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Influence of Biomass Composition and Microwave Pyrolysis Conditions on Biochar Yield and its Properties: a Machine Learning Approach

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Abstract
The investigation of microwave pyrolysis behavior and interactive effects of process parameters through machine learning is necessary to systematically determine the combined effects on the yield and characteristics of biochar. This study involves the prediction of microwave biochar yield and its property using various machine learning approaches. Based on the input data of feedstock characteristics (elemental and proximate composition) and operating conditions of microwave pyrolysis (microwave power, time, weight, absorber), the output targets like biochar yield and higher heating value (HHV) have been predicted. The results suggested that eXtreme Gradient Boosting (XGB) model with optimal hyper-parameters could predict the yield and HHV of microwave-derived biochar with higher correlation coefficient (R^2) of 0.91. The impact of each factor on output target and their interactions during microwave pyrolysis has been observed from SHAP (SHapley Additive exPlanations) dependence plots. The study outcome revealed that microwave power is the most significant feature influencing the yield of biochar and its property (HHV). The present work gives an insight through computational approach in improving microwave pyrolysis of biomass for enhanced biochar yield and its properties.

Keywords Biochar yield · Biomass · Heating value · Machine learning · Microwave pyrolysis

Introduction

The extensive exploration of renewable resources like solar, wind, and biomass energy is being carried out recently as alternative for conventional energy sources that have adverse environmental impacts. Biochar, a carbonaceous product obtained from biomass through thermochemical conversions is gaining sharp attention in recent decades owing to its extensive applications as solid fuel [1], land reclamation [2], contaminant removal [3, 4], wastewater treatment [5, 6], soil conditioner to improve crop productivity [7, 8], carbon sequestration [9, 10] and as catalyst for biodiesel production [11, 12]. The potential utilization of biochar for different applications is likely owing to its properties of higher porosity, surface area, cation exchange capacity, functional groups, and stability. The properties of biochar are heterogeneous based on the type of feedstock used and process conditions subjected whereas the characteristic features of biochar determine its feasibility for final applications [13, 14]. Pyrolytic conditions involving reaction temperature, time, and heating rate are the major determining factors that affect the yield and property of biochar. Pyrolytic temperature and time are negatively correlated with the yield of biochar since the higher temperature and time enhances the volatilization rate [15]. At higher temperature, both pH and electrical conductivity of biochar tend to increase owing to the release of inert ash components [16]. The H/C and O/C ratio of biochar also decreases with increase in temperature. Fixed carbon content of biochar increases with increase in temperature and time, which also leads to increased higher heating value [17]. On other hand, the organic structure and composition of feedstock also affects the reactivity of pyrolysis process [18].

Microwave-assisted pyrolysis (MAP) is one of the effective thermochemical conversions utilizing dielectric heating mechanism to produce biochar with better characteristics than conventional heating which has limitations associated to heat transfer and reduced energy efficiency. Thermochemical reactions in MAP occur at lower temperature compared

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to conventional pyrolysis owing to mechanism of volumetric heating and energy conversion technique rather than heat transfer [19, 20]. The biochar produced through microwave pyrolysis possesses relatively higher surface area and better porous characteristics [21, 22], higher carbon content, and calorific value [23, 24] compared to conventionally produced biochar. Mohamed et al. [25] reported that volatile releasing rate at low temperature is higher in microwave heating than conventional method and most of the minerals are retained in biochar surface which would be beneficial for sorption of contaminants and nutrient utilization for plants. Foong et al. [26] reported that microwave and solar pyrolysis are energy efficient pyrolytic technique compared to other advanced pyrolysis processes that are developed to reduce reaction temperature, enhancing product yield and quality, higher energy efficiency, and reducing production cost. Selvam and Paramasivan [27] has summarized the comparative studies on conventional and microwave assisted pyrolytic characteristics and concluded that biochar production through microwave heating is more carbon-negative than conventional process, and biochar possess better surface characteristics. Based on these perspectives, it could be inferred that microwave pyrolysis of biochar production is the promising technique in terms of quality and quantity.

However, the economic viability of MAP is still a concern. As estimated by International Biochar Initiative through a survey of 326 companies, the biochar market is incrementing yearly, whereas the companies commercializing the biochar often deploy conventional pyrolysis. Haeldermans et al. [24] has identified that conventional pyrolysis is more feasible than microwave pyrolysis; however, 20% price increase of biochar makes the MAP viable with increased carbon content of 5% and BET-specific surface area of 50 m^2 g^{-1} owing to improved quality. However, Lo et al. [28] has reported that energy return on investment through microwave pyrolysis is feasible in terms of energy and economy for a sustainable society. The production of superior quality of biochar with higher carbon content, cation exchange capacity, low contaminant content, and higher energy recovery is essential to make the process feasible [25, 26].

Machine learning (ML) algorithm is a computational method that processes the different input parameters in repetition and gets adapted to produce a desired outcome of higher accuracy from random datasets [29]. Utilization of machine learning aids in forecast prediction of biomass [30] and pyrolytic product characteristics using the datasets associated with the pyrolysis process and feedstock [31] that enable the readers to understand the correlation between process conditions and the products. The main limitation of machine learning algorithm is its black box nature which inhibits the model interpretability. Also, the quality of datasets and number of decision trees needs optimization to avoid overfitting and erroneous results for improving the performance of the model [32].

Machine learning prediction of biochar yield and its characteristics obtained through microwave pyrolysis paves the way to understand the factors influencing the yield and characteristics of biochar and also aids in designing the prototype for superior quality biochar production in large scale. Machine learning prediction of conventional pyrolytic biochar yield has been done by many authors [33–35] whereas the literatures predicting the microwave biochar yield along with its characteristics through machine learning models are sporadic. Narde and Remya [36] used quadratic model to predict the microwave biochar yield and reported that volatile matter, ash content, and temperature could be used as predictor variables to determine biochar yield with regression coefficient of 0.89. Huang et al. [37] has recently studied performance of different machine learning models for prediction of yield and HHV of char produced through direct, microwave, infrared and solar heating. Most of the studies on ML related to microwave pyrolysis have utilized one or more ML algorithms to predict the biochar yield encompassing few input variables. Also, none of the studies to the best of the authors' knowledge on ML have detailed the interactive influence of the input parameters on microwave biochar yield and its properties.

Thus, the present study utilized a comprehensive range of input data comprising of the feedstock characteristics (volatile matter, ash content, fixed carbon content, carbon, oxygen, hydrogen, nitrogen contents) and operating conditions of microwave pyrolysis (feedstock amount, microwave power, time, absorber) to predict the influence on yield and property (HHV) of biochar. Also, to avoid bias and erroneous interpretation of the predictions, the present research has considered 4 different supervised learning ML algorithms (Linear Regression (LR), eXtreme Gradient Boosting (XGB), Random Forest (RF), and Support Vector Machine (SVM)). Further, the correlation and influence of input variables and their impact on output targets have been detailed via analysis of SHAP (SHapley Additive exPlanations) dependence plots. Considering, limited amount of scientific literature available on ML of microwave pyrolysis, the study will surely contribute in making appropriate decision-making while controlling the process variables during the deployment of large-scale microwave pyrolysis units.

