors. Finally, the output of the model comes within the 0–1 range. There are several different variants of an ANN model presently available in the open literature whose architectures have been modified slightly to suit more sophisticated datasets. Recursive neural network (RNN), convolutional neural network (CNN), multilayer perceptron (MLP), and recurrent neural network (ReNN) are the examples of regularly utilized ANNs on more complex datasets. These derivatives are distinct from each other despite possessing some characteristics in common due to the principles applied to their creation and purpose. As a result, ANNs can be employed alone or in conjunction with other algorithms. A layout of a typical ANN is depicted in Fig. 2.

Because of the initial layer structures in artificial neural network algorithms, they have the capacity to take numerous properties of fire retardants at the commencement of the algorithmic layers. These properties are then examined throughout subsequent calculations in the following layers, leading to improved predictions in the final layer. Consequently, the influence of each property on the flame retardancy characteristics of polymer composites can be investigated with greater accuracy. However, the proper selection of the number of nodes and intermediate layers is crucial, as their inappropriate choice can adversely affect the prediction process. For instance, it may result in prolonged processing times or give rise to issues related to overtraining. This can be viewed as a drawback when employing them to address the flammability of polymer composites, especially when dealing with a multitude of variables.

3.2. Lasso and ridge and their combination with ANNs

Chen et al. [36] developed a new scheme illustration algorithm

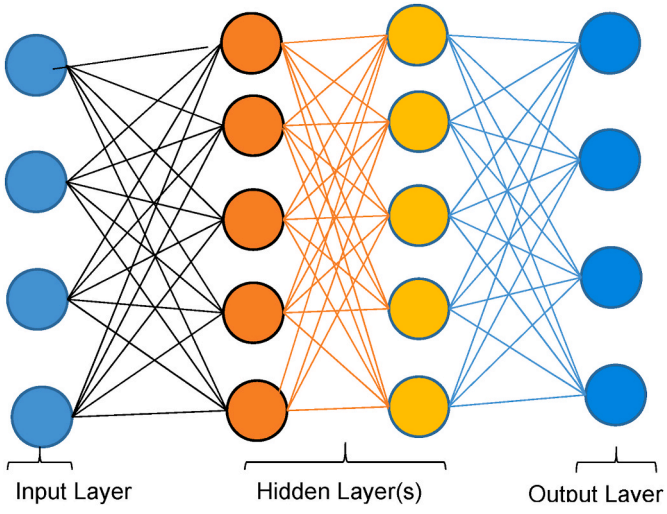

Fig. 2. Framework of an artificial neural network.

(L-ANN) by combing linear regressions (Ridge, Lasso) and ANN to achieve a more accurate model to predict the limiting oxygen index of material. The innovative distinction of the newly developed L-ANN is the incorporation of ANN and linear regression, which fully utilizes linear and nonlinear techniques. Biased estimation regression techniques, such as Ridge and Lasso, are frequently utilized in collinear analysis. By forgoing the objectivity of least squares method, the Ridge regression is a dependable regression that may get regression coefficients at the cost of some information and accuracy. It also has a great capacity to fit inadequately conditioned data [58]. The least absolute selection and shrinkage operator, often known as the least absolute value selection and shrinkage operator, are the full name of the Lasso regression. To achieve the goal of the variable selection, it can compress the regression coefficients and make some of them 0 by creating a penalty function [58].

The goal of the Lasso regression is to find the variables and accompanying regression coefficients that result in a model with the least amount of error in the prediction. This is done by placing a restriction on the parameters of model that "shrink" the regression coefficients in the direction of zero, or, more specifically, by requiring that the total absolute value of the regression coefficients to be smaller than a predetermined value (λ) [59]. This limits the complexity of model practically. The model does not include variables having a regression coefficient of 0 following shrinkage. An automated k-fold cross-validation method is typically used to select the value of λ. The dataset is randomly divided into k equal-sized sub-samples for this method. The remaining sub-sample is utilized to validate the prediction model created by the k-1 sub-samples. Each of the k sub-samples is used for validation and the remaining ones for model development as this process is repeated k times. By aggregating the k individual validation results for a range of values λ and selecting the preferred λ, an overall result is generated that is then utilized to choose the final model. This technique has the specific benefit of reducing overfitting without limiting the usage of a subset of the dataset only for internal validation [59]. The repeated process of cross-validation hence allows for a more robust evaluation of the model, resulting in improved accuracy and reliable evaluation metrics. Additionally, this technique allows for the selection of a hyperparameter λ which is optimal for the given dataset, as it takes into account the variability of the data and the underlying patterns. This further allows for a better understanding of the data and the model's performance.

Integrating the ridge and lasso methods with artificial neural networks offers a solution to the challenge of insufficient data, thereby enhancing prediction accuracy. This integration proves advantageous in tackling the flammability of polymer composites and identifying the influential parameters in the composition of fire retardants. However, as mentioned earlier, the improper selection of nodes and intermediate layers in neural networks can lead to overfitting, posing a potential drawback that may adversely affect the prediction process.

3.3. Sure independence screening and sparsifying operator (SISSO)

Ouyang et al. [60] developed an approach called the sure independence screening and sparsifying operator (SISSO), which is a subfield of artificial intelligence, especially a fusion of compressed sensing with symbolic regression. The compressed sensing feature of SISSO enables it to locate sparse linear models from tens to thousands of data points [61]. One of the main obstacles to effective material development is the absence of trustworthy techniques for determining descriptors, the sets of parameters that capture the underlying mechanisms of material behavior. The SISSO deals with large and correlated feature spaces, and it converges to the best result by combining properties related to the desired features of the materials [60]. SISSO takes on expansive spaces while preserving compressed the efficacy of sensing. SISSO is designed to function even when there are just a few training sets available, albeit this is not a requirement. The descriptor-property relationship is defined by SISSO in terms of an analytical equation [60].

