




Research Article

Predicting Carbon Residual in Biomass Wastes Using Soft Computing Techniques

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In recent decades, the development of complex materials developed a class of biomass waste-derived porous carbons (BWDPCs), which are used for carbon capture and sustainable waste management. It is difficult in understanding the adsorption mechanism of CO₂ in the air as it has a wide range of properties associated with its diverse textures, functional group existence, pressure, and temperature of varying range. These properties influence diversely the adsorption mechanism of CO₂ and pose serious challenges in the process. To resolve this multiobjective formulation, we use a machine learning classifier that maps systematically the CO₂ adsorption as a function of compositional and textural properties and adsorption parameters. The machine learning classifier helps in the classification of various porous carbon materials during the time of training and testing. The results of the simulation show that the proposed method is more efficient in classifying the porous nature of the CO₂ adsorption materials than other methods.

1. Introduction

To reduce CO₂ emissions, carbon capture and storage (CCS) has been widely accepted [1–4]. As the concentration of carbon dioxide (CO₂) in the atmosphere continues to rise [5], CCS has been regarded as an essential technique. Due to the expense of CO₂ capture [6], more than half of the entire

CCS cost is still accounted for by CCS systems. Aside from precombustion and postcombustion, oxy-fuel combustion is the third most cost-effective method of CO₂ capture from industrial emission point sources [7, 8].

This technique, however, has a major barrier due to the low CO₂ concentration in postcombustion flue gases. Regenerative amine solution techniques for postcombustion CO₂ capture

are expensive and plagued by corrosion, solvent loss due to degradation, and environmental toxicity [9]. Researchers are trying to produce cost-effective membranes with high CO₂ permeability for extracting CO₂ from flue gas, but this is still a long way off. In the second generation of carbon capture, solid porous carbon-based CO₂ adsorption is usually considered the most promising method [1, 8, 10].

In addition, it is inexpensive, has minimal energy consumption, and is stable in the cyclic mode. Biomass waste has a number of advantages for making porous CO₂ adsorbents, including sustainability, cost-effectiveness, and abundance [2, 11]. The environmental contamination produced by improper biomass waste management can be reduced with the use of BWDPCs for CO₂ collection, as can climate change mitigation through decarbonization and negative emission technologies [9].

More and more research has been done on BWDPC CO₂ adsorption isotherms at various temperatures in order to decipher and optimise CO₂ adsorption process thermodynamic features [12]. Solid carbon adsorbents are vulnerable to adsorption settings with limited CO₂ selectivity because CO₂ adsorption is predominantly dominated by physisorption [10].

Carbonization and activation, followed by heteroatom doping, have a substantial role in increasing CO₂ adsorption capacity and CO₂ selectivity. Carbonization and activation are the two main processes in the production of porous carbon from biomass waste. Carbonization has been a major focus of thermochemical techniques [11].

Chemical and physical activations have received a lot of attention [13, 14]. The fundamental active sites of porous carbons can also be increased by heteroatom doping treatments [15–18]. Acid–base interactions improve CO₂ adsorption and selectivity over other gases. Some hazardous or greenhouse gases are released during thermochemical reactions.

Aside from carbon dioxide, the handling of nitrogen oxides emitted must be carefully studied because NO_x is both harmful and one of the most common greenhouse gases [18]. In the last decade, BWDPCs under varied carbonization/activation settings and diverse adsorption parameters have largely been treated in similar ways [1, 14], determining whether or not BWDPCs can be effectively employed to absorb CO₂. It is currently uncertain how to optimise the synthesis process by combining carbonization and activation with a realistic guideline.

Furthermore, the textural properties and functional groups of porous carbons are widely regarded as the most important factors influencing CO₂ capture performance [1, 11, 16, 19, 20]. However, it is still unclear how to prioritise these three qualities; a prioritising technique would be advantageous for guiding the synthesis of porous carbons from biomass waste.

Waste-to-energy, biochar for metal and organic compound sorption [21, 22], municipal solid waste treatment [23, 24], and micropollutant oxidation [25, 26] have all recently received a lot of attention due to the potential for machine learning.

Tree-based ML models are a subclass of supervised ML methods that leverage recursive binary splitting of data in a manner that minimises the residual sum of squares [19].