Materials and Methods

Data Collection

The literatures available on MAP have been searched using the keywords like "microwave pyrolysis", "biochar", and "char" using Boolean operators. A total of 240 datasets have been collected which include MAP of different feedstocks, under varying operating parameters. The selection of manuscript is carried out in such a way it covers all the essential parameters. The data was acquired from tables, figures extracted through Plot digitizer 2.6.9 in publications and corresponding supplementary materials. Since a few of the literatures have not reported either the proximate or ultimate composition, the missing entries of biomass composition alone have been imputed through mode values. The missing values in process parameters and outliers have been removed. The processed dataset has been subjected to machine learning algorithms like Linear Regression (LR), eXtreme Gradient Boosting (XGB), Random Forest (RF), Support Vector Machine (SVM) techniques using scikit python version 3.7.12. The model input parameters were a proximate composition of biomass which includes volatile matter (VM) (%), ash content (AC) (%), fixed carbon (FC) (%) contents, ultimate composition of biomass like carbon (C) (%), hydrogen (H) (%), oxygen (O) (%), nitrogen (N) (%), and process conditions like amount of feedstock (g), microwave power (W), time (min), and microwave absorber (categorical variable). The output includes biochar yield (%) and its HHV (MJ kg−1). Statistical data analysis with reference to mean, standard deviation, maximum and minimum value for all the features was performed.

Model Development

Machine learning algorithm models especially those based on supervised learning often use optimized, statistical and probabilistic methods to derive specific pattern of relation between the unstructured and complex datasets. Since the accuracy of prediction depends on the data as well as the estimation efficiency of the ML model, often the use of a single algorithm might provide biased and erroneous results leading to inappropriate decision-making. Therefore, the present research with the aim to predict the influence of operational conditions of microwave pyrolysis on biochar yield, utilized 4 different supervised ML models like LR, XGB, RF, and SVM. The present study selected the above-mentioned supervised training ML algorithms as also utilized in the study for predicting the pyrolytic gas yield and composition [38], higher heating value [30], and gasification reactions [32]. LR-based ML algorithm is simple and easy to implement with no need of feature scaling. SVM learning is an efficient algorithm utilized for classification and regression in a high-dimensional space and provides different results based on linear, polynomial, and radial/sigmoid kernel function. RF is an ensemble classification technique that fits several decision tree classifiers in parallel on different subset of data and uses average as an outcome, thus reducing overfitting issues, thereby increasing accuracy and control. XGB is a fast ML algorithm to handle large datasets that uses a more detailed approximation to perform regularization, minimize overfitting, improving model generation and performance. The study selected these algorithms as they were easy, simple and effective to implement on a complex dataset considering the diversity of factors impacting the microwave pyrolysis-based biochar. These models also had little impact of outliers with no overfitting of data, thereby provided better performance with less errors.

The datasets were randomly split into 3:1 ratio for training and testing group respectively and subjected to selected machine learning algorithms. These algorithms were used to train and optimize the prediction model for biochar yield and its HHV through scikit-learn python library. These non-linear and ensemble-based algorithms have been used by many authors for predicting the output target [38, 39]. In each prediction model, the hyperparameters involved were tuned for the dataset considered. In case of XGB model, learning rate which measures the upgradation of model weight in each run, maximum depth of tree and the ratio of samples from training dataset used in each update has been used as hyperparameters which formed the basis of forming decision trees. For RF algorithm, the number of tress (*n_tree*), maximum depth of tree, and randomness state act as hyperparameters based on which the *n_tree* bootstrap samples were randomly drawn from training data. At each split node denoting randomly selected feature, decision tree was built and average performance of all decision trees were counted. And for SVM, the accuracy of prediction is mainly related to epsilon, regularization parameter, and the kernel function. Hence, the modeling was tried with different kernel function like “linear”, “poly” (polynomial), and “rbf” (radial basis function). These functions aid to plot each point of data in n-dimensional space and search the hyper-plane which segregates the classes significantly [40]. These hyperparameters were tuned to strengthen the model to avoid overfitting.

Evaluation of Model Prediction Accuracy

The performances of developed models were evaluated based on the regression coefficient (R^2) and root mean square error (RMSE) for the training and testing data. These coefficient metrics indicate the two sides of an algorithm’s accuracy. R^2 explains the fitness of the model i.e., the efficiency which increases from 0 to 100% whereas RMSE gives an idea of how the model reflected the data mistakenly with the absolute perfection sets at 0. The calculation formulas of R^2 and RMSE were shown as the following in Eq. (1) and Eq. (2), respectively.

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left(Y_i^{exp} - Y_i^{pred}\right)^2}{\sum_{i=1}^{N}\left(Y_i^{exp} - Y_{avg}^{-exp}\right)^2} \tag{1}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(Y_i^{exp} - Y_i^{pred}\right)^2} \tag{2}$$

where, Y_i^{exp} and Y_i^{pred} are the experimental and predicted entries respectively and, Y_{avg}^{exp} is the average of the experimental entries. The model showing higher R^2 and lower RMSE was selected and used further for feature evaluation.

Evaluation of Feature Impact on Output Target

The evaluation of feature importance on target is carried out once the models were developed, performance predicted, and interpreted. Owing to the black box nature of the model, this is often a challenging task. In order to illustrate the effect of each input feature on output target, SHAP dependence plot has been used to represent the interaction of crucial factors on biochar yield and HHV. Each dataset will be plotted in dots for an input parameter range in X-axis and its SHAP value on Y-axis, and the relative importance of a feature could be determined [35]. Here in this study, tree SHAP has been used which is accurate and a fast method for predicting the contribution of each feature (either positive or negative) to the target. The combination of feature importance plot with SHAP dependence plot has been presented as summary plots. The input features were marked in y-axis on the basis of their influence, i.e., the most influential variable placed at top. SHAP values were placed in x-axis represented in level of significance from low to high. From these plots, the influential factors and their interactive effects could be interpreted to illustrate the process design for enhancing the biochar yield and its property.

Results and Discussion

Analysis of Input and Output Features of Microwave Biochar

Out of 240 datasets collected, the data points being missed and outliers for microwave pyrolysis process conditions have been removed. This leads to drastic reduction in datasets to 157 since few manuscripts didn't report entire conditions employed for microwave-assisted biochar production. The collected data contains the feedstock's proximate and ultimate composition, microwave pyrolysis conditions, biochar yield, and HHV. A descriptive analysis of input features and output targets derived from the compiled dataset has been presented in Tables 1 and 2 for yield and HHV, respectively. Different metrics like count, mean, standard deviation (std), minimum (min) and maximum (max) have been calculated. Count refers to total number of datasets considered for the study and mean indicates the average of dataset of each variable, and standard deviation refers to deviation from average value. These two indicators aid in understanding the distribution pattern of data. The minimum and maximum values indicate the range of the associated parameters.