Building the feature space and identifying the descriptors are the two parts of SISSO [62]. To create a large new feature space from the previous feature space, the first part of method, known as feature space construction, is utilized; otherwise, it is an increasing dimension approach. The process of finding the best descriptors and matching coefficients from the feature space created in the first phase is called descriptor identification and it is considered second part. The two stages of descriptor identification are sure independence screening (SIS) [63] and sparsifying operation (SO) [60,64]. SISSO has already been used in the fields of catalysts, perovskites, and topological insulators [65,66].

In case of discovering the properties of materials, SISSO has been specifically designed to work with high dimensional feature spaces. For the characteristics of flame retardant polymer composites, it can be said that since a huge number of variables can be effective in determining the flame retardant properties, SISSO can be used as an effective tool. Moreover, this algorithm can be used for small training datasets [60] and identifies the optimal descriptor by evaluating combinations of features, particularly physical properties. It possesses the ability to discern irrelevant descriptors for the given problem, allowing for further optimization of the feature space [60]. However, presently, the sole challenge associated with SISSO pertains to the necessary computer memory for managing the feature space. Ongoing endeavours are focused on developing more efficient implementations to address this concern [60].

3.4. Extreme gradient boosting (XGB)

Tianqi Chen and Carlos Guestin [67] created the extreme gradient boosting (XGB) regularizing gradient boosting framework. They suggested a brand-new algorithm for dealing with sparse data as well as a theoretically supported weighted quantile sketch for approximate learning. In addition to utilizing the structure of hardware to speed up computation and improve memory use, XGB incorporates regression penalties into the boosting equation (for example, elastic net) [38]. As described by Chen [67], XGB is a scalable machine learning system for tree boosting. In numerous machine learning and data mining problems, the influence of algorithm has been extensively acknowledged. A tree ensemble model employs K additive functions to forecast the output for a given data set with n examples and m features $\mathscr{D} = \{(x_i, y_i)\}$ $(|\mathscr{D}| = n, x_i \in R^m, y_i \in R)$.

$$\widehat{y}_i = \sum_{k=1}^{K} f_k(x_i), f_k \in \mathscr{F} \tag{4}$$

In equation (4), $\mathscr{F}$ represents the space of regression trees (also known as CART) and f_k is an independent tree structure with leaf scores. The regularized objective to optimize is represented in equation (5):

$$\mathscr{L}(\varphi) = \sum_i l(\widehat{y}_i, y_i) + \sum_k \Omega(f_k) \tag{5}$$

where $\Omega(f) = \gamma T + \frac{1}{2}\lambda\|\omega\|^2$.

In equation (5), the difference between the target y_i and the forecasted $\widehat{y}_i$ is measured by a differentiable loss function, called l. The second is a regularization term Ω, which deters over-fitting by penalizing model complexity. In this term, the number of leaves and the score on each leaf are, respectively, denoted by T and ω. γ and λ are employed to control the degree of regularization.

Given the intricate patterns and relationships within the dataset of flame retardant polymer materials, utilizing XGBoost can prove beneficial due to its notable predictive accuracy. The algorithm's capability to capture non-linear behaviours aligns well with the potentially complex nature of flammability in flame retardant polymer composites. It's important to note, however, that optimizing XGBoost performance requires careful adjustment of various hyperparameters. This tuning

process, especially for complex datasets assessing the flammability of fire retardant polymer composites, may demand a significant investment of time and effort.

3.5. Support vector machine (SVM)

Cortes and Vapnik [68] developed the Support Vector Machine (SVM) as an innovative form of a learning machine. Support Vector Machines (SVM) exhibit numerous appealing characteristics and demonstrate promising empirical performance. In comparison to conventional neural networks, SVM boasts significant advantages [69]. The algorithm's robust theoretical foundation contributes to a strong ability for high generalization and avoidance of local minima. Moreover, a solution is guaranteed and can be efficiently obtained using a standard algorithm, specifically quadratic programming. Besides, there is no requirement to pre-determine the network topology; it can be automatically derived upon the conclusion of the training process. Support Vector Regression involves the fundamental concept of transforming the input data x into a high-dimensional feature space F using a nonlinear mapping Φ, followed by conducting linear regression within this feature space. One can show the input data and output data as follows:

$$\{(x_i, y_i)\} \quad (x_i \in R^n, y_i \in R) \tag{6}$$

The decision function *f(x)* is expressed as follows:

$$f(x) = \sum\nolimits_i (c_i - c_i^*)\Phi(x_i).\Phi(\mathrm{x}) + b \tag{7}$$

In equation (7), c_i and c_i^* are the Lagrange multi pliers. The parameter b refers to the bias of the regression function. $\Phi(x_i).\Phi(\mathrm{x})$ is the kernel function and by substituting in the decision function formula (7), the following equation is obtained:

$$f(x) = \sum\nolimits_i (c_i - c_i^*)K(x, x_i) + b \tag{8}$$

The Kernel function can take different forms such as linear kernel, polynomial kernel, sigmoid kernel and so on. However, the typical kernel function commonly used by researchers is the Gaussian kernel (or radial basis function). The Gaussian kernel can be written as follows:

$$K(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right) \tag{9}$$

In equation (9), the parameter σ controls the generalization of the algorithm by adjusting the width of the kernel.

Support Vector Machines (SVM) can be employed as one of the most useful algorithms to design new fire retardants for polymeric materials. In fact, SVMs possess high generalization ability, which shows SVMs can perform well on unseen data. One can train a dataset collecting effective parameters using SVM, then use the model to predict the properties of new fire retardants. Support Vector Machines (SVMs) are adept at addressing the challenge of outliers, a common issue when collecting training datasets for fire retardant data. Specifically, obtaining completely outlier-free, high-quality data is nearly impractical. Nonetheless, the utilization of SVMs can be a practical approach to mitigate the model's sensitivity to outliers. Support Vector Machines (SVMs) may exhibit drawbacks when employed to predict flame retardancy properties. One such limitation lies in the potential negative impact on the learning process if the choice of kernel and regularization parameter is not appropriately tuned.