Random forest, decision trees, light and gradient boosting decision trees, and extreme gradient boost are some of the most popular models. With their capacity to cope with tiny datasets, resistance to overfitting, and ability to overcome noisy features, the last three boosting tree-based models have witnessed a spike in popularity in scientific research [27].

Boosting trees have advantages over traditional RF [28], such as global predictions, nonbiased feature weighting, and efficient processing of unevenly distributed datasets. It has also been found that these boosting tree techniques are more efficient in tuning hyperparameters than the more commonly used SVM algorithms when working with relatively small datasets.

The SVM classifier used in this study maps CO₂ adsorption as a function of compositional and textural features, as well as adsorption parameters, to resolve this multiobjective formulation. During training and testing, the machine learning classifier assists in the classification of diverse porous carbon materials. The simulation results suggest that the proposed method is more effective than existing ways of categorising CO₂ adsorption material porous nature.

The major contributions of the work involve the following:

- (i) First, we need to collect the information from the database BWDPCs for CO₂ capture was carried out using various keywords (such as biomass waste, porous carbon, biochar, CO₂ adsorption, and capture). Further, it will lead to preprocessing where we eliminate the duplication, similar data, null set, etc.; the rest of the other data will be forwarded to the next stage
- (ii) The proposed method FCN extracts and selects the contents from an input image by constructing an accurate data split
- (iii) The simulation is conducted to test the efficacy of the model that integrates the contextual information for optimal segmentation of optical cup and disc

2. Data Collection

With the use of major databases, a comprehensive literature analysis of BWDPCs for CO₂ capture was carried out using various keywords (such as biomass waste, porous carbon, biochar, CO₂ adsorption, and capture). 632 data points were gathered from 76 peer-reviewed papers published in the last decade. Biomass waste-derived porous carbons (BWDPCs) are a class of complex materials that are widely used in sustainable waste management and carbon capture. BWDPCs have been extensively used to synthesise CO₂ adsorbents, and the most important requirements for their development were good adsorption and selectivity, steady working capacity, cost-effectiveness, recycling, facile regeneration, and quick adsorption–desorption dynamics. This is worth emphasising.

As a result of this, we focused largely on the CO₂ adsorption capacity of BWDPCs at various temperatures and pressures, as well as the textural and compositional features of BWDPCs.

- (1) A lack of data on the working capacity, kinetic characteristics, and regeneration of adsorbents was found in most of the articles evaluated, resulting in the inability to create ML models for all of the aforementioned important attributes
- (2) Due to a lack of environmental effects and techno-economic evaluation, performance standards for the other categories were lacking

As a result, when gathering data, the following hypotheses and tactics were employed:

- (i) There was no initial judgement or bias on the validity of the data that was initially accepted
- (ii) The vast majority of the data was gleaned from published study publications. It was essential to extract the relevant data from the figures using the Web-PlotDigitizer software for those data points that were not explicitly listed in a table. An extensive screening process ensured that all data was unique and free of duplications or duplicated submissions
- (iii) For the purposes of this study, the input features were divided into three general categories: (1) textural properties; (2) BWDPC elemental compositions; and (3) adsorption parameters, such as CO₂ adsorption temperature and pressure
- (iv) It is important to note that the BWDPC surface area (SA), total pore volume (TPV), micropore volume (MPV), and elemental compositions of carbon, hydrogen, nitrogen, and oxygen were all examined
- (v) Different adsorption parameters were employed to determine the CO₂ uptake by the BWDPCs. There are 288 data points and 344 data points from different publications for heteroatom-doped porous carbons

3. Proposed Method

Input features were correctly detected and labelled based on the data collected. Data preprocessing was carried out after the gathering of data to enable effective SVM prediction performance. Figure 1 illustrates the data processing and data classification methodology to improve the quality of information.

3.1. Data Preprocessing. The first stage in machine learning is data preprocessing. Many concerns must be resolved before any further analysis can take place. These include ensuring that the data is clean and free of noise or missing numbers. Machine learning algorithms are constantly being improved to be able to perform well in the presence of miss-

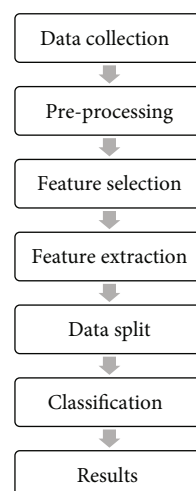


FIGURE 1: Proposed workflow schematic.

ing values or noise, but the quality of the outcomes is still affected by the input data.