The mean carbon and hydrogen content is found to be 42.05% and 5.77%, respectively, which was found to be comparable to that lignocellulosic biomass, algae, and other feedstock [41]. The effect of elemental composition is also an important factor since it affects the yield of pyrolysis

Table 1 Descriptive statistics of input features for microwave biochar yield

	Volatile	Fixed carbon	Ash	Carbon	Hydrogen	Nitrogen	Oxygen	Weight	Power	Time	Yield
count	157	157	157	157	157	157	157	157	157	157	157
mean	65.14	18.00	6.13	42.05	5.77	1.73	45.81	63.07	668.82	20.83	32.85
std	18.34	9.75	10.35	6.05	1.05	1.60	8.94	89.50	369.66	11.37	22.01
min	25.7	0.12	0.38	19.9	0	0	17.8	5	100	3	0.77
max	97	34	55.5	73.1	10.4	5.92	56.5	388	2310	60	95

Table 2 Descriptive statistics of input features for microwave biochar HHV

	Volatile	Fixed carbon	Ash	Carbon	Hydrogen	Nitrogen	Oxygen	Weight	Power	Time	HHV
count	67.00	67.00	67.00	67.00	67.00	67.00	67.00	67.00	67.00	67.00	67.00
mean	60.41	15.33	4.53	43.28	6.11	2.10	43.98	76.85	528.80	19.77	23.3
std	22.83	8.66	3.96	4.44	1.05	2.32	8.79	78.7	254.17	6.87	4.21
min	25.70	6.40	0.41	37.10	4.50	0.00	31.43	8.00	100.00	15.00	17.25
max	81.97	34.0	23.900	53.21	10.40	5.92	56.50	300	1000	40	33.3

products as also reported by Nzediegwu et al. [42]. The mean fixed carbon content and volatile matter are of 18% and 65.14%, respectively, and maximum of 34% fixed carbon containing biomass has been included in the study which indicates that alternative fuel with rich carbon could be produced from these types of biomass [43]. In case of microwave process conditions, the minimum weight of biomass used for the study has been observed to be 5 g and maximum amount was 388 g. Microwave power was observed to range between 100 and 2310 W with time-period varying from 3 to 60 min which indicates that all regime of pyrolysis conditions has been accounted for the study. Based on these input parameters considered, the yield of biochar produced through microwave pyrolysis ranged from 0.77 to 95%. The mean value of 32.85% biochar yield was observed with the mean value parameters of 63.07 g of feedstock subjecting to 668.82 W of microwave power for 20.83 min. The statistical result obtained for HHV is similar as that for yield, and the maximum HHV reported was of 33.3 MJ kg^{-1}. The mean value of HHV obtained was 23.3 MJ kg^{-1} with conditions of 76.85 g of feedstock weight subjecting to 528.80 W of microwave power for 19.77 min. The relation between the input features and output targets has been given in Pearson correlation coefficient matrix (Fig. 1). From the matrix, it could be inferred that fixed carbon, and total carbon contents are positively correlated with both biochar yield and HHV whereas microwave power is negatively correlated. However, in order to understand the in-depth effects of characteristics of feedstock and microwave pyrolytic conditions on biochar yield and HHV, high accurate prediction model was built using machine learning methods. In addition, relative importance of each factor and the interactions among input variables has been discussed in the subsequent sections.

Model Development and Hyperparameter Tuning

Different machine learning models like XGB, RF, SVM, and LR were developed using the dataset obtained to achieve higher regression coefficient (R^2) and lower root mean square error (RMSE). Initially by subjecting the original dataset without any imputation, low R^2 and higher RMSE were obtained through all methods employed. Then, the dataset with mode imputed values was subjected to algorithms to obtain a model that best predicts the output targets (Table 3). The scatter plot for experimental and predicted values of XGB model has been given in Fig. 2a–d. In case of XGB model, the number of estimators (n_estimators) [10 to 100], depth of tree (1 to 5) and randomness state (random_state) has been optimized. By increasing the number of estimators, it was observed that the value of R^2 was increased and RMSE was decreased. The maximum of 100 estimators was set to achieve a R^2 of 0.91 and RMSE of 6.47 from 0.78 of R^2 and 10.29 of RMSE executed with 10 estimators. Similarly, when increasing the randomness state starting with 1, it affects the R^2 positively and RMSE in negative manner. After increasing the random_state beyond 4, RMSE was observed to increase. Hence, random_state has been set to 4. By increasing the depth of tree, R^2 was observed to increase until 5 and after that, it decreased. Hence, the optimal hyperparameter was set with 100 estimators and maximum depth of tree as 5 and randomness state of 4 to achieve a R^2 of 0.91 and RMSE of 6.47 (Fig. 2c). The R^2 obtained was relatively higher than reported by Narde and Remya [15] who obtained R^2 of 0.89 using quadratic model using the biomass composition and process conditions as input features for microwave biochar yield prediction. The converse of observation was noted in RF algorithm compared to XGB model. An initial R^2 of 0.74

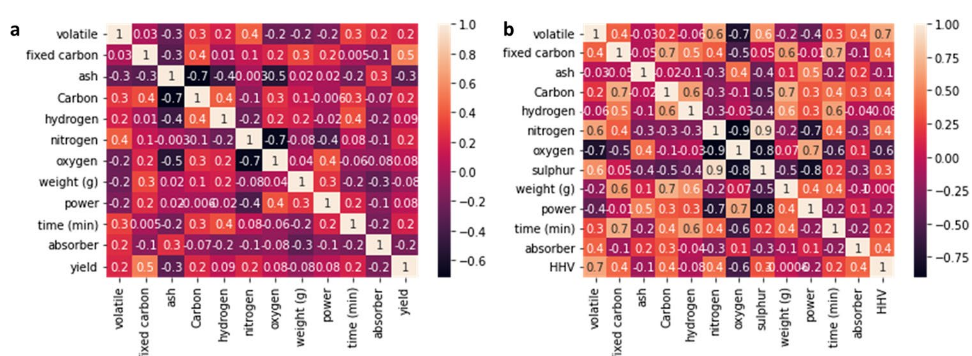

Fig. 1 Pearson correlation coefficient matrices for relationship between input and output parameters of (**a**) microwave derived biochar yield, and its (**b**) HHV

Table 3 Statistical interpretation of machine learning models in for microwave biochar yield and its HHV prediction

	Dataset	XGB R^2	XGB RMSE	RF R^2	RF RMSE	SVM R^2	SVM RMSE	LR R^2	LR RMSE
Without imputation (yield)	103	0.71	8.98	0.73	8.67	0.44	18.9	0.23	14.7
After imputation (yield)	157	0.91	6.47	0.89	7.03	0.69	12.6	0.21	21.5
After imputation (HHV)	67	0.89	1.04	0.89	1.5	0.49	2.75	0.63	2.5

