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ORIGINAL ARTICLE

Rough set-based machine learning for prediction of biochar properties produced through microwave pyrolysis

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Abstract

Biochar, a carbon-rich compound, has a plethora of applications being explored in soil improvement, wastewater treatment, catalysis, and more. It is produced through pyrolysis process involving biomass carbonization in limited oxygen using conventional or microwave heating. However, the relationship between biomass characteristics, microwave pyrolysis operational variables, and the biochar properties is scarcely understood. The present study uses a data-driven rough set-based machine learning model to generate rules and classify biochar yield and its properties. The conditional attributes included biomass properties (volatile matter, fixed carbon, ash content, carbon, hydrogen, nitrogen, oxygen) and pyrolysis conditions (microwave power (P), residence time (t), biomass loading (W), microwave absorber dosage (MWA)) in the study. The biochar yield and its higher heating value (HHV) were taken as the decision attributes. The rules generated were validated using certainty and coverage values to achieve scientific accuracy. The cores of the dataset were found to be biomass load, microwave power, time, absorber dosage and microwave power, time, absorber dosage for predicting microwave-derived biochar yield, and its HHV respectively. The algorithm predicted that the biochar yield of class 1 (yield $\leq$ 20%) could be produced when feedstock fixed carbon content ranged between 15-35%, with nitrogen content less than 0.5% is processed under microwave power of 900–1200 W and it corresponds to HHV > 30 MJ kg^{-1}. The study would act as the baseline model for selecting optimal feedstock properties and pyrolysis conditions for achieving microwave biochar production and facilitating commercialization.

Keywords Biochar · Biomass · Higher heating value · Microwave pyrolysis · Rough set · Yield

Abbreviations

RSML	Rough set-based machine learning
SHAP	Shapely additive explanations
R^2	Regression co-efficient
HHV	Higher heating value
ROSE2	Rough sets data explorer
IND	Indiscernibility
Cer	Certainty
Cov	Coverage
VM	Volatile matter content of biomass
FC	Fixed carbon content of biomass
Ash	Ash content of biomass
C	Carbon content of biomass
H	Hydrogen content of biomass
O	Oxygen content of biomass
N	Nitrogen content of biomass
P	Microwave power
T	Microwave reaction time
W	Weight of biomass
MWA	Microwave absorber

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1 Introduction

Biomass is emerging as a promising renewable energy source in alternative to conventional fossil fuels causing environmental degradation. Being produced at 140 billion metric tonnes annually, it is widely used for various heating and value-added product applications through thermochemical and biological conversions [1]. Biochar is receiving attention from various stakeholders over the decade due to its physicochemical characteristics of large surface area with porous structure, mineral content, and functional groups. It leaves its footprints in energy utilization [2],

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conditioning of soil [3], wastewater treatment [4], and catalytic transformations [5, 6].

Of thermochemical conversions, pyrolysis is an established technique for biochar production which involves heating the biomass in a closed environment with limited air [7, 8]. It is an endothermic process requiring heat at temperatures of 300 to 900 °C to decompose biochemical components of biomass [9]. Advanced pyrolytic methods also came into existence which utilizes lower reaction conditions producing better yield and quality of products. The selective heating of biomass is enhanced; secondary reactions are reduced and process will be of higher energy efficiency and cost-effective. Microwave pyrolysis is one of the advanced forms of pyrolytic process where biomass is subjected to rapid, selective volumetric heating using microwave irradiation for shorter time compared to conventional process [10]. The dipole rotation and ionic conduction are the principle mechanisms for dielectric heating of biomass. Microwave pyrolysis has been widely used for different types of biomass involving agro-residues [11], forestry residues [12], plastic [13], sewage sludge [14], and so on. The biochar produced through microwave pyrolysis possesses higher surface area, porous structure, and carbon content compared to conventional process [15]. The characteristics and yield of biochar produced are mainly influenced by feedstock type and process conditions involving microwave power, retention time, and microwave absorber [16]. The trade-off between product attributes and the process conditions indicates the need of optimal parameters for prototype design and process scale-up.

Modeling of biomass pyrolysis aids in clear understanding and accurate predictions of product formation leading to higher process controllability. The development of a model that encloses the complex kinetics and thermodynamics of biomass pyrolysis in predicting the product distribution with higher accuracy is often carried out [17]. Machine learning (ML)-based approach is one of the viable techniques to study the interactive effects of process parameters on biochar yield and its quality since these models are accurate and flexible. ML models are being used to derive better solutions for interpreting the complexities in thermochemical treatment processes through forward and reverse optimization methods [18, 19]. Machine learning-based prediction of biochar yield and its composition has been carried out by Zhu et al. [20], Li et al. [21], and Leng et al. [22]. Shafizadeh et al. [23] have predicted the quality and quantity of hydrochar using biomass composition and process conditions using decision tree regression algorithm with $R^2 > 0.88$ and RMSE < 6.8. The effect of input factors on target attributes has been interpreted using contour diagrams, and the optimization was carried out using a genetic algorithm to be used for different applications.

Previous studies on machine learning-based understanding of microwave pyrolysis have been documented by different research groups. Recent study by Yang et al. [24] has predicted the pyrolytic product yield and its composition produced under microwave irradiation using 14 descriptors comprising of feedstock type and reaction conditions. The authors observed that gradient boosting regressor gave better performance with $R^2 > 0.822$. The developed model has also been interpreted using SHAP plots with an understanding of the importance of features on output and reported that microwave power, operating temperature, and time contributed more to decision prediction. Narde and Remya [25] have utilized quadratic regression model with R^2 of 0.894 for the prediction of microwave-derived biochar yield and validated with laboratory experimental results. Several research groups like Potnuri et al. [26] and Terapalli et al. [27] had analyzed the design of experiments with machine learning model to understand the influence of pyrolytic factors on product yields. For instance, research group of Potnuri et al. [26] has analyzed the effect of pre-treatment of sawdust for microwave-assisted pyrolysis using KOH catalyst and graphite absorber through polynomial-based machine learning regression model. The product yield and the energy requirement have been evaluated by varying catalyst loading, pretreatment temperature, and found to be similar with experimental values. Huang et al. [28] have studied the effect of different heating sources on char yield and its higher heating value (HHV) using five different machine learning models where gradient boosting algorithm gave better prediction performance. A comprehensive summary of recently published machine learning studies related to microwave pyrolysis for the prediction of biochar properties is tabulated in Table 1.