3.6. Random forests

Random Forests (RF) represent an amalgamation of machine learning algorithms [70]. Breiman [71] invented random forests for the first time, where each tree's dependency on values is determined by a randomly sampled vector. The sampling is independent, and all trees in the forest share the same distribution. The essence of the Random Forest regression model can be succinctly described as follows: within the sample space X and classification labels Y, the construction of random forests for regression involves growing trees that are contingent on the random variable Φ. In relation to each category label, the tree h(x, Φ) yields an outcome [72]. If $\mathscr{L} = \{(x_1, y_1), (x_2, y_2), \ldots\ldots, (x_M, y_M)\}$ indicates the training data, a training data $\mathscr{L}_j$ of size *N* would be separated from $\mathscr{L}$. Obviously, it can be said that $N < M$ and a decision tree is formed to train with $\mathscr{L}_j$. As previously stated, RF consisted of a number of decision trees h(x, Φ) which each of them predicts a result. The final prediction of the algorithm is achieved as follows:

$$f(x) = \frac{1}{J}\sum_{j=1}^{J} \mathrm{h}(\mathrm{x}, \Phi) \tag{10}$$

In other words, the final prediction of random forests would be obtained by taking average over K of the trees $\mathrm{h}(\mathrm{x}, \Phi)$.

Random forests (RF) can be suggested for datasets consisting of large number of samples, RF can indicate satisfactory since they divide the dataset into smaller training datasets and achieve the final prediction by averaging the results predicted for smaller training datasets. This can increase the accuracy of final prediction for high-number sample datasets. However, it is crucial to understand that the selection of an appropriate number of trees significantly influences the algorithm's predictions. Opting for a large number of trees can result in prolonged processing times and less accurate outcomes. Moreover, one challenge of random forests (RF) in predicting flammability of fire retardant composite is the interpretability. Due to the mechanism of RF, the specific impact of each property on the target variable might be less considered which might be a disadvantage for using it to predict the flammability of fire-retardant polymer composites.

4. Comparison study for the use of machine learning algorithms to predict flame retardant properties

In this section, the performance of the above algorithms in predicting flame retardant properties (LOI and cone calorimetry results) of polymeric materials are studied [73]. Moreover, the advantages and the disadvantages of each algorithm will be discussed.

4.1. The usage of ANN and L-ANN in predicting LOI of polymer composites

LOI is a key indicator for flame retardancy of materials [73,74]. Typically, a greater LOI value corresponds to higher flame retardancy [73]. Chen et al. [36] created a database including 233 items from experiments and handbooks to train ANN and L-ANN. To investigate the flame retardancy of composites, both halogen and halogen-free flame retardants were used to blend with the matrix for experimental results. Due to the extensive use of PP, they focused their emphasis mostly on it as the composite matrix. Although antimony trioxide (Sb_2O_3) can improve the flame-retardant properties of decabromodi phenylethane (DBDPE), the use of Sb_2O_3 is prohibited due to its harmful effects on the environment and human health. The following halogen-free flame retardants were selected for testing: magnesium hydroxide (MH), 9, 10-dihydro9-oxa-10-phosphaphenanthrene-oxide-phosphonamidate (DOPO), zinc stannate (ZS), and zinc hydrostannate (ZHS). As for the handbook data, there are numerous formulations about halogen and halogen-free flame retardants. Hexabromocyclododecane (HBCD), 1, 2-bispentabromophenoxy (BPBPE), and other substances are among the halogen flame retardants. Ammonium polyphosphate (APP), aluminum hydroxide (ATH), and other substances are examples of halogen-free flame retardants. As additional partial data for base data resources, 80 formulations about flame-retardant PP were gathered from handbooks. As a result, the initial dataset had 233 pieces of information that can be utilized to train algorithms (ANN and L-ANN) [36]. For the first run of algorithm training, Fig. 3a and b shows the scatterplots of

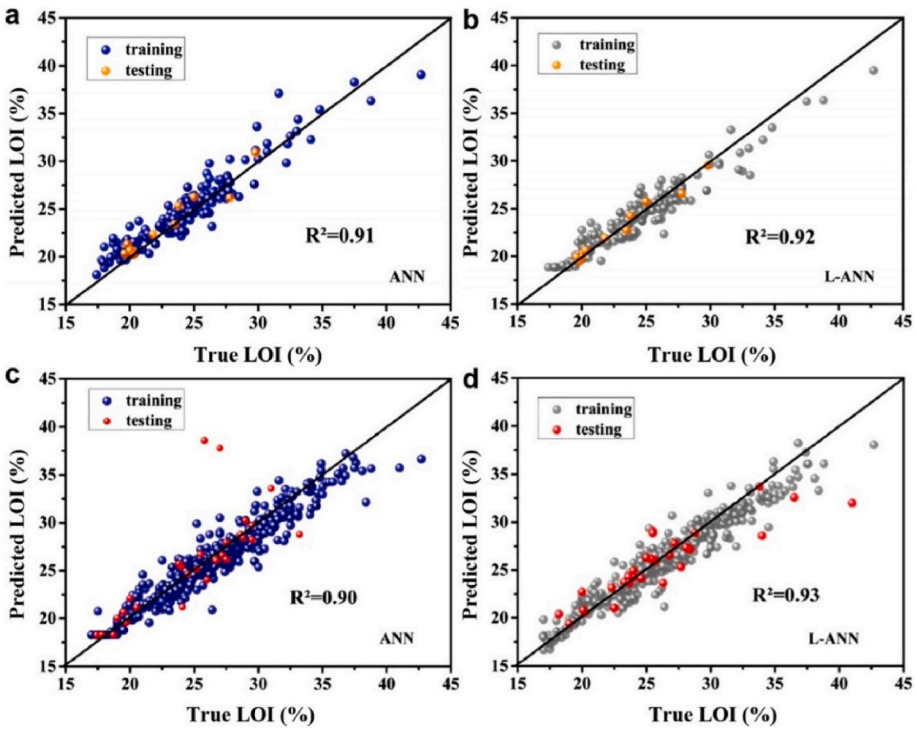

Fig. 3. The scatter plots of predicted versus true LOI by (a, c) ANN method, (b, d) L-ANN method and their corresponding R^2 values for the first and second runs. Adapted with permission form ref. [36].

predicted versus true LOI for ANN and L-ANN methods. The high degree of correlation between ANN and L-ANN is demonstrated by the R^2 values of 0.91 and 0.92 for ANN and L-ANN, respectively. This demonstrates that both algorithms are capable of accurately predicting the LOI values of the dataset, with the ANN being slightly more accurate. Additionally, the results indicate that the training process was successful since a strong degree of correlation between the predicted and true LOI values was observed. For the second run of algorithm training, they added 339 new samples from published papers to the initial dataset to build an augmented dataset. The scatter plots between predicted versus true LOI by ANN and L-ANN methods and their corresponding R^2 values are depicted in Fig. 3c and d. L-ANN and ANN have extremely high R^2 values of 0.93 and 0.90 in the second run of algorithm training.