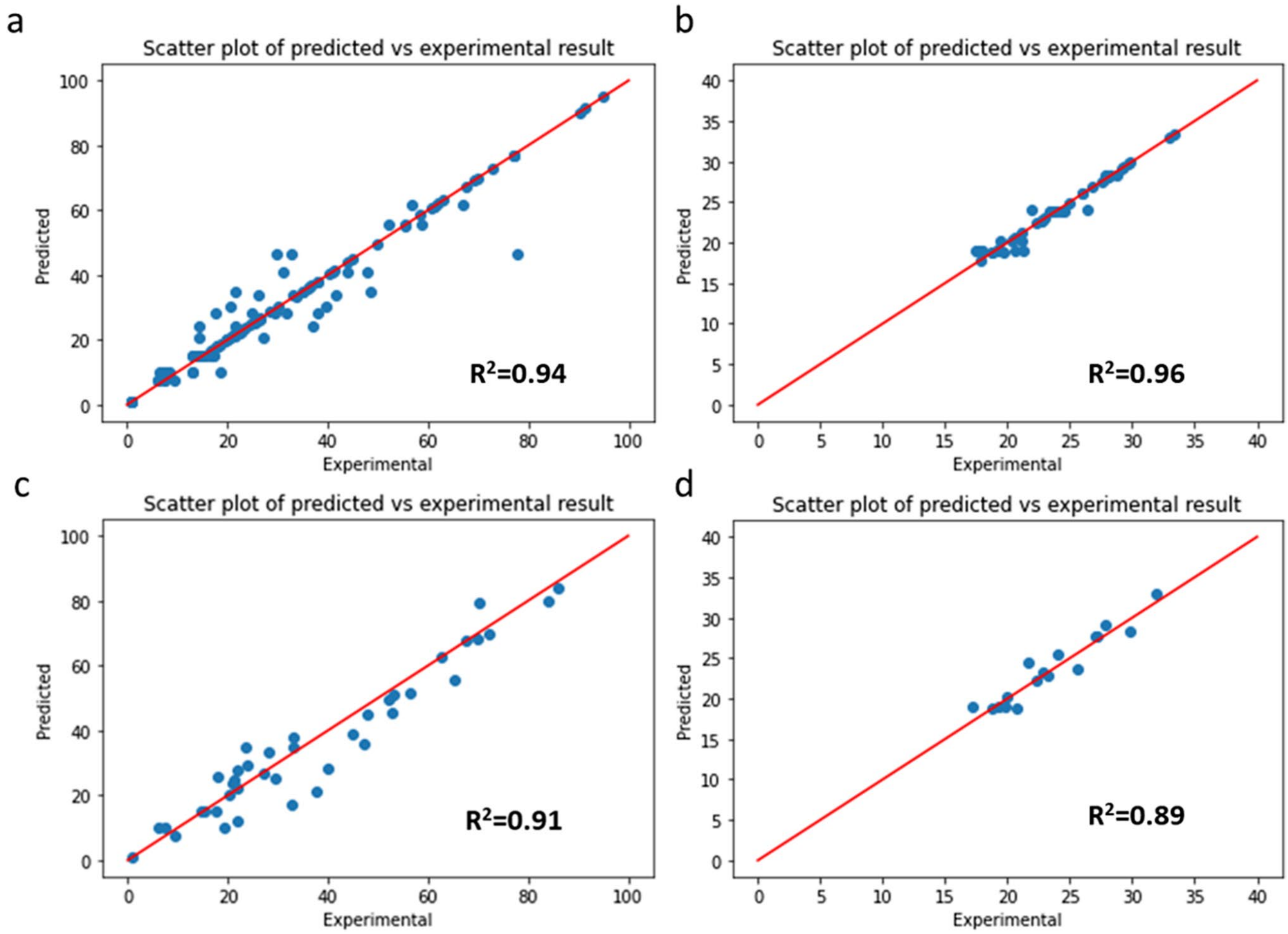

Fig. 2 Predicted vs experimental values of XGB model prediction on training dataset for microwave-derived (**a**) biochar yield (**b**) HHV and, testing dataset for microwave derived (**c**) biochar yield (**d**) HHV

and RMSE of 10.51 was obtained with 10 estimators, and it was observed to decrease further until n_estimators reached 50. After 50, both R^2 and RMSE were tending to increase and decrease in an insignificant manner and final R^2 and RMSE of 0.89 and 7.03, respectively, were obtained. In case of SVM, the hyperparameters optimized were of regularization parameter and epsilon value with linear kernel function. In case of linear kernel function, the RMSE values decreased until epsilon of 0.5, and then increased with the increase of epsilon, but showed no significant decrease in RMSE values when the regularization parameter was increased. Final R^2 and RMSE of 0.69 and 12.6, respectively were obtained with epsilon of 0.5 and regularization parameter of 4. In linear regression model, very low R^2 of 0.21 and RMSE of 21.5 were obtained.

In case of HHV, while subjecting the imputed dataset to XGB algorithm initially with 10 estimators, R^2 of 0.35 was obtained; however, with increase in number of estimators, R^2 increased up to 40 estimators and did not increase any further. However, the RMSE value decreased with continuous increase of estimators until 100. A similar trend was also observed while optimizing the maximum depth of tree. The optimized hyperparameter of 100 estimators with maximum depth of tree as 5 and randomness state of 5 resulted in R^2 of 0.89 and RMSE of 1.04 (Fig. 2d). With regard to RF algorithm, by increasing the number of trees, R^2 was observed to increase with decrease in RMSE; however, with increase in number of estimators from 10, R^2 was observed to decrease. With optimized hyperparameters of 10 estimators, maximum depth of tree as 10 and random state of 5, R^2 of 0.89 and RMSE of 1.5 were achieved. In case of LR and SVM algorithms, comparatively low R^2 of 0.49 and 0.63, respectively, and higher RMSE of 2.75 and 2.5, respectively, were obtained. From these observations, it could be inferred that XGB model showed higher R^2 and lower RMSE for both yield and HHV of biochar. Hence, this model was further used to predict the importance of the factor associated with the process and their interactive effects. Also, similar to the present study, Li et al. [41] also utilized R^2 and RMSE to evaluate the accuracy of ML models for prediction of hydrochar and pyrochar properties.