3.2. Missing Value Imputation. Our initial step is to deal with the issue of missing data and impute the values that were not found during our preliminary analysis of the data.

There are many ways to deal with the problem of missing numbers in weather data, some of which are more involved than others. In order to deal with missing values, it is helpful to know the reason for their absence in the dataset, and this is based on their unpredictability.

The last two types are the most challenging to work with since the substituted value may not accurately reflect the original observation. This is the most straightforward technique to deal with a missing value. There may be too few complete examples to justify removing partial features. It is also possible that the discarded values include valuable information, and deleting them could have a negative impact on the outcome.

We do not have to remove features that have missing values; instead, we can “impute” new values to the missing data. The apparent option is to remove the features with missing values, but this can result in the loss of valuable data. Because of this, we can utilise imputation methods to automatically fill in the blanks with new data.

This allows us to evaluate more characteristics rather than eliminate all the observations with missing values. We can use missing values. To ensure that the entire dataset is included, missing values might be inserted to ensure that the results are not skewed. It can, however, have a small impact on the final outcome. For those missing variables, we opted to use mean imputation to fill in those that were not included in the original dataset.

Means of observed values are utilised to fill in missing values in each feature in this method, which is one of the most accessible and often used strategies. It is worth noting that filling in the blanks is a critical part of data preparation because it serves as the basis for subsequent operations. From linear correlation to support vector regression, there are increasingly complex imputation approaches.

3.3. Feature Selection with Correlation. Selecting features that are not correlated with each other but still predictive of the class is what feature selection is all about. If a variable is not predictive of the class, it can be deleted. An evaluation of the dataset inner feature correlation and its contribution to classification models is carried out to establish the value of this task.

Data interdependencies can be assessed using Pearson's correlation coefficients, which are simple to calculate. Assuming x_i is the number of observations (i^{th}) and y is the class label, the Pearson correlation coefficient can be defined as

$$R_{(i)} = \frac{\text{cov}(x_i, y)}{\sqrt{\text{var}(x_i) \text{var}(y)}}, \quad (1)$$

where cov is covariance and var is variance.

Mathematically, the complete formulation is

$$R_{(i)} = \frac{\sum_{k=1}^m (x_{k,i} - \bar{x}_i)(y_k - \bar{y})}{\sqrt{\sum_{k=1}^m (x_{k,i} - \bar{x}_i)^2 \sum_{k=1}^m (y_k - \bar{y})^2}}. \quad (2)$$

A correlation map is used in the implementation to demonstrate the correlation between the columns. One adsorption feature is dropped from each pair in this algorithm. A classification algorithm is then used to see how the classifier performs when we add a new subset to our dataset. A closer look at the strongly connected group of attributes is useful at this point. Because of this, feature selection by a correlation coefficient of adsorption relies heavily on trial and error and does not produce optimal results.

3.4. Recursive Feature Elimination with Cross-Validation. In most circumstances, RFE and cross-validation can be used to pick a new subset of characteristics for adsorption in most circumstances, because the preferred number of features is often unknown. Once the model has been fitted, cross-validation scores can be compared to determine the best number of features for classification accuracy. Prior to classification, RFE can be used to identify the intercorrelated features and patterns in the dataset. Unnecessary and redundant data are removed quickly with RFE. But there are certain disadvantages to this approach. It is important to think about computational intensity. Before training the data, the user must choose the number of features to be used in RFE. Other feature selection strategies have been employed to overcome this issue and arrive at the ideal dataset.

3.5. Feature Extraction. PCA is a popular feature extraction technique that uses principal component analysis to determine a lower-dimensional basis from the original dataset that captures most of the data variation. For the lower-dimensional basis, the correlated features are transformed into fewer uncorrelated ones by linear transformation into principal components.

The goal of PCA is to discover the lowest-dimension surfaces onto which to project the data in order to minimise the

projection error. Using vectors, we may describe the lower-dimensional surfaces. Two conditions must be met for a surface to be considered good. The first two goals are to maximise anticipated variance and decrease mean squared error. All dimensions must meet these parameters. It is these dimensions or directions that account for the greatest amount of variance in PCA vectors, which are known as principal components.