Despite the fact the ANN and L-ANN algorithms indicated a satisfactory coefficient of determination in this study, it would be better to express them individually for both training and test sets. This enables other researchers to have better insight toward the performance of the developed model. To be more specific, the difference between the coefficient of determination of training and test sets can indicate how well it has been trained. For instance, if the difference is considerably high, then it might be interpreted that an overfitting issue happened. In order to confirm the performance of their algorithm with a new unseen set of dataset, they added two samples to predict LOI. The result of this prediction for LOI has been reported in Table 1. Assessing a model's performance with new unseen data is crucial. If a model demonstrates satisfactory accuracy in predicting target variables for a new dataset, it signifies generalization and adds to the credibility of the developed model. In this study, two additional samples were employed for this evaluation, affirming the model's high accuracy in predicting LOI. While this supports the model's reliability, a more extensive inclusion of samples would further enhance confidence in the generalizability of the predictions.

Table 1
The prediction of the model for two new samples. Adapted with permission from Ref. [36].

Samples	PP0 (g)	APP (g)	DPER (g)	ZS (g)	AO (g)	LOI-pre (%)	LOI-Exp (%)
ADZ5	700	250	83.3	5	5	28.56	29.2
ADZ10	700	250	83.3	10	5	28.42	29.5

In another study, Yan et al. [75] recruited a machine learning approach by developing a self-enforcing deep neural network (SDNN) to forecast the flammability of flame-retardant epoxy resins. This algorithm is a specific type of artificial neural networks which has a considerable number of hidden layers. The term "deep" refers to the high number of hidden layers between input and output layers. The authors of this research paper have not clearly expressed the "self--enforcing" term but they announced that they have been inspired by Vaswani et al. [76] work. In this research, they define a term called "self-attention" which might have the same concept with the term "self-enforcing". They have defined the "self-attention" term as a mechanism that focuses on various positions within a single sequence to generate a comprehensive representation of that sequence.

They created three types of datasets for three different parameters including LOI, PHHR and THR. The input data was created by fingerprinting 2D chemical structures by Morgan fingerprinting [77]. This then leaded to a high dimensional binary vector which then was combined with molar ratio of flame retardants. For the database of LOI, 163 combinations have been achieved along with 126 combinations for PHRR and 131 for THR. After training the datasets with SDNN algorithm, the results have been depicted in Fig. 3. Based on their results, the coefficient of determination R^2 was 0.98 for the training data of LOI and 0.86 for the test set. Regarding PHRR, the training set had R^2 of 0.93 and 0.87 for the test set. As for THR, R^2 was 0.92 for the training dataset, and it is reported 0.85 for the test set. There are two other metrics on the scatter plots, percentage of correct point (PCP) and mean average percentage error (MAPE). PCP indicates the percentage of points that were predicted correctly. For each parameter, they considered a percentage error as an acceptable range. This was 10 % for LOI and 20 % for PHRR and THR. As for MAPE, MAPE measures the percentage difference between predicted and actual values. These two parameters are also

depicted in Fig. 4. They claimed that to prevent overfitting, the MAPE difference between the test and training sets of data should typically not be greater than 20 %. The MAPE difference between the training and test data for LOI is only 2 %, suggesting a well-fitted model with no signs of overfitting. Moreover, the MAPE discrepancies for PHRR and THR between the training and test data, both at 10 %, are deemed satisfactory, especially considering the limited size of the training dataset. While the model's performance is deemed satisfactory in this study, the researchers have not presented any information about the utilization of a novel dataset to validate the model's generalization. It is