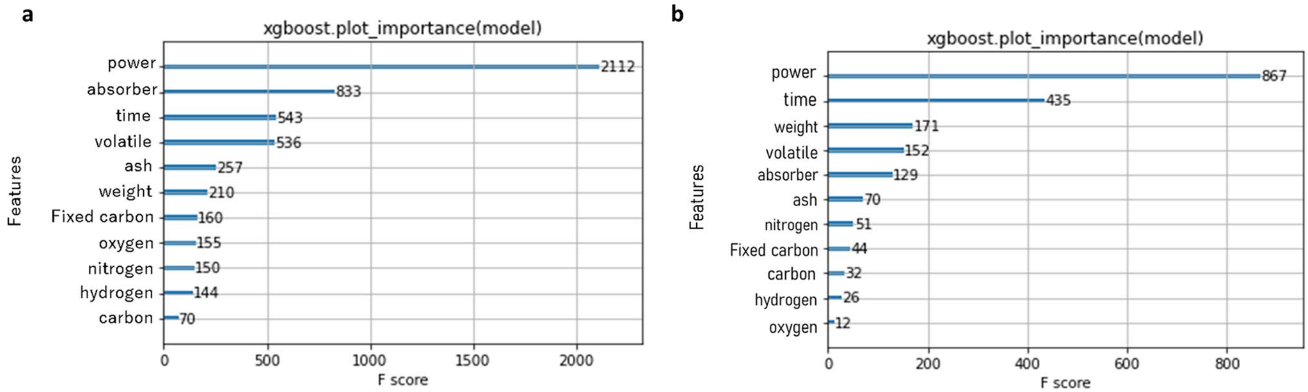

Fig. 3 Feature importance plot of all input parameters on MAP derived (**a**) biochar yield, and (**b**) HHV

Impact of Input Features on Biochar Yield

The importance of each input features on biochar yield has been given in Fig. 3a. As observed, microwave power is found to be most influential factor affecting the biochar yield and the results are also comparable to the inferences obtained by Abd et al. [44], who has reported that microwave power is a more significant parameter than microwave absorber and biomass particle size influencing the biochar yield. This could be corroborated from the F-score (measure of impact/importance of an input feature on output feature) of 2112 obtained in case of microwave power. Since most of the biomass materials have low dielectric property, the addition of microwave absorber (833) is more important in order to enhance the heating profile and in turn increase the biochar yield. Salema et al. [45] has observed that without

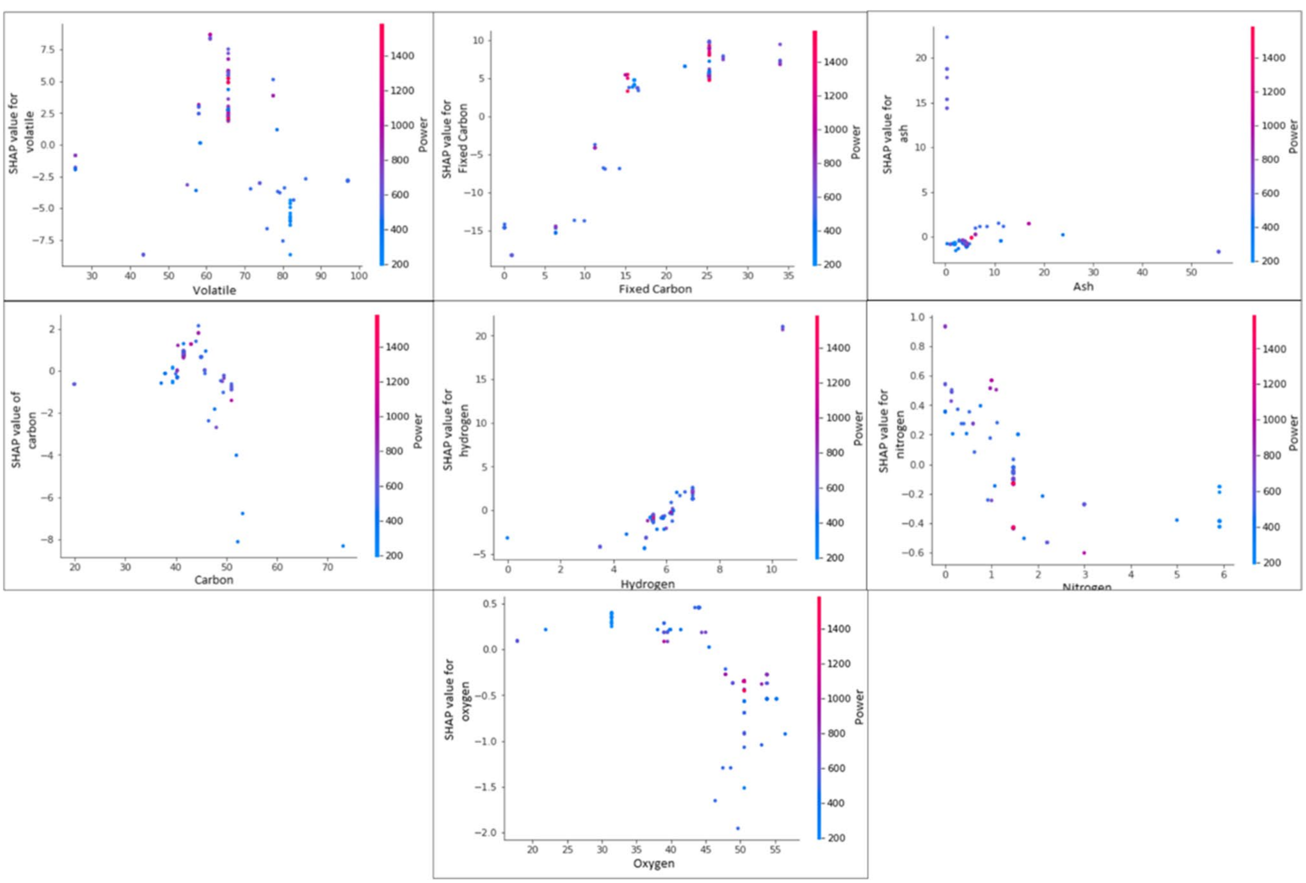

Fig. 4 SHAP Dependence Plots for the combined effect of power and biomass composition on MAP-derived biochar yield by XGB model

the presence of microwave absorber, no product formation happened until the microwave power of 450 W. However, after the addition of biochar as microwave absorber, the temperature profile was increased and resulted in product formation. Fodah et al. [46] reported that by using Na_2CO_3 catalyst, a significant effect was observed on maximum temperature during the biomass pyrolysis. However, increased temperature also decreases the yield of char as reported by Zhao et al. [47] and Zhang et al. [48]. The microwave time (543) is the next influential factor that influences the biochar yield. Since higher or lower retention time might change the product formation pathway, hence, optimal time is required to attain sufficient amount of biochar. As reported in literatures, higher retention time will lead to lower yield of biochar since it facilitates the devolatilization process rather than carbonization [49]. Low microwave power and long heating time result in increased biochar yield with higher carbon content owing to the improved carbonization, absence of secondary pyrolysis reactions, and thermal cracking [50]. After time, follows the feedstock amount (210) which is also significantly influencing the biochar yield. Since lignocellulosic biomass is of low dielectric materials, the sufficient amount of feedstock should be available for creating substantial power density that is required to initiate the pyrolysis reaction. The power density depends on the strength of electric field within the biomass and also depends on applied power and geometry of the reactor. Mathiarasu and Pugazhvadiv [51] reported that time required to achieve maximum temperature varied with the power density which also influences the yield of char. The elemental composition of biomass influences the product yield as reported by Gahane et al. [52] since the biomass composition is varied for different types of biomass, and it is dependent on temperature function to decompose during the pyrolysis reaction which in turn determines the product yield. The above-described influential factors predicted by ML determine the microwave biochar yield.