PCA is a linear transformation that rotates the points into a new coordinate system, erasing the association between them in the mathematical sense. By projecting the data into a lower dimension and reducing the mean squared projected error, PCA performs the transformation by minimising the difference between the original and projected data. The formula for calculating the average squared projection error is as follows:

$$\text{Mean square projection error} = \frac{1}{m} \sum_{i=1}^m \|x^i - x_{\text{approx}}^i\|^2. \quad (3)$$

Component variance is calculated by ensuring that the mean squared projection error over total variance is less than 1% for the 99% criterion.

$$\frac{1/m \sum_{i=1}^m \|x^i - x_{\text{approx}}^i\|^2}{1/m \sum_{i=1}^m \|x^i\|^2} \leq 0.01. \quad (4)$$

For a particular threshold α , the steps of the PCA algorithm are as follows:

- Step 1: the mean should be calculated from the data
- Step 2: data should be the focus
- Step 3: take the covariance matrix and run it through
- Step 4: eigenvectors must be computed
- Step 5: the eigenvectors can be computed
- Step 6: calculate the percentage of the overall variation that is accounted for

Step 7: in order to reduce the overall variance to less than 1%, choose a dimensionality that has the fewest components

A smaller base and less dimensionality are now possible. Reduced dimensionality using PCA can keep the variance and accuracy of the classifier but also helps learning algorithms run more effectively and reduce computation time because many features in real-world datasets are correlated or redundant.

3.6. Classification—Support Vector Machines. In fraud detection, identifying cancer cells from healthy ones, face recognition, weather forecasts, etc., SVM is a common classification algorithm. For this reason, the SVM is referred to as a supervised learning classifier since it uses data that has already been labelled by the supervisor.

In order to maximise speed while retaining generalisation for unknown data, classification methods are used. In other words, the model potential to generalise is compromised in favour of better fitting the data. Data classification is done by finding a hyperplane that separates the two classes in SVM. This method is summarised in a single sentence:

$$\hat{y} = \text{sign}(H(x)). \quad (5)$$

In this formulation, the decision function $H(x)$ is used. Any location on the separating hyperplane can meet the following requirement:

$$\begin{aligned} H(x) &= w^T x + b = 0, \\ x, w &\in \mathbb{R}^n, \end{aligned} \quad (6)$$

and

$$b \in \mathbb{R}, \quad (7)$$

where x is feature vector, w is weight vector, and b is offset.

The hyperplane position in space is determined by the linear equation weight vector for adsorption. Weight vector is perpendicular to the hyperplane, and b is the hyperplane offset, or distance from the origin. The input space is divided into two halves by the hyperplane: $H(x) > 0$ in one half space and $H(x) = 0$ in the other. For all data points on the hyperplane, the critical property of this hyperplane is $H(x) = 0$. On this hyperplane, which is used to divide the test data into two groups, $H(x) > 0$ corresponds to a +1 label, and $H(x) < 0$ corresponds to a -1 label on this hyperplane.

$$\hat{y} = \begin{cases} 1 & w^T x + b > 0 \\ -1 & w^T x + b < 0. \end{cases} \quad (8)$$

The margin of separation is defined as the distance between the nearest adsorption data point in the training set and the separating hyperplane. The hyperplane with the greatest separation between the two classes is unique and can only be identified by optimization, even when several hyperplanes satisfy the criteria. Maximising the largest margin of separation is essential because it boosts a model generalisation or ability to better handle noise in the test data, and the data points that are classified based on their position in the band are classified.

The term support vector is also a key component of this method name. A support vector is a set of data points whose distance from the separating hyperplane is equal to one after normalisation.

3.7. Parametric Modeling. An algorithm known as SVM can be used to forecast the future. However, it may require a lot of time and resources. A regularisation parameter known as C is used to adjust the model parameters in order to get the best results from SVM. There are two goals to be met: minimise the error term and weight vector norm and maximise the margin of separation. The regularisation parameter governs this trade-off. The SVM classifier performance can be significantly impacted by fine-tuning this parameter. Grid search is a common method for tweaking parameters in SVM, as there are few other options. The model is trained on a collection of hyperparameters to discover the best parameters for the given model before performing a grid

search for parameter selection. An expensive and time-consuming method of searching huge datasets, grid search constructs many models with given parameter values and chooses the optimal one after comparing outcomes for all combinations.