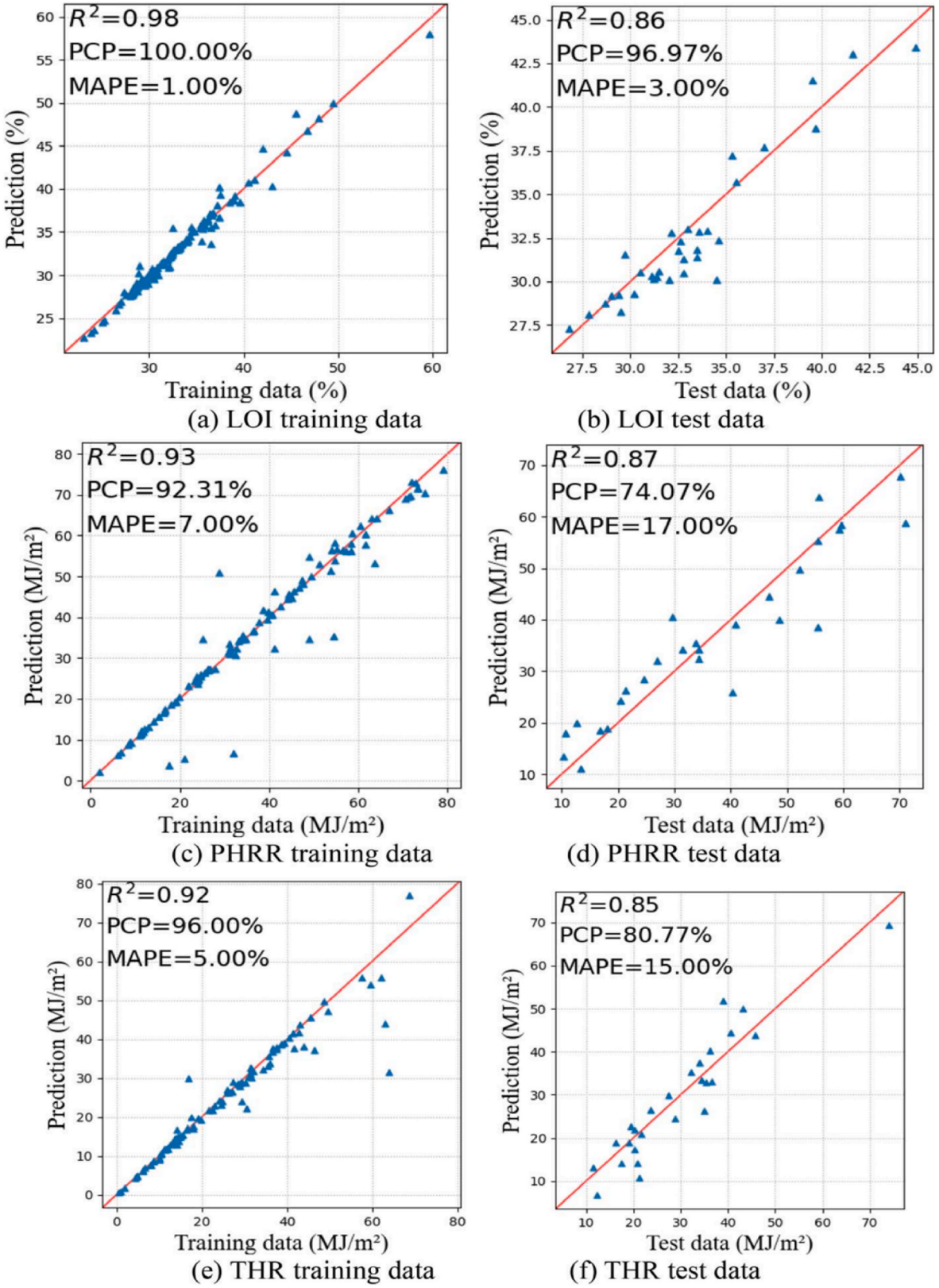

Fig. 4. Scatter plots of training and test sets of SDNN model: (a) LOI (b) PHRR (c) THR. Adapted with permission from Ref. [75].

acknowledged that models, despite displaying excellent performance on training and test sets, may exhibit lower accuracy when applied to entirely new datasets. In contrast to the prior study, which introduced new samples for assessing generalization, the current study lacks any reported details in this regard. However, in this study, the model's performance was distinctly presented for the training and test datasets. This approach is considered more favourable when compared to the prior study, where the coefficient of determination was reported for both training and test sets in a single scatter plot, leading to challenges in assessing the model's performance.

4.2. The usage of SISSO in predicting LOI of polymer composites

Chen et al. [39] have developed an effective flame retardant (ZHS@GO), nano graphene oxide (GO) wrapped micro zinc hydroxystannate (ZHS), to improve the mechanical properties and flame retardancy of PP composites. Then, they learned a straightforward equation for the LOI using the SISSO and 20 composite samples they prepared. They first created composites with varying ratios of ammonium polyphosphate (APP), pentaerythritol (PER), and ZHS@GO, and then they initially assessed the flame-retardant performances of these samples using LOI. The PP composites with various fractions of APP, PER, and ZHS@GO exhibited different LOI values.

The percentages of APP, PER, and ZHS@GO, as well as the LOI values from experiments and machine learning, are denoted by x_1, x_2, x_3, y-Exp LOI and y-ML LOI, respectively. After training the above dataset using SISSO, a training root-mean-square-error (RMSE) of 0.868 and the coefficient of determination (R^2) of 0.95 are achieved. A scatter plot between predicted versus true LOI using SISSO is depicted in Fig. 5. Moreover, experiments were performed on two new samples derived from 3D scatters of anticipated LOI. Due to the limited number of samples in the dataset, the researchers opted not to split it into training and test sets. While it is generally recommended to perform this division to mitigate overfitting, the use of SISSO can potentially overlook this concern, especially when dealing with small training datasets. For experimental validation of their model, and confirming the generalization, they employed two new samples and predicted LOI with the algorithm. The results of this study have been presented in Table 2. Despite the limited number of training samples, the model demonstrated commendable accuracy in predicting new samples, suggesting effective training. However, additional samples may be necessary for prediction to thoroughly assess the model's generalization capabilities.

'The experiment excellently confirms the one prediction ($x_1 = 20$, $x_2 = 5$, and $x_3 = 5$), demonstrating the strong predictive ability of SISSO.

Table 2
Experimental validation of LOI for two new samples. Adapted with permission from Ref. [39].

No	APP(%)	PER(%)	ZHS@GO(%)	Predict-LOI	Experiment-LOI
Exp1	20	5	5	26.82	28.40
Exp2	25	10	5	36.13	29.5

In another study, Chen et al. [78] employed SISSO algorithm to identify new flame retardant polymeric composites. They gathered different types of flame retardants including halogen and halogen-free ones used for polypropylene (PP) as the matrix of composites. A total of 153 flame-retardant polymer composites (FRPC) incorporating at least two of the six fillers—ZS, ZHS, DBDPE, Sb2O3, Mg(OH)2, DOPO—were synthesized. Subsequently, all the composites underwent testing for four performance metrics: LOI, TS, Dsmax, and VOF4. The input features for all subsequent machine learning analyses included the content of the six fillers: ZS, ZHS, DBDPE, Sb2O3, Mg(OH)2, and DOPO. They specified 80 % of the 153 samples for the training and the rest for the test set. After training the model with the provided dataset, a coefficient of determination (R^2) of 0.83 has been achieved for the test set. The scatter plot for comparison study between experimental and prediction results has been shown in Fig. 6. The researchers have not reported the coefficient of determination for training set, which can make it a little bit challenging to assess the performance of the model. However, they have provided 10 more samples to assess the generalization of the model. In fact, this action can help researchers have better insight towards the performance of their developed model. The results of this comparison study have been reported in Table 3. Regarding other three target variables, researchers reported R^2 less than 0.5 which might suggest that these properties may need better impactive variables as input in the dataset. In contrast to the prior study that also employed the SISSO algorithm, this current study exhibited higher accuracy in predicting new datasets. This observation implies that while SISSO can achieve satisfactory predictions with a limited number of datasets, its accuracy can be enhanced with a larger sample size.