Impact of Input Features on Biochar HHV

In case of HHV, microwave power (867) is the most influencing parameter and then follows microwave time (435) and the biomass load (171) (Fig. 3b). HHV will be improved significantly with increasing the microwave power [46]. And one more added advantage of MAP is that similar HHV value could be obtained at lower temperature in comparison with conventional

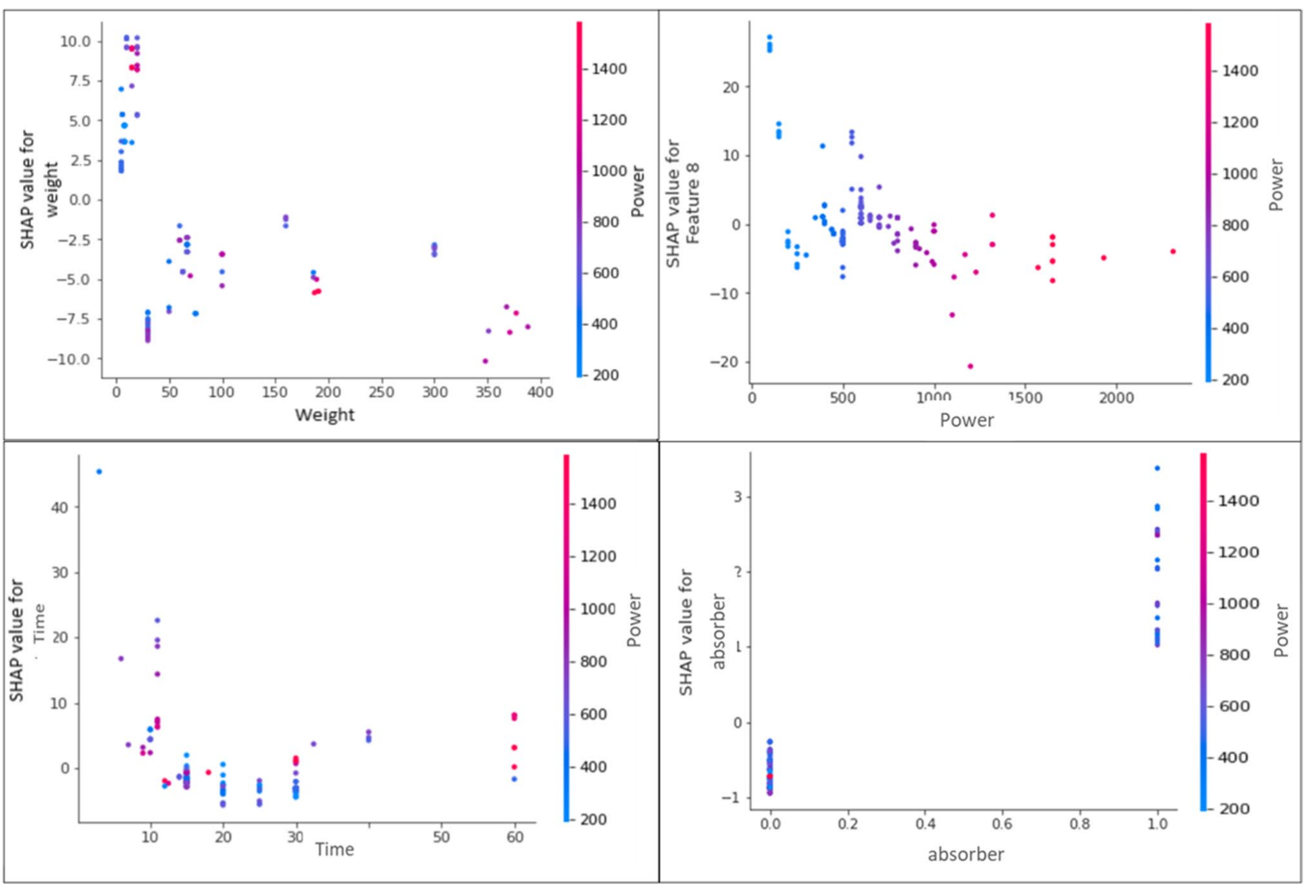

Fig. 5 SHAP Dependence Plots for the combined effect of power and microwave pyrolytic conditions on biochar yield by XGB model

pyrolysis [53]. Biochar obtained with higher HHV leads to higher energy recovery potential as mentioned by Zhouet al. [54]. Huang et al. [55] reported that microwave power levels of 150–200 W are sufficient to produce biochar with higher yield and HHV. The increased HHV of biochar formed during pyrolysis also seems to catalyze the pyrolytic reaction. Liew et al. [56] described that more amount of heat energy was produced at higher power owing to the interaction between microwave energy and its absorbing material. Retention time is also one of the factors that influences the HHV of biochar. With the increase in microwave heating time, the devolatilization reaction would be facilitated thereby increasing the heating value of the biochar [55]. The composition of biomass also influences the HHV of biochar. The biomass containing higher amount of hydrogen and oxygen reduces the energy value since the bond association between carbon and hydrogen is lower than carbon -carbon bond. Chen et al. [57] reported that HHV of microalgal biochar is lower than lignocellulosic biochar. This is due to the fact that microalgal biochar contained lesser carbon content than lignocellulosic biochar. The author also projected that supplementing the algal biomass with microwave absorber like activated carbon did not have any significant impact on HHV of char produced. This was also validated by Said et al. [58] who reported that higher carbon content present will lead to higher amount of HHV. Based on these perspectives, the importance of each feature on microwave biochar yield and HHV could be interpreted.