In this paper, we present a method based on the parametric simplex method for exhaustively searching the solution path and determining the optimal regularisation parameter value. A parametric simplex approach can be used to obtain all possible values for the parameter in this work using the SVM algorithm, which is a linear programming problem. We can then select the best value from a small number of possible values.

The parametric simplex approach can be applied in a variety of ways, each with a somewhat different set of variables to update. The approach suggested in this paper solves the linear programming issue at a global level.

There are a few terms that need to be defined before we can get into the method further. Algorithms begin by solving augmented forms of the original issue to ensure that the problem can be successfully solved. The optimal values of the choice variables in the enhanced LP are the result of solving this problem. The LP corner-point solution is a simple one. Whether or not the basic answer is practical, it is referred to as a “basic, feasible solution.”

The sole difference between the corner-point solution and a basic solution is the inclusion of slack variables. There are two types of variables in the corner-point solution: basic and nonbasic. These are the variables whose values are set to zero in the basic solution, while the remaining variables are considered nonbasic. The basis is a collection of all the variables that are essential to the model. When minimising the objective function, it is necessary to lower the coefficients in order to get the optimal value. The reduced cost vector is another word that needs to be defined.

Support vector machines with L1-norm kernels are used to classify the indivisible data and the problem is stated as

$$\text{Min}_{w,b,\zeta} \left\{ \lambda_1 \sum_{i=1}^l |w_i| + \lambda_2 \sum_{i=1}^l \zeta_i \right\} \text{ s.t. } y_i \left[\sum_{j=1}^l w_j \cdot k(x_i, x_j) + b \right] \geq 1 - \zeta_i, \quad (9)$$

where $\zeta_i \geq 0$, $w_i \geq 0$, $\lambda_1 + \lambda_2 = 1$, and $\lambda_1, \lambda_2 \geq 0$.

A multiobjective problem can be solved in a variety of ways. The weighted sum of two goal functions that we are seeking to minimise simultaneously is the objective function. We are trying to figure out the best values for λ_1 and λ_2 to achieve this. Let the study set $\lambda_1 = \lambda$ and $\lambda_2 = 1 - \lambda$ to make the problem compatible with the form described in Section 4.

4. Results and Discussions

Section 2 shows the data collection, and the proposed SVM is compared with existing methods in terms of various performance metrics that include the accuracy, precision, and recall of the percentage error.

Figure 2 shows the results of precision between conventional machine models and proposed SVM. The results of

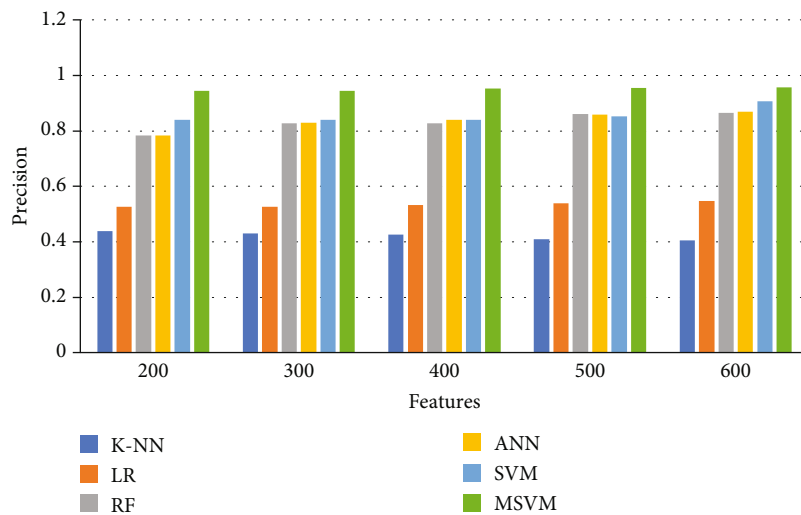


FIGURE 2: Precision.