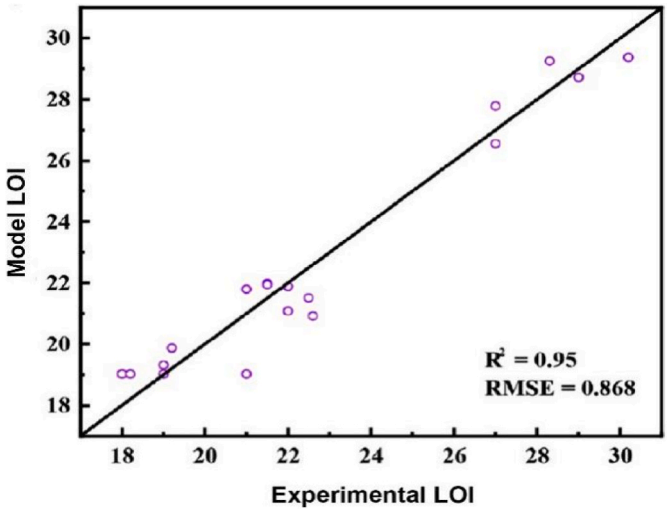

Fig. 5. A scatter plot of the predicted versus true LOI using SISSO for 20 composite samples. Adapted with permission from Ref. [39].

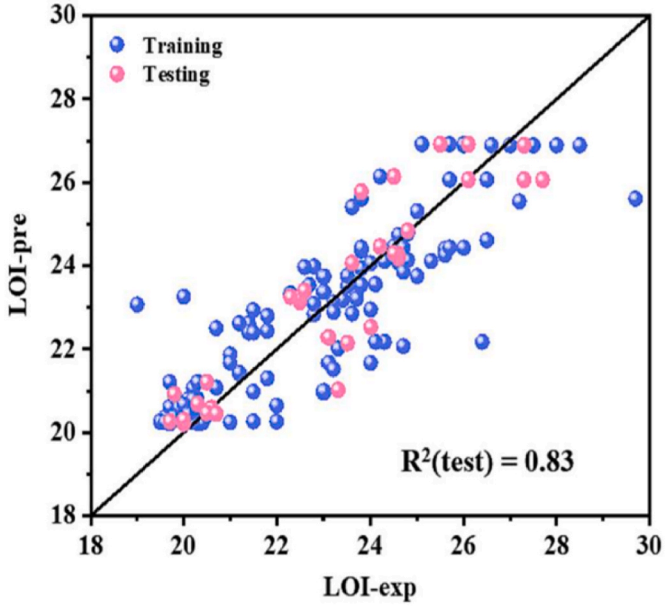

Fig. 6. A scatter plot of the predicted versus experimental LOI. Adapted with permission form ref. [78].

Table 3
The assessment of performance for SISSO for the selected samples. Adapted with permission from Ref. [78].

Sample	DBDPE(%)	$Mg(OH)_2$(%)	DOPO(%)	LOI(%)Pre/Exp
1	22.5	0	1.5	26.06/26.7
2	22.5	0.35	1.5	25.48/25.6
3	22.5	0.35	2	25.49/26.3
4	21	0	1	26.01/25.5
5	21	0.35	1	25.44/25.4
6	21	0	0.5	26.01/25.2
7	19.5	0	1.5	25.95/25.8
8	19.5	0.35	1.5	25.37/25.7
9	16.5	0.35	1.5	25.14/24.9
10	16.5	0	1.5	25.71/25.4

4.3. The usage of ridge models with RFE for feature selection in predicting LOI of polymer composites

Chen et al. [37] developed a machine learning model employing Ridge regression as an inner estimator and RFE for feature selection [79]. They gathered information from the existing literature on the LOI values of epoxy resin (EP) composites containing organophosphate flame retardants (OPFRs) from 2005. In order to make the structural data suitable for ML modeling, a simplified molecular-input line-entry system (SMILES) string was utilized to encode the structural information into a numerical list [80]. The SMILES helped them to investigate the relationship between the structure and the addition amount of OPFRs with the LOI values of EP composites. Based on the LOIs of the reported EP composites, a trained ML model was obtained and used to forecast a novel 9,10-dihydro9-oxa-10-phosphaphenanthrene-10-oxide (DOPO) derivative (BDOPO), which was later confirmed through experiments. Their LOI database had a total of 1053 data points. The fitting outcomes of the LOI ML model on the training and test sets are displayed in Fig. 7. The training and test sets' coefficient of determination (R^2) values are 0.844 (790 data points) and 0.642 (263 data points), respectively. The outcome of their model is an indication that the relationship between the FR structure, the amount of addition, and the LOI of EP composites can be accurately predicted.

To evaluate the model's generalization and further scrutinize its prediction accuracy regarding LOIs, BDOPO was designed and synthesized. The outcomes of the model were subsequently compared with experimental results. While the model did not exhibit a high R^2 for the test set, it appeared to demonstrate satisfactory accuracy when applied

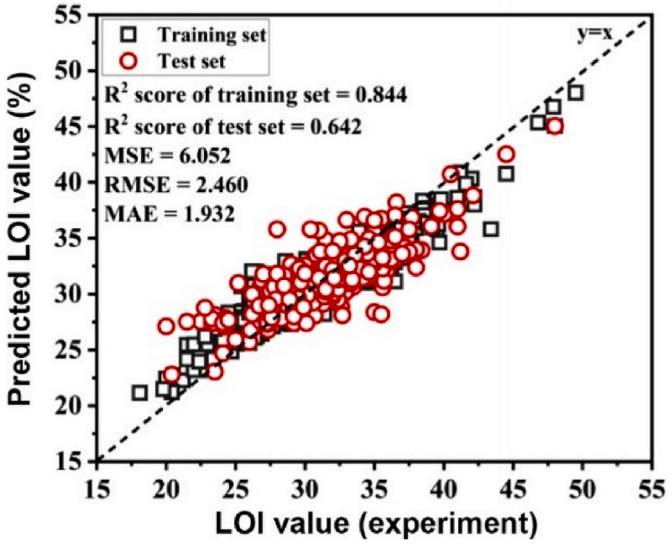

Fig. 7. The performance of the LOI ML model on training and test datasets. Adapted with permission from Ref. [37].