Analysis of Interactive Effect of Input Features

Interactive Effect of Input Features on Biochar Yield

The interactive effect of each factor on biochar yield could be interpreted through SHAP dependence plots. From the feature importance plots, microwave power is found to be the most influential factor and hence its interactive effect with other factors was analyzed through SHAP dependence plots (Figs. 4 and 5). It was seen that with an increase in fixed carbon content of biomass above 15%, the biochar yield increased since the data points having lower fixed carbon have negative SHAP values and are in blue color whereas the data points containing higher fixed carbon had positive SHAP values and are in pinkish-red color. Moderate power of 400 –600 W with higher fixed carbon

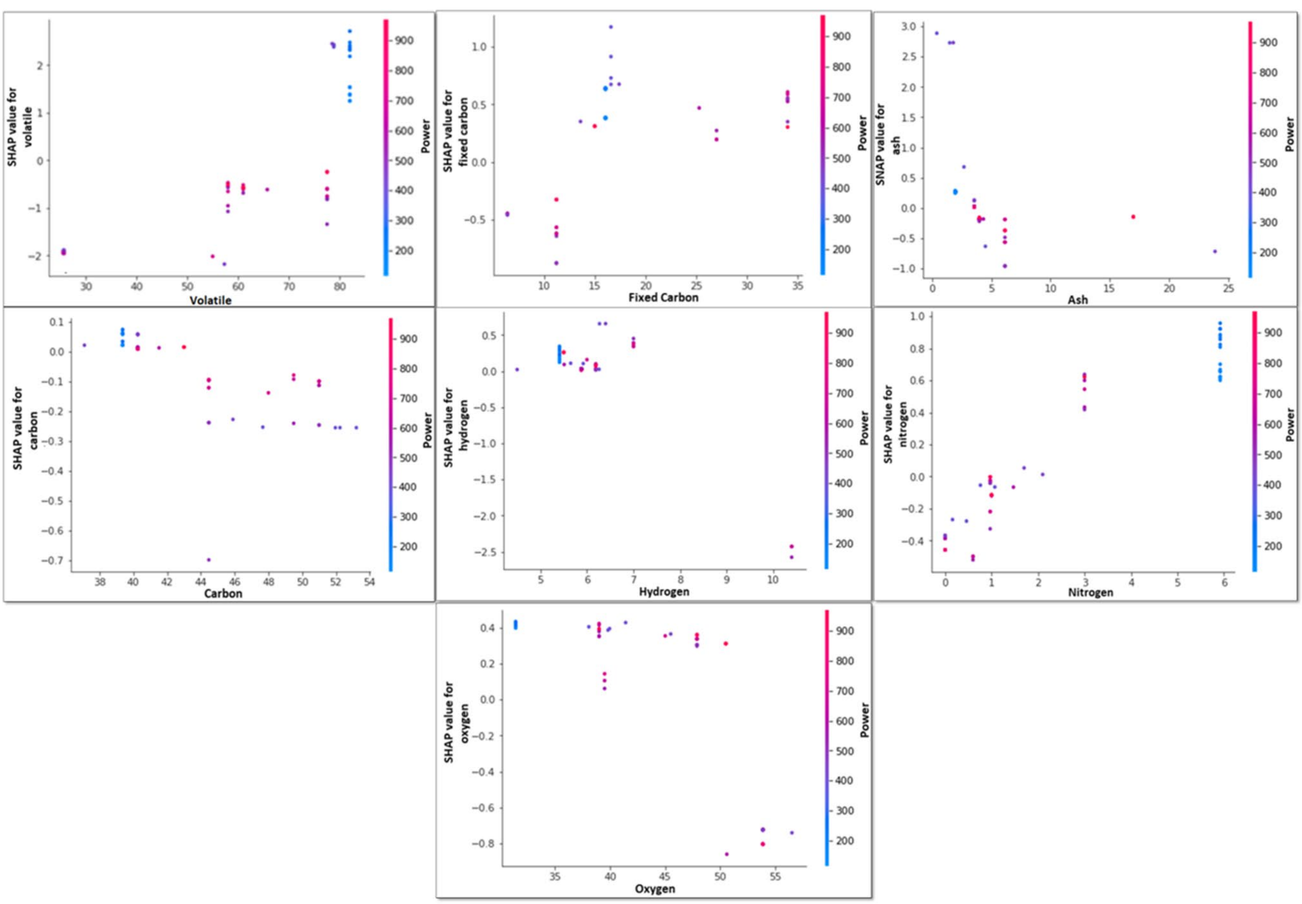

Fig. 6 SHAP Dependence Plots for the combined effect of power and biomass composition on microwave biochar HHV by XGB model

content results in higher yield of biochar and the similar trend is applicable to total carbon content. With regard to ash, the distribution of data points is converged in the initial region of 10–30% range, representing a positive correlation with the yield. Ash content of biomass consists of inorganic elements like sodium (Na), potassium (K), magnesium (Mg), and calcium (Ca) which catalyze the pyrolytic reactions and increases the biochar yield [11]. Hydrogen content of biomass consisted of all data points mostly near negative SHAP value irrespective of microwave power which indicate that the parameter is a less influential factor in biochar yield prediction. In perspective of process conditions, feedstock amount of more than 50 g resulted in negative SHAP irrespective of microwave power. Microwave time of 10–30 min with moderate power of 400 W consisted of positive SHAP value revealing the optimized conditions for higher yield of biochar. Sahoo and Remya (2020) [15] analyzed the interactive effect of microwave power and time, and reported higher yield (68%) of biochar under optimal conditions of 473 W and 19 min. With constant power and at increasing residence time, heat and mass transfer effect enhances, leading to more devolatilization resulting in lower yield of biochar [59]. The elementary composition of biomass also affects the biochar yield. Elementary oxygen and hydrogen content decreases with increase in microwave power owing to weaker bond cleavage. Hence, biomass containing lower oxygen and hydrogen content is favorable for higher yield of biochar production since degradation of biomass components will be lower at specific microwave power [42].

Interactive Effect of Input Features on Biochar HHV

The interactive effects of influential factors on microwave biochar HHV could be visualized through SHAP dependence plots (Figs. 6 and 7). HHV of biochar is observed to increase with increase in microwave power as also reported by Huang et al. [55]. Biomass containing fixed carbon content of higher than 15% and microwave power of higher than 500 W consists of higher HHV as visualized through positive SHAP values and the trend follows the same for total carbon content of biomass. Nzediegwu et al. [42] also