Despite of growing interest in machine learning-based analysis of microwave pyrolysis of biomass, the recommendations for operating parameters and biomass type for specific biochar yield and its properties have not been highlighted yet so far. Furthermore, the current machine learning algorithms (like random forest, extreme gradient boast, and support vector machine) possess some serious disadvantages like high complex, bias, overfitting, and lack of transparency. A rule-based prediction model is required to drive the production of biochar with desired characteristics. Rough set-based machine learning (RSML) is a rule-based algorithm that works on *if–then* rules to classify the attributes for decision prediction (Fig. 1). Rough sets theory (RST) was first introduced by Pawlak as an extension of set theory, which is a mathematical approach to overcome vagueness, imprecision, inconsistencies, and uncertainties in information and knowledge. Chong et al. [30] have carried out RSML-based prediction of parameters for pH and HHV of bio-oil where the authors listed validated rules comprising the range of proximate and ultimate composition of biomass and temperature. Ang et al. [31] and Tang et al. [32] have developed predictive model for analyzing biochar surface properties and energy potential respectively

Table 1 Features of published machine learning studies related to microwave pyrolysis for prediction of biochar yield and properties

Biomass	Input features	Output targets	Models used	Training and testing method	Evaluation metrics			Inference	Reference
					Best model	R^2	RMSE		
Biomass feedstock	Elemental composition; proximate content; reaction temperature, time; percentage, dielectric constant, and dielectric loss factor of microwave absorber	Syngas yield H_2, CO, CO_2, CH_4 Bio-oil yield Biochar yield H/C ratio H/N ratio O/C ratio Calorific value	Support vector regressor (SVR), Random Forest Regressor (RFR), and Gradient Boost Regressor (GBR)	*k*-fold resampling method	GBR	0.908 0.963, 0.944, 0.882, 0.849 0.906 0.857 0.980 0.823 0.986 0.985	6.177 3.462, 5.846 6.248, 3.984 4.287 4.714 0.056 12.381 0.132 1.340	GBR model showed better prediction performance in the quantity and quality of pyrolysis products	[24]
Polystyrene	Mass of polystyrene, catalyst (KOH) amount	Oil, gas yield Char yield Pyrolysis time Heating rate SME SMP MEC CHL	Support vector machine (SVM)	Data set is divided into training and testing, leave-one-out method was used to cross-validate the model	SVM	1.00, 1.00 0.99 0.99 0.99 0.98 0.99 0.99 0.88		The experimental values were closely replicated by the developed model	[27]
Biomass, solid waste, plastic, tires	Feedstock type, size, heating source, heating rate, final temperature, dwelling time	Ln (char yield) HHV	Linear Regression (LR), Polynomial Regressions (PR), *k*-Nearest Neighbor (kNN), Artificial Neural Networks (ANN), and Gradient Boosting (GB)	Training — 70%; validation — 30%	GB		0.186 (train) 0.249 (valid) 1.186 (train) 2.345 (valid)	Gradient boosting model is the best to estimate Ln (char yield) and HHV with high accuracy compared to other models used in the study	[28]
Agricultural biomass	Percentage of C, H, N, S, O, proximate characteristics of feedstock like percentage of VM, AC, and FC, and process parameters included total reaction time, temperature, and microwave power	Biochar yield	Linear Rregression (LR), Interactive Regression (IR), and Quadratic Regression (QR) were performed	80% training data and 20% testing data	QR	0.913		Quadratic regression was the best fit model compared to others VM, AC, *t*, *T*, and *P* had high variance and may be used as predictor variables	[25]

Table 1 (continued)

Biomass	Input features	Output targets	Models used	Training and testing method	Evaluation metrics			Inference	Reference
					Best model	R^2	RMSE		
Biomass, plastics	Elemental analysis, proximate analysis, blending ratio, heating rate, pyrolysis temperature, pyrolysis time, microwave power, name of catalyst	Bio-oil yield, biochar yield, biogas yield	Support vector machine (SVM)	155 data samples Leave-one-out (LOO) cross-validation	SVM	0.96 0.93 0.91	3.58 4.06 4.96	Considering a broader range of input features leads to better prediction performance for all product yields One-way and two-way partial dependence plots were used to analyze the impact of factors on product yield	[29]

SME, specific microwave energy; *SMP*, specific microwave power; *MEC*, microwave energy conversion; *CHL*, conductive heat losses

using rough sets; however, the heating source has not been defined. The prediction rules or set of recommendations for microwave pyrolysis of biomass for biochar production and obtaining desired physicochemical characteristics have not been addressed yet. In this study, RSML-based analysis of biomass composition involving proximate and ultimate content, process conditions of microwave pyrolysis involving microwave power, amount of feedstock, retention time, and percentage of microwave absorber used has been taken into account to predict the biochar yield and higher heating value. The statistical performance of the rules has been observed through its accuracy, coverage, and strength after validation. The generated rules provide a research framework for future researchers and other stakeholders to design the microwave pyrolysis with optimal parameters for desired yield and features of biochar.