to a new set of data. They prepared samples with 2, 3, 5, 10, 11, 15 and 20 % addition amount. During the experiments, the Limiting Oxygen Index (LOI) of the EP/BDOPO composites initially rises from 24.8 % in pure EP to 27.1 % in the 2 wt%, 29.4 % for 3 wt%, 30.6 % for 5 wt% and 31.7 % for 10 wt%. At the same time, the predicted LOI was 29.03 % for 2 wt%, 31.77 % for 3 wt%, 32.4 % for 5 wt%, and 33.1 % for 10 wt%. Subsequently, the predicted LOI exhibits variations, reaching approximately 33.98 % at 11 wt%. Beyond this point, with addition amounts higher than 11 wt%, the predicted LOI shows an incremental trend at a slower pace compared to the 1–11 wt% range. The peak predicted LOI, around 34.15 %, is achieved at 20 wt% BDOPO, marking a marginal increase of 0.17 % from the value at 11 wt%. The experimental LOI values for EP/11BDOPO and EP/15BDOPO stand at 32.7 % and 32.6 %, respectively, representing an increase of approximately 1 % compared to EP/10BDOPO. The observed trend in LOI within the 10 to 15 wt% range aligns closely with the predicted LOIs. EP/20BDOPO records the highest LOI at 33.1 %, consistent with the model's predictions. Furthermore, as per the model's prediction, minimal LOI variations occur beyond 11 wt%. While the LOI model slightly overestimates the impact of BDOPO in enhancing EP LOI, with an error reaching up to 7.1 % and an average error of 5.1 %, it accurately predicts the experimental LOI trends, showcasing a steady increase below 11 wt% and a constant trend after this threshold.

Although the developed model could not predict the LOI for each sample with high accuracy, it could predict the trend almost accurately. However, there remains uncertainty regarding the model's ability to predict additional samples, given its less-than-optimal performance on the test set. One possible explanation could be the limitations of the algorithm employed by researchers for LOI prediction, which, despite a large sample size, did not yield highly successful results on the test set. In contrast to the other algorithms examined thus far, this particular algorithm struggled to capture the relationship between input data and the target variable. Perhaps adopting a more advanced algorithm, such as Artificial Neural Networks (ANNs) or SISSO, could potentially enhance accuracy on the test set. The high difference between R^2 score of training and test sets might suggest that the algorithm might not be well-trained. Possibly, the issue lies in the extensive number of training samples, and a resolution could involve the utilization of the recommended algorithms or even alternative ones which specifically has been developed for dealing with high-number datasets.

4.4. The usage of XGB in predicting cone calorimetry results

Zhang et al. [38] have employed five machine learning algorithms, including support vector machines (SVM), multiple linear regression (MLR), random forest (RF), k-nearest neighbors algorithm (k-NN), and extreme gradient boosting (XGB) to predict the flame retardancy index (FRI, a non-dimensional parameter derived from cone calorimetry test) values of different flame-retardant polymer nanocomposites. Vahabi et al. [81] proposed the flame retardancy index, which was utilized to quantify the flame retardant performances of various polymer composites using a set of trustworthy data. The FRI was described as the ratio between pure polymer and the corresponding flame-retardant composite in terms of total heat release (THR), peak heat release rate (pHRR), and time to ignition (TTI). The FRI is shown in equation (6):

$$FRI = \frac{\left[THR \times \left(\frac{pHRR}{TTI}\right)\right]_{Pure\ Polymer}}{\left[THR \times \left(\frac{pHRR}{TTI}\right)\right]_{Composite}} \quad (6)$$

In this case, the outcome of machine learning-driven approaches is heavily influenced by the independent variables, which are numerical expressions of the flame-retardant system. Information on the experimental settings, filler characteristics, thermal stability of nanocomposites, and flammability of polymer is contained in the

independent variables. The multiple linear regression (MLR) approach was used by Zhang et al. [38] as a performance benchmark. The MLR trend misrepresented the correlation between numerous variables, which resulted in inaccurate outcome predictions [82]. Then, they used four different regression techniques (k-NN, SVRM, RF, and XGB) for the purpose of predicting flame retardancy. The statistical evaluation results of the forecasting models are listed in Table 4. Their database consisted of 799 samples, divided into training set and test set, which the first one contained 639 sample the second one had 160 samples.

As presented in Table 4, the highest percentage of the coefficient of determination (R^2) belonged to the XGB algorithm, which reached 0.935. In comparison to other algorithms, XGB indicated the highest accuracy in predicting the FRI. Besides, the R^2 values were 0.97 and 0.815 for the training and testing sets, respectively.

Additionally, since the number of samples is large during training the algorithms, XGB and RF come out as better candidates which might suggest they have better prediction in comparison to others. In order to prove the generalization ability of their model (XGB), and to find out how much this model can be effective for designing puroposes, they embedded IiO-66, as a type of metal−organic frameworks (MOFs), into A poly(methylmethacrylate) PMMA. In order to obtain the independent variables consisting the input, the samples were examined by Thermogravimetric Analysis and Differential Thermal Analysis TGA/DTG, and FTIR spectra. Large-scale fire tests were not conducted, and the sample size were as small as a few milligrams to perform TGA (Thermogravimetric Analysis) and DTG (Differential Thermal Analysis) tests. Ultimately, the flame retardant characteristics of both pure PMMA and the nanocomposite were thoroughly assessed using the cone calorimeter, encompassing parameters such as Time to Ignition (TTI), Peak Heat Release Rate (pHRR), and Total Heat Release (THR). For a sample with 1 wt% loading, the logarithmic transformation FRI_{exp} was −0.22, while the model predicted it to be −0.207. The error was only 6 %. In another sample, they changed the loading wright percentage to 1.5 wt%, the FRI_{exp} achieved to be 0.198 while the model predicted it to be 0.142, which has an acceptable accuracy.