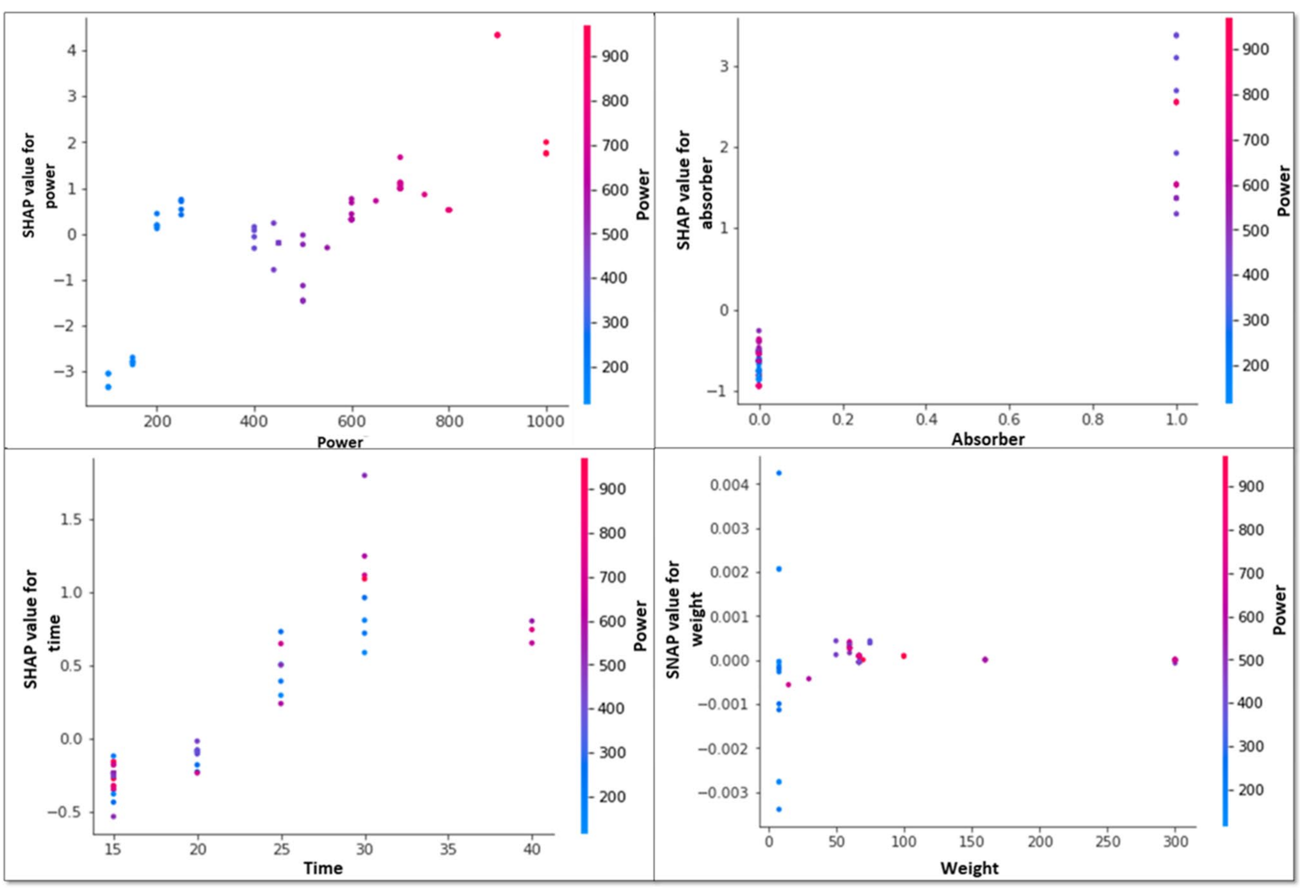

Fig. 7 SHAP Dependence Plots for the combined effect of power and microwave pyrolytic conditions on biochar HHV by XGB model

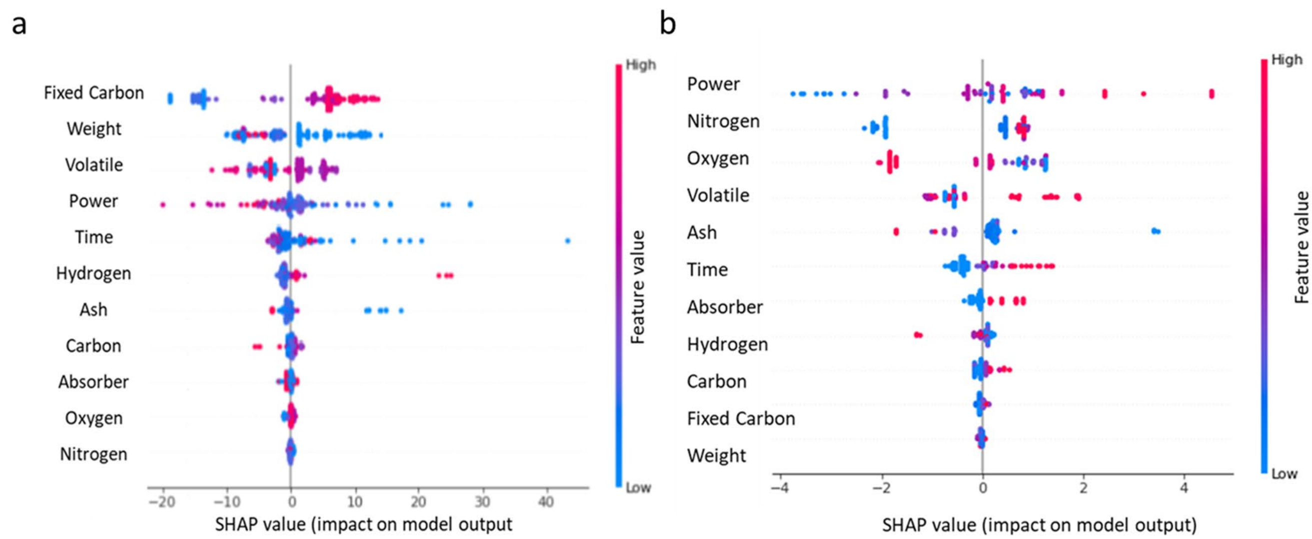

Fig. 8 Summary plot of different input parameters for (**a**) microwave biochar yield, (**b**) HHV of microwave biochar by XGB model

suggested that MAP of lignocellulosic biomass at 500 °C would result in higher carbon densification. Also, lower ash content and moderate microwave power of 500–600 W had positive SHAP values. This is in correlation with the study by Chaturvedi et al. (2021) reporting that wood-based biochar had higher HHV than lignocellulosic biochar owing to lesser amount of ash content. Higher nitrogen content biomass with low microwave power could be visualized in the region containing positive SHAP values. Microwave time range of above 20 min and moderate microwave power of 500 W resulted in positive SHAP values. Huang et al. [55] reported a similar trend of increasing HHV with higher residence time and microwave power. These entries indicate that microwave power of 500–600 W with retention time of 20–30 min will produce biochar with higher HHV from biomass containing higher carbon content.

The above-mentioned interpretations could be correlated well with the observations from summary plots (Fig. 8). From summary plot, it could be understood that the higher the fixed carbon content, microwave power and time, the higher will be the yield of biochar and HHV. Similarly, the significance of all input features based on their influential characteristics could also be understood through summary plot. These observations aid the researchers in process design for higher biochar production before spending huge time and money during scale-up.

Conclusion

This study presents the machine learning prediction of microwave biochar yield and its HHV. Out of 4 models executed, XGB algorithm performed best with higher correlation coefficient of 0.91 and root mean square error of 6.47 for biochar yield, and 0.89 and 1.04 for HHV, respectively, with optimized hyperparameters. The interactive effects between the input features and output target have been studied using SHAP dependence and summary plots. Moderate microwave power of around 500 W with lower reaction time of 20–30 min could be able to produce higher biochar yield and HHV using biomass containing higher carbon content. This study aids the researchers and primary stakeholders in designing the prototype for higher production of biochar with significant fuel property during field scale implementation.

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Author Contribution All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by [Mari Selvam S], [Balasubramanian P]. The first draft of the manuscript was written by [Mari Selvam S] and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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Data Availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Competing Interests The authors declare no competing interests.

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