2 Methodology

2.1 Data collection

The data on microwave pyrolysis of different biomass has been collected from the previously published literature. The data comprises feedstock composition of volatile matter, fixed carbon, ash content, and ultimate composition including carbon, hydrogen, oxygen, and nitrogen. The second set of inputs include microwave pyrolysis process conditions consisting of microwave power, biomass load, retention time, and microwave absorber (%). These data sets constitute the conditional attributes; on the other hand, the biochar yield and its higher heating value were regarded as the decision attributes. Total dataset of 212 and 113 has been collected comprising of various lignocellulosic, woody, and other biomass and a wide range of process conditions for prediction of microwave-derived biochar's yield and HHV, respectively (Table S1). The distribution of data under each attribute was plotted as violin plots using the seaborn package in python. The violin plots illustrate the distribution of data through box-plot and emergence of peaks through kernel density distribution for the input and output features [33]. The mean of carbon, hydrogen, nitrogen, and oxygen contents for abovementioned feedstock was estimated to be 43.05%, 5.85%, 1.83%, and 44.60% respectively. The means of volatile matter, fixed carbon, and ash content were found to be 68.66%, 15.32%, and 6.02% respectively.

2.2 Development of rough set machine learning model

The rough set-based model relies on specific assumptions, including the discretization or categorization of dataset

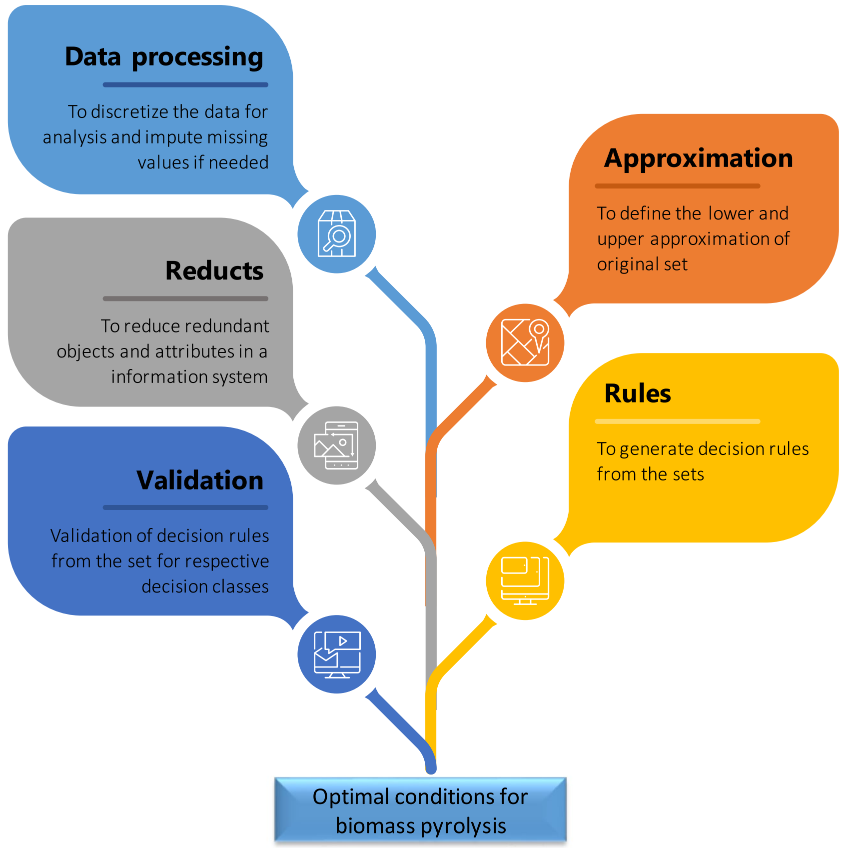

Fig. 1 Schematic flowchart of steps followed in rough set analysis

attributes, conditional independence, data completeness, and the presence of an indiscernibility relation. The model is used primarily for classification tasks rather than regression or continuous prediction. It can identify the patterns and rules in data; however, there exists a trade-off between the interpretability and accuracy of rules. The inflexibility of varying data split ratio and hyperparameter tuning also affect the model efficiency.

Subsequent with data collection, the objects of the conditional attributes were arranged into a form of information table with classified decision attributes based on literary references. The dataset of similar feedstocks has been grouped together and classified into different classes as shown in Table S2. The categorization of decision attribute is based on Tang et al. [32] and it has been shown in Table 2. The information table is represented as $S = (U, A)$ where $U = \{x_1, x_2, \ldots x_n\}$ is a universal set of non-empty finite objects and $A = \{a_1, a_2, \ldots a_n\}$ is non-empty finite set of attributes where a: $U \rightarrow V_a$ and $a \in A$. The columns and rows of the information table depict the biomass properties with process conditions (conditional attributes), biochar yield, HHV (decision attributes), and the behavior of biomass in corresponding conditions respectively. RSML algorithm could predict the decision rules based on training data where it explicates the class of output provided the set of conditional attributes are satisfied. The rough set-based machine learning model uses entire data set for training and the validation was done by internal sampling through *k*-fold validation method.

Table 2 Categorization of decision attribute of microwave-derived biochar yield and HHV into different classes

Decision attributes	Values	Class
Yield (%)	≤ 20	1
	$20 < \text{yield} \leq 30$	2
	$30 < \text{yield} \leq 40$	3
	$40 < \text{yield} \leq 60$	4
	> 60	5
HHV (MJ kg^{-1})	HHV ≤ 15	1
	$15 < \text{HHV} \leq 20$	2
	$20 < \text{HHV} \leq 25$	3
	$25 < \text{HHV} \leq 30$	4
	HHV > 30	5

Once the information table is discretized, approximation, reduction, and rule generation were carried out in an open source ROSE2 software [33]. The reduction of set is performed based on indiscernibility (IND) of objects which depicts the relation between two or more objects with dissimilar target conditional attributes (C1, C2, C3). The main purpose of this step is to negate the attributes which have no effects on decision and to keep the influencing conditional attributes. By defining R ({C1, C2, C3}) as the family of equivalence relation, the equation of indiscernibility of object B1 to B6 is presented in Eq. (1).

$$\mathrm{IND(R)} = \{\mathrm{B1, B5}\}, \{\mathrm{B2, B3}\}, \{\mathrm{B4}\}, \{\mathrm{B6}\} \tag{1}$$

Furthermore, conditional attributes can also be distributed into dispensable and indispensable attributes by implementing the object's indiscernibility concept. The indiscernibility of attributes C2 and C3, C1 and C3, and C1 and C2 are shown in Eqs. (2) to (4).

$$\begin{aligned}\mathrm{IND(R} - \{\mathrm{C1}\}) &= \mathrm{IND}(\{\mathrm{C2, C3}\}) \\ &= \{\mathrm{B1, B5}\}, \{\mathrm{B2, B3}\}, \{\mathrm{B4}\}, \{\mathrm{B6}\} = \mathrm{IND(R)}\end{aligned} \tag{2}$$

$$\begin{aligned}\mathrm{IND(R} - \{\mathrm{C2}\}) &= \mathrm{IND}(\{\mathrm{C1, C3}\}) \\ &= \{\mathrm{B1, B2, B3, B5}\}, \{\mathrm{B4}\}, \{\mathrm{B6}\} \neq \mathrm{IND(R)}\end{aligned} \tag{3}$$

$$\begin{aligned}\mathrm{IND(R} - \{\mathrm{C3}\}) &= \mathrm{IND}(\{\mathrm{C1, C2}\}) \\ &= \{\mathrm{B1, B5}\}, \{\mathrm{B2, B3}\}, \{\mathrm{B4}\}, \{\mathrm{B6}\} = \mathrm{IND(R)}\end{aligned} \tag{4}$$

From the above illustrations, it could be interpreted that attributes C1, C3 are dispensable and C2 is indispensable. Both the indiscernibility of attributes set {C1, C2} and attributes set {C3, C2} were equivalent to the indiscernibility relation of R, IND (R). This reveals that the attributes C1 and C3 are dispensable indicating that removing these attributes does not affect the set. The dependency between the two pairs is found to be independent with each other since IND ({C1, C2}) ≠ IND ({C1}) and IND ({C2}) and hence, {C1, C2} is called as reduct and similarly, {C3, C2} is another reduct of the set.

2.3 Validation of rules obtained through rough set-based machine learning

The generated rules through RSML might not be deterministic for few instances and hence, the evaluation metrics like coverage, certainty, and strength are used to predict its performance. The strength of a rule is described as adherence of objects of set for a specific rule (supp_x (C, D)) over total number of objects (card (U)) (Eq. 5). The certainty of rule (cer_x) is defined by its probabilistic relation of fitting of objects for a set of characteristics that are classified into decision class (Eq. 6). Rule coverage (cov_x) tells the number of objects used for a classification for specific class supp_x (C, D) over the total number of objects for the same decision class card $(D(x))$.

$$\mathrm{Strength} = \frac{\mathrm{supp}x(C, D)}{\mathrm{card}(U)} \tag{5}$$

$$\mathrm{Certainty} = \frac{\mathrm{supp}x(C, D)}{\mathrm{card}(C(x))} \tag{6}$$

$$\mathrm{Coverage} = \frac{\mathrm{supp}x(C, D)}{\mathrm{card}(D(x))} \tag{7}$$

The rules were then validated by using dataset and the performance of the rules was assessed by the above-mentioned metrics (Eqs. 5, 6, and 7). The rules of higher certainty (>60%) and higher coverage have been selected for interpretation and rules having lower coverage are given in supplementary section. In addition to that, scientific coherency of the model has also been considered to evaluate the logical consistency, interpretability, and meaningfulness of the rules generated by rough set-based model. This validation method focuses on ensuring that the extracted rules accurately represent the underlying patterns in the data and align with domain knowledge and expectations. The schematic representation of the methodology followed is given in Fig. 2.

2.4 Validation of model

The validation of trained model was done using *k*-fold cross-validation technique, since it is one of the simple and comprehensible cross-validation methods. The entire dataset will be divided randomly and splited into *k* groups ($k = 10$), where in each iteration, one *k* group will act as test set and rest of the groups as training sets. The trained model is being validated by passing the test and training sets on each iteration and the efficiency of the model in classifying each class of data is analyzed through confusion matrix. The confusion matrix is a $N \times N$ 2-dimensional matrix, where N is the number of target classes, which can provide interpretable results of the model validation. The data of each which were predicted accurately will be placed on the diagonal while the mispredicted data will be found on the either side of the diagonal, providing a detailed overview of the model performance. The higher the values in the diagonal represents better accuracy while the off-diagonal elements indicate classification errors. Furthermore, the accuracy, precision, recall, and F1 scores were calculated from the confusion matrix using the following Eq. 8–Eq. 11:

$$\mathrm{Accuracy} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}} \tag{8}$$

$$\mathrm{Precision} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}} \tag{9}$$

$$\mathrm{Recall} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} \tag{10}$$

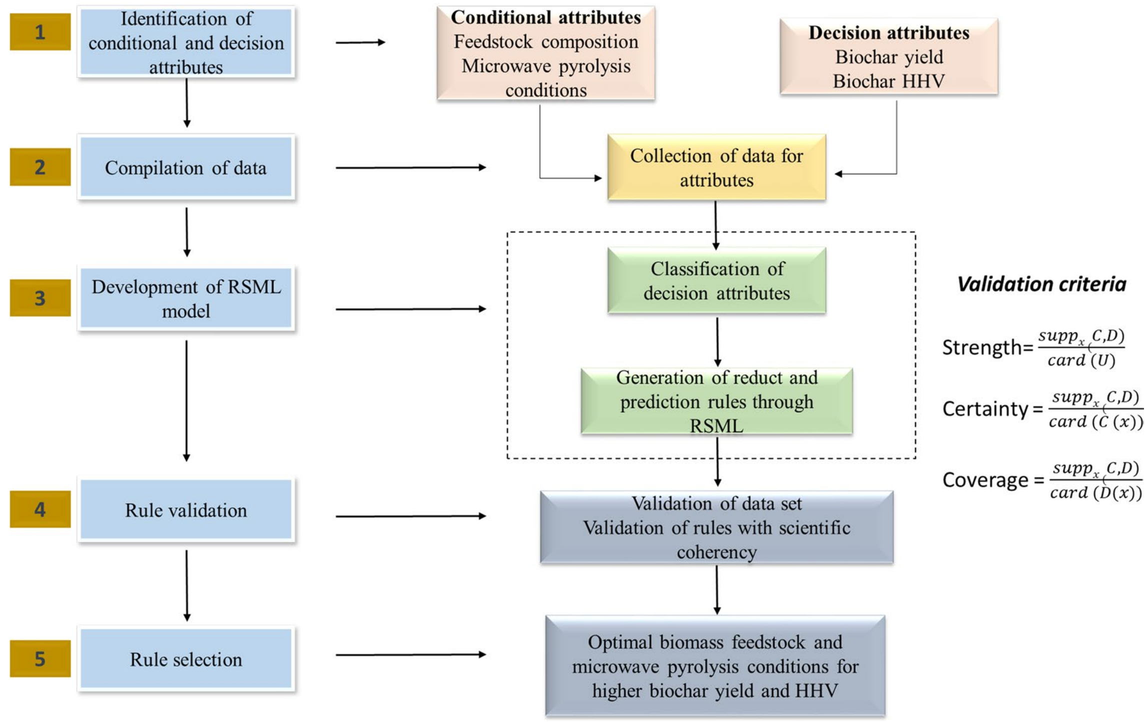

Fig. 2 Methodology followed in rough set analysis for rule induction for decision attributes

$$\text{F1score} = 2 * \frac{\text{Precision} * \text{Recall}}{\text{Precision} + \text{Recall}} \tag{11}$$

where TP, TN, FP, and FN represent true positive, true negative, false positive, and false negative respectively.

3 Results and discussion

3.1 Analysis of data features for prediction of yield and higher heating value of microwave-derived biochar

The violin plots for the dataset considered for predicting microwave-produced biochar's yield and HHV are described in Figs. 3 and 4 respectively. From the plot, it could be inferred that the proximate and ultimate composition of biomass exhibits a wide range indicating the higher divergence of feedstock resource and its composition. This includes categories such as "woody," "agro-residues," "lignocellulose," "biosolids," and "others" (includes algae, paper waste). All variables were concerted around the median with data range including volatile matter (25.70–97%), fixed carbon (0.12–34.10%), ash content (0.23–55.50%), carbon content (19.90–75.13%), hydrogen content (2.36–11.07%), oxygen content (0.60–56.50%), nitrogen content (~0–10.92%) similar to Zhu et al. [20] and Li et al. [21], weight (4–3500 g), power (60–3000 W), time (3–120 min), microwave absorber (0–116%). The mean value of these diverse datasets offers a valuable opportunity to develop a rough set-based prediction rules that can generalize well [26]. A similar trend of variable ranges was also observed with the datasets that has been taken for analyzing the prediction rules for HHV of microwave-derived biochar (Fig. 4).

3.2 Assessment of cores and reducts

As observed from software analysis of ROSE2, there were 11 and 12 reducts comprising of parameters involving biomass composition and process conditions in different combination sets for predicting the rule for microwave-derived biochar's yield and HHV, respectively. The obtained reducts and cores are listed in Table 3. The cores of the set include mainly the process parameters of microwave pyrolysis of biomass involving feedstock weight, microwave power, retention time, and percentage of microwave absorber; however, the feedstock weight has not been accounted in the case of HHV of microwave-produced biochar. These findings are well relatable with the study carried out by Yang et al. [24] where the gradient boosting regressor-based prediction

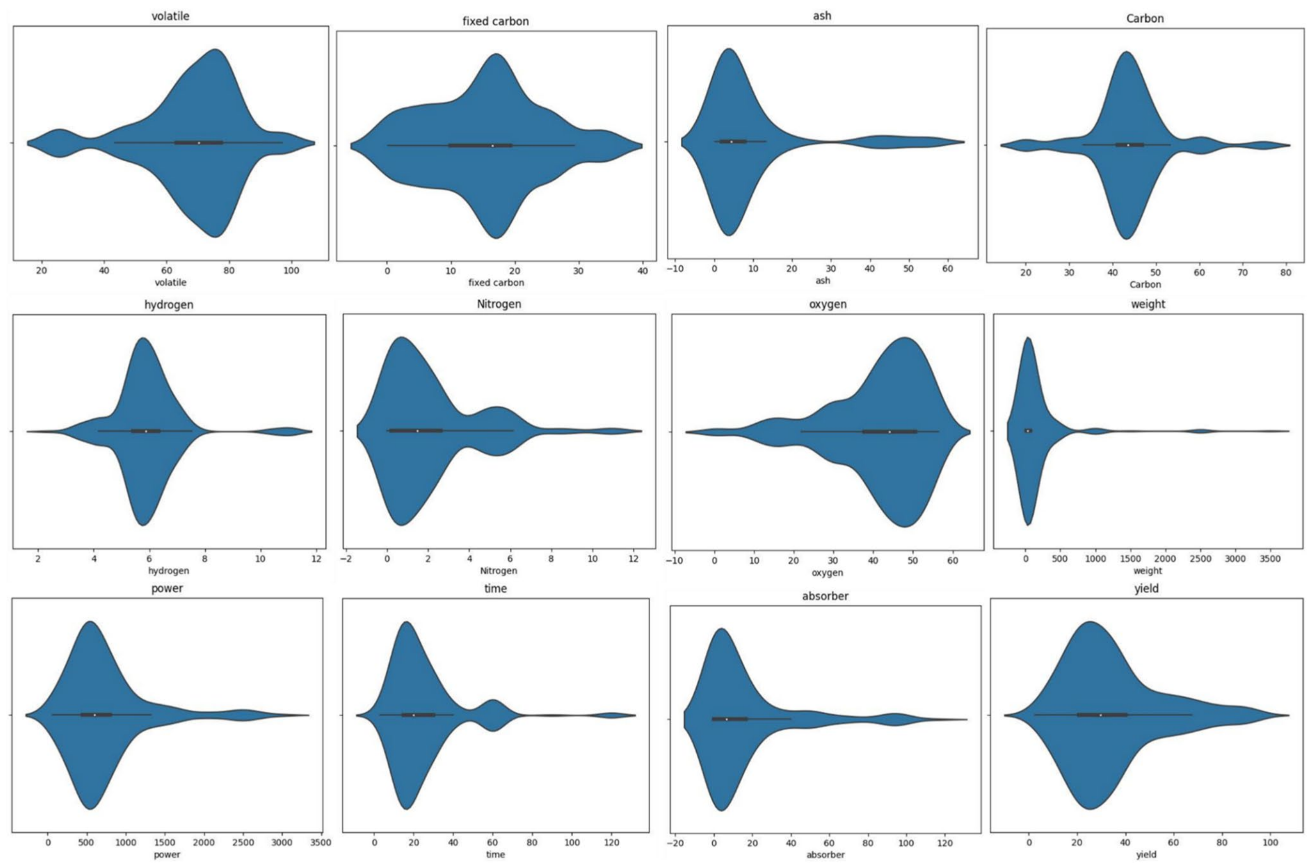

Fig. 3 Violin plot for the conditional and decision attributes considered for analyzing the microwave-derived biochar yield (*volatile — volatile matter, fixed carbon — fixed carbon content, ash — ash content, carbon — carbon content, hydrogen — hydrogen content, oxygen — oxygen content, nitrogen — nitrogen content, weight — weight of feedstock, power — microwave power, time — retention time, absorber — microwave absorber percentage used, yield — MAP-derived biochar's yield)

revealed through SHAP plots that microwave power, operating temperature, and reaction time exhibited significant contribution in determining the microwave pyrolysis of biomass. Huang et al. [28] also reported that process temperature is found to be most influencing parameter for predicting the natural logarithm of char yield of biomass under the influence of different heating sources with its process conditions determined through linear, polynomial, and other machine learning models. From these observations, it could be interpreted that determination of influencing parameters through rule-based models relies on estimating the relationship between the attributes and the target whereas it is also consistent with the domain knowledge.

3.3 Generation and validation of rules

The rules for the decision attribute biochar yield derived through microwave pyrolysis have been selected and validated from the ROSE2 software based on domain knowledge and statistics metrics. A total of 73 rules have been generated from 212 datasets, where, the selected rules of 9 rules contribute to class 1, 24 rules constitute class 2, 17 rules describe class 3, 9 rules for class 4, and 7 rules for class 5. The number of rules generated for each class is non-linear and independent with each other and it is merely dependent on input objects. The selected rules with respect to domain knowledge and scientific coherent for prediction of microwave-derived biochar yield are listed in Table 4, where it could be interpreted that rule number 5 corresponding to reduct 9 for class 1 is (Biomass = woody) & ($15 \leq$ FC < 20) & (N < 0.5) & ($1200 < P \leq 2000$). In other words, woody biomass containing fixed carbon content greater than or equal to 15% but less than 20% and microwave power of greater than 1200 W but less than 2000 W leads to production of class 1 biochar (yield $\leq$ 20%) [34]. The coverage and certainty of the rule are 3.17% and 100% respectively. The strength and coverage of the rules for prediction of yield and HHV of microwave-derived biochar are given in Fig. 5. The similar range of values of strength and coverage for the rules have also been reported by Tang et al. [32].

It could be noted that with increase in classes of biochar yield, the microwave power required is decreasing which

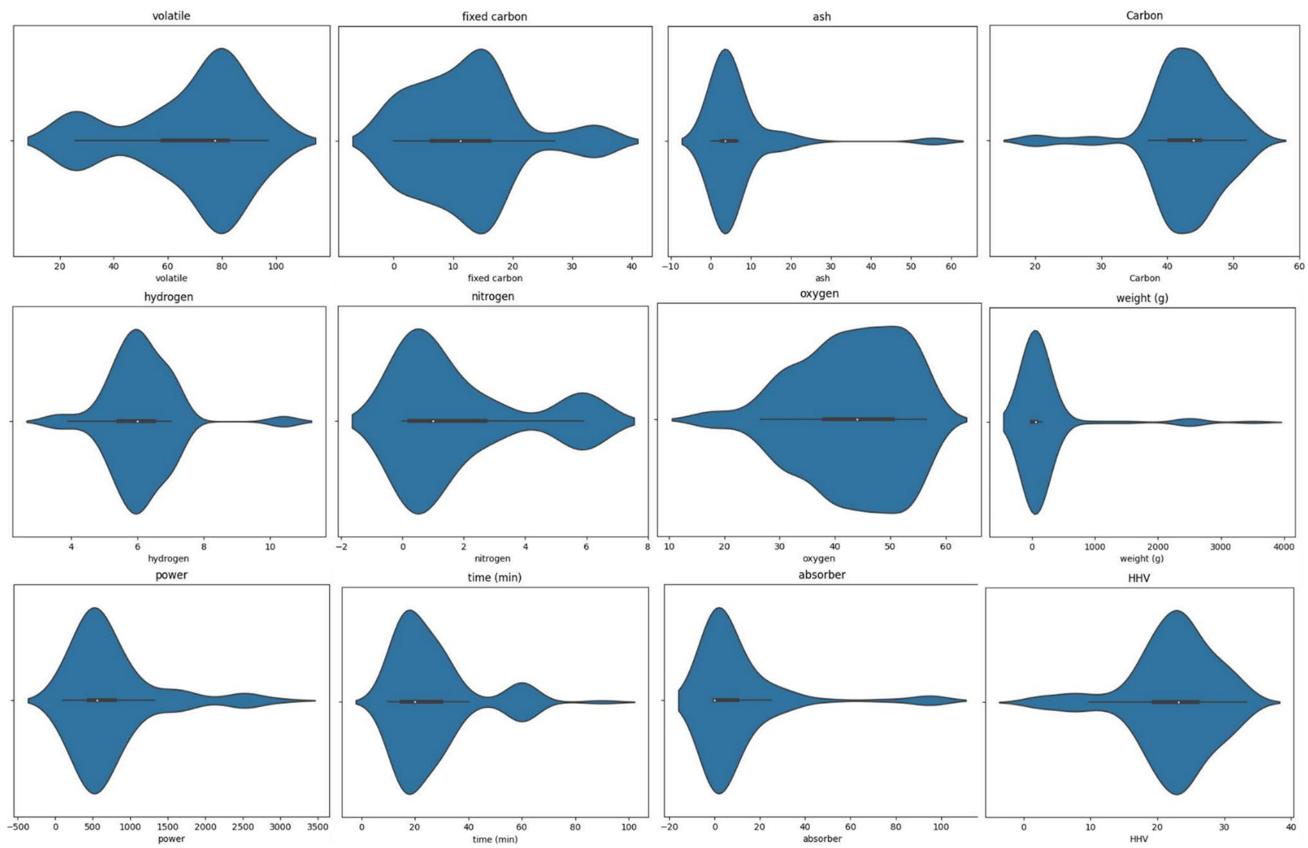

Fig. 4 Violin plot for the conditional and decision attributes considered for analyzing the microwave-derived biochar HHV (*volatile — volatile matter, fixed carbon — fixed carbon content, ash — ash content, carbon — carbon content, hydrogen — hydrogen content, oxygen — oxygen content, nitrogen — nitrogen content, weight — weight of feedstock, power — microwave power, time — retention time, absorber — microwave absorber percentage used, HHV — MAP-derived biochar's HHV)

validates the fact of inversely proportional to biochar yield. From Table 4 and Table S3, it could be inferred that the required microwave power to produce class 1 of biochar is moderately higher (500–2000 W). And it requires the addition of microwave absorber with dosage of 10–30%. This study is correlated to Ellison et al. [35] where the authors reported that higher microwave power and higher microwave absorber dosage increase the carbonization reactions and decrease the biochar production. Fodah et al. [36] have reported that microwave pyrolysis of corn stover (oxygen content — 47.88%) at 500–900 W resulted in decreased yield of biochar with increase in power. This difference in microwave power could distinguish the yield of microwave-derived biochar into class 1 and class 2 (rules 4 and 17) respectively. As per Ellison et al. [35], in presence of 10–20% char as microwave absorber under microwave power greater than 900 W, the yield of biochar is less than 20%, corresponding to class 1 of biochar (rules 2 and 8).

In case of class 2 (yield of microwave-derived biochar), the power required is of moderate except in few entries like rule 19 which corresponds to biomass that requires higher microwave power density for its decomposition into pyrolytic products. Nhuchen et al. [37] have analyzed the effect of biomass loading and microwave power level on biochar properties of wood pellets. The authors have reported that yield of biochar decreased from 32.4 to 26.2% when microwave power is increased from 2000 to 3000 W for processing 2.5-kg biomass. This difference in microwave power could distinguish the microwave-derived biochar into class 2 and class 3 (rules 19 and 43) respectively. Wang et al. [38] have compared the yield of biochar obtained through microwave pyrolysis of peanut shell and microalgae at 390 W for 10 min using lignite char as microwave absorber. Microalgae contains higher volatile matter and lower fixed carbon than peanut shell and thus lead to lower yield of biochar corresponding to class 2 (rule 18) compared to latter being classified in class 5 (rule 71). Huang et al. [39] have analyzed product yield of leucaena wood biochar under different microwave power levels of 100–250 W and processing time of 15–30 min. The yield of biochar falls under class 2 (rules 13, 21,

Table 3 List of cores and reduct parameters generated for predicting microwave-derived biochar yield

Decision attributes	Core	Reducts
Yield	W, P, T, MWA	#1 = {C, N, O, W, P, T, MWA} #2 = {VM, N, O, W, P, T, MWA} #3 = {C, H, N, W, P, T, MWA} #4 = {VM, H, N, W, P, T, MWA} #5 = {C, H, O, W, P, T, MWA} #6 = {Biomass, VM, H, O, W, P, T, MWA} #7 = {FC, C, H, W, P, T, MWA} #8 = {VM, C, H, W, P, T, MWA} #9 = {Biomass, C, H, W, P, T, MWA} #10 = {Ash, C, O, W, P, T, MWA} #11 = {Biomass, VM, Ash, O, W, P, T, MWA}
HHV	P, T, MWA	#1 = {VM, Ash, C, P, T, MWA} #2 = {FC, Ash, C, P, T, MWA} #3 = {Ash, H, P, T, MWA} #4 = {Ash, N, P, T, MWA} #5 = {VM, Ash, O, P, T, MWA} #6 = {FC, Ash, O, P, T, MWA} #7 = {H, O, P, T, MWA} #8 = {N, O, P, T, MWA} #9 = {Ash, C, W, P, T, MWA} #10 = {Ash, O, W, P, T, MWA} #11 = {H, W, P, T, MWA} #12 = {N, W, P, T, MWA}

VM, volatile matter; *FC*, fixed carbon; *AC*, ash content; *C*, carbon content; *H*, hydrogen content; *O*, oxygen content; *N*, nitrogen content; *W*, weight of feedstock; *P*, microwave power; *T*, retention time; *MWA*, microwave absorber percentage used

and 26) and both microwave power and processing time affect the mass and energy yield of biochar. The microwave pyrolysis of biomass having carbon content of 43–45% at 600–700 W with 10% of microwave absorber leads to class 2 yield (rule 27) of biochar which also correlates to Dong et al. [40] and Fodah et al. [36].

With respect to class 3, rule 38 has higher strength and coverage of 13 and 20% respectively which depicts the importance the proximate and ultimate composition of biomass on the yield of microwave-derived biochar. The volatile matter, hydrogen, and oxygen content of sludge [41] and oil palm fiber [42] biomass satisfy the rule for obtaining class 3 yield of microwave-derived biochar; however, it is also significantly dependent on process conditions. The processing of agro-residues like sugarcane bagasse and empty fruit bunch at 500–600 W with higher dosage of microwave absorber yields class 3 of biochar (rules 39 and 40). Kuan et al. [43] have obtained microwave-derived sugarcane bagasse biochar of yield 37.62% at 500 W for 30 min using 10% microwave absorber. Mubarak et al. [44] have pyrolyzed empty fruit bunch at 600 W for 11 min with 50% microwave absorber and obtained class 3 yield of biochar (38%) (rule 39); however, increasing microwave power to 900–1200 W leads to class 4 yield (41–45%) of biochar (rule 61).

The rule 56 reveals the influence of reaction time and microwave absorber dosage in yield of microwave-derived biochar. The microwave reaction time of 15–20 min and higher microwave absorber dosage result in class 4 yield of biochar. The rule is supported by Fodah et al. [36] where microwave pyrolysis of corn stover at 900 W for 15 min with the presence of sodium carbonate as catalyst resulted in 50% biochar yield. Also, Dominguez et al. [45] reported 44% of biochar from microwave pyrolysis of coffee hull at 270 W for 20 min with 20% microwave absorber. The yield fractions are similar to conventional pyrolysis in the study conducted by authors. The study by Dominguez et al. [45] and Luo et al. [41] satisfies under the rules 56 and 58 respectively. The rule 66 implies the effect of ash content, nitrogen content, and microwave power, and the range of the parameters is supported by Hossain et al. [42] and Foong et al. [46]. Besides the microwave pyrolysis process conditions influencing the biochar's characteristics, feedstock composition also plays a major role in the determination of biochar properties [47]. As could be interpreted from Table 4, rules 30 and 39, the different biomass of algae/biowaste and agro-residues processing at microwave power of $500 <= P < 600$ distinguished into two different classes of yield of biochar. This is owing to the difference in biochemical composition of feedstock where algae contain mostly volatile matter and less fixed carbon content than agro-residues and thereby results in lower yield than later [48].

The confusion matrix provides a clear representation of how each class was classified and highlights the differences between the predicted and actual classes. The confusion matrix generated for prediction of microwave produced biochar yield is given in Table 5. It allows to analyze the performance of a classifier by examining the correct and misclassified instances. The average accuracy of classifier for separating the rules into desired classes is of 81.84% (Table 6). The precision of classifier for class 1 and class 5 separation is 72.41% and 61.11% respectively and the precision is low for other classes which could be improved by processing higher number of datasets.

The rules generated for predicting the HHV of microwave-derived biochar have been given in Table 7 and Table S4. Twenty-eight exact rules have been generated from processing 112 number of datasets. Out of 28, the selected rules of two correspond to class 1 HHV of biochar. Four rules belong to class 2, 10 rules belong to class 3, 7 rules for class 4, and 3 rules for class 5 and the rules generated are given in Table 7. The power required is of moderate range

Table 4 Selected rules for the prediction of biochar yield obtained through microwave pyrolysis

Rule no	Reducts	Rule	Strength	Relative strength	Coverage	Certainty
Class 1						
2	1	(15 < = FC < 20) & (N < 0.5) & (900 < P < = 1200)	2	2	3.17%	100.00%
4	7	(FC < 10) & (60 < = W < 80) & (700 < P < = 900)	8	8	12.70%	100.00%
5	9	(Biomass = woody) & (15 < = FC < 20) & (N < 0.5) & (1200 < P < = 2000)	2	2	3.17%	100.00%
8	6	(45 < = O < 50) & (10 < = W < 20) & (700 < P < = 900)	2	2	3.17%	100.00%
Class 2						
13	7	(5.5 < = H < 6) & (P < 200) & (10 < T < = 15)	4	4	4.82%	100.00%
17	9	(Biomass = Agro-residue) & (60 < = W < 80) & (700 < P < = 900)	3	3	3.61%	100.00%
18	11	(Biomass = Others) & (50 < = VM < 70) & (3 < = N < 11)	6	6	7.23%	100.00%
19	8	(80 < = VM < 100) & (2000 < P < 3000)	5	5	6.02%	100.00%
21	7	(200 < = P < 400) & (15 < T < = 20) & (MWA = 0)	2	2	2.41%	100.00%
26	9	(200 < = P < 400) & (10 < T < = 15) & (MWA = 0)	2	2	2.41%	100.00%
27	1	(43 < = C < 45) & (600 < = P < = 700) & (MWA < = 10)	3	3	3.61%	100.00%
Class 3						
38	11	(50 < = VM < 70) & (10 < = Ash < 20) & (5.5 < = H < 6) & (50 < = O < 57)	13	13	20.00%	100.00%
39	6	(Biomass = Agro-residues) & (500 < = P < 600) & (30 < MWA < = 50)	2	2	3.08%	100.00%
40	9	(Biomass = Agro-residues) & (500 < = P < 600) & (10 < MWA < = 30)	1	1	1.54%	100.00%
43	3	(5.5 < = H < 6) & (1200 < P < = 2000) & (10 < T < = 15)	3	3	4.62%	100.00%
Class 4						
56	9	(15 < T < = 20) & (20 < MWA < = 50)	4	4	10.81%	100.00%
58	1	(3 < = N < 11) & (20 < T < = 30) & (10 < MWA < = 30)	4	4	10.81%	100.00%
61	9	(Biomass = Lignocellulose) & (45 < = C < 50) & (30 < MWA < = 50)	1	1	2.70%	100.00%
Class 5						
66	10	(20 < = Ash < 55) & (2 < = N < 3) & (600 < = P < = 700)	6	6	17.65%	100.00%
71	11	(200 < = P < 400) & (T < = 10)	2	2	5.88%	100.00%

VM, volatile matter; *FC*, fixed carbon; *AC*, ash content; *C*, carbon content; *H*, hydrogen content; *O*, oxygen content; *N*, nitrogen content; *W*, weight of feedstock; *P*, microwave power; *T*, retention time; *MWA%*, microwave absorber percentage used