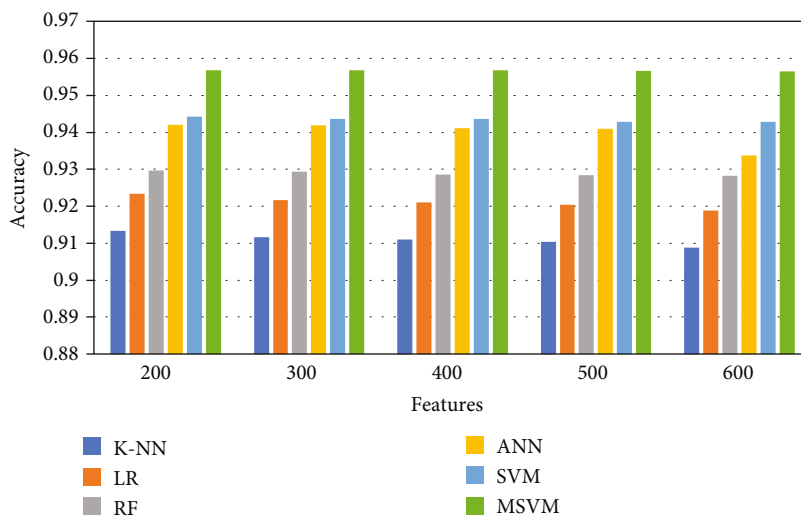


FIGURE 3: Accuracy.



FIGURE 4: Recall.

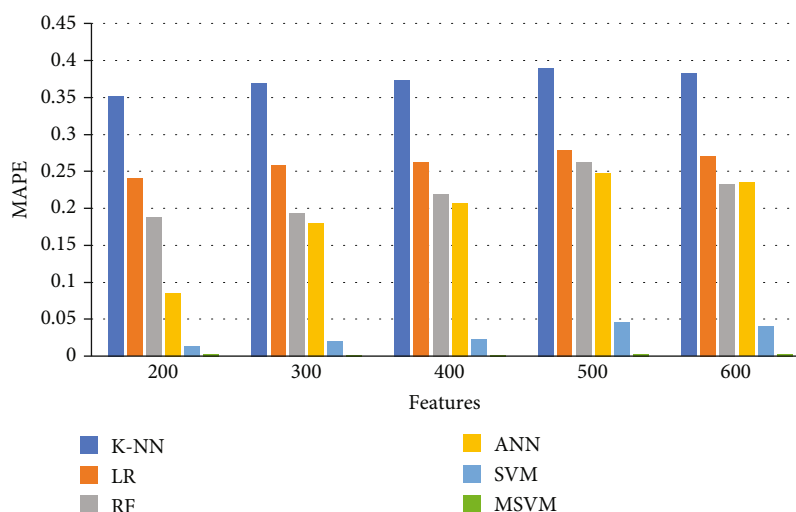


FIGURE 5: Mean average percentage error (MAPE).

the simulation show that the proposed SVM achieves a higher rate of segmentation performance with high precision than other methods.

Figure 3 shows the results of accuracy between conventional machine models and proposed SVM. The results of the simulation show that the proposed SVM achieves a higher rate of classification performance with high accuracy than other methods.

Figure 4 shows the results of recall between conventional machine models and proposed SVM. The results of the simulation show that the proposed SVM achieves a higher rate of segmentation performance with high recall than other methods.

Figure 5 shows the results of MAPE between conventional machine models and proposed SVM. The results of the simulation show that the proposed SVM achieves a reduced rate of MAPE than other methods.

5. Conclusions

An SVM-based multiobjective formulation is presented in this study, which shows how changes in composition, texture, and other adsorption characteristics affect CO₂ adsorption. During training and testing, the machine learning classifier assists in the classification of diverse porous carbon materials. The simulation results suggest that the proposed method is more effective than existing ways of categorising CO₂ adsorption material porous nature.

In addition, these data-driven models provided certain mechanistic knowledge about the real CO₂ capture process, which raised confidence in their adoption because their findings and inferences were supported by the existing literature.

This study has provided us with a framework for our next steps, which include developing a strategy to maximise the CO₂ adsorption of BWDPCs by optimising the adsorption parameters and textural properties of the BWDPCs and testing the optimizer, which will be done by incorporating new experimental data points into the database and

making it freely available for use by other researchers in the community.

Data Availability

The datasets used and/or analyzed during the current study are available from the corresponding authors on reasonable request.

Conflicts of Interest

There is no conflict of interest.

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