5. Conclusion and perspectives

5.1. Conclusions

This review paper discusses different available algorithms currently used for predicting the flame-retardant properties of polymer composites. The accuracy of each algorithm is compared based on their respective R^2 values. The SISSO algorithm has the highest R^2 of 0.95, but it is based on a small dataset of only 20 samples. This demonstrates that SISSO is capable of achieving high and satisfactory accuracy, especially in scenarios with a limited number of datasets. As mentioned earlier, while SISSO is effective in addressing the challenge of a low number of samples in datasets, having a larger number of samples can enhance the model's accuracy in predicting the flammability of fire-retardant polymer composites. However, according to the findings presented in our paper, SISSO did not successfully predict other target variables such as TS, Dsmax, and VOF4. It is important to note that SISSO is specifically designed for the discovery of new materials and has demonstrated satisfactory predictions for LOI. Therefore, the lack of success in predicting other properties may be attributed to the characteristics of the database rather than a limitation of the algorithm itself. The ANN and L-ANN algorithms have R^2 values of 0.92 and 0.91, respectively, in the first run, and their performance improves when additional samples are included in the training set. The L-ANN algorithm utilizes both linear and nonlinear algorithms effectively, addressing the issue of data scarcity. Moreover, the newly developed algorithm, SDNN, demonstrated its proficiency in predicting LOI, PHRR, and THR. The coefficient of determination for the test set was 0.86, 0.87, and 0.85, respectively, indicating the algorithm's high accuracy and performance. However, since researchers have not assessed the generalization property of their newly developed model by predicting unseen data, we cannot make clear judgements about the generalization of SDNN. On the other hand, the RFE algorithm, which uses ridge regression, achieves lower R^2 values of 0.84 for the training set and 0.64 for the test set, indicating lower accuracy in predicting LOI. However, it is still useful for small sample sizes and since the generalization was almost accurate, it might be a good candidate for predicting the flammability of fire-retardant polymer composites. Overall, the ANN and L-ANN algorithms outperform others in predicting LOI and are promising for the development of next-generation fire retardants. However, using SISSO can be more practical since it can deal with low number samples in datasets and still shows high accurate predictions. In addition, the purpose of developing SISSO was discovering new materials and predicting their chemical and physical properties. Thus, SISSO can be considered as a better candidate in predicting the flammability of fire-retardant polymer composites. In summary, SISSO and artificial neural networks (ANNs) (along with other recently developed models like L-ANN and SDNN) have demonstrated superior performance as algorithms capable of capturing the intricate relationship between input data and output when predicting the flammability of polymer materials.

In terms of predicting cone calorimetry results, the XGB model exhibits the highest accuracy among the algorithms. It achieves a coefficient of 0.935, making it an excellent choice for accelerating the design of fire retardants. The XGB algorithm's strength lies in its ability to accurately predict experimental outcomes by identifying intricate patterns in complex and unstructured data. This capability makes it highly powerful for this application, as it can expedite the development process of new fire retardants by providing more precise predictions.

Table 4
The accuracy of machine learning algorithms used for flame retardancy prediction. Adapted with permission from Ref. [38].

model	training set		training set		overall	
	R^2	RMSE	R^2	RMSE	R^2	RMSE
MLR	0.308	0.538	0.430	0.533	0.335	0.537
k-NN	0.418	0.508	0.460	0.520	0.426	0.510
SVRM	0.550	0.437	0.583	0.461	0.557	0.442
RF	0.916	0.207	0.783	0.343	0.886	0.241
XGB	0.970	0.115	0.815	0.304	0.935	0.171

5.2. Perspectives

While AI modeling can be a powerful tool for predicting fire behavior, it is not without limitations. One significant drawback of existing algorithms is the scarcity of data, which hinders the development of models based on AI/ML for predicting fire-retardant materials behavior. Machine learning algorithms require large amounts of data to train and improve their accuracy. Without enough fire test data, these models cannot accurately predict fire behavior in different scenarios, making it challenging to develop reliable machine learning (ML)-driven new materials. In summary, we introduced some challenges and some suggestions to overcome them below. To address these challenges, there is a great need of a better understanding of designing fire-retardant polymeric materials.

(1) In order to tackle the sacristy of data, it is crucial to invest in more fire testing to enable the development of accurate and reliable AI/ML models using large amounts of data. This requires extensive collaborative work among researchers in this field.
(2) To solve the problem with making AL models with more dynamic between inputs and outputs, both experimental and AI modeling approaches are necessary to develop a comprehensive understanding of fire behavior and develop effective fire-retardant systems. By combining the strengths of AI modeling and fire

experiments, one can improve the ability to predict, prevent, and mitigate the devastating effects of fires.

(3) Apart from the above, numerical moldering approaches, such as the finite element method (FEM) [83], can be employed along with AI modeling and experimental research to obtain more reliable and accurate results for designing the next-generation fire retardants.

(4) It is important for researchers to construct models with the ability to predict outcomes for previously unseen datasets. The model's generalization can serve as a valuable tool for designing and discovering novel materials with optimized properties.

(5) Future research in this field should focus on key aspects such as the creation of high-quality datasets, the development of multi-objective prediction models, and enhancing the interpretability of models.

CRediT authorship contribution statement

Pooya Jafari: Data curation, Formal analysis, Writing – original draft. **Ruoran Zhang:** Formal analysis, Methodology. **Siqi Huo:** Methodology, Supervision. **Qingsheng Wang:** Methodology, Writing – review & editing. **Jianming Yong:** Software, Writing – review & editing. **Min Hong:** Writing – review & editing. **Ravinesh Deo:** Methodology, Writing – review & editing. **Hao Wang:** Supervision, Writing – review & editing. **Pingan Song:** Conceptualization, Funding acquisition, Supervision, Writing – review & editing.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used CHATGPT in order to be assured of the readability and language. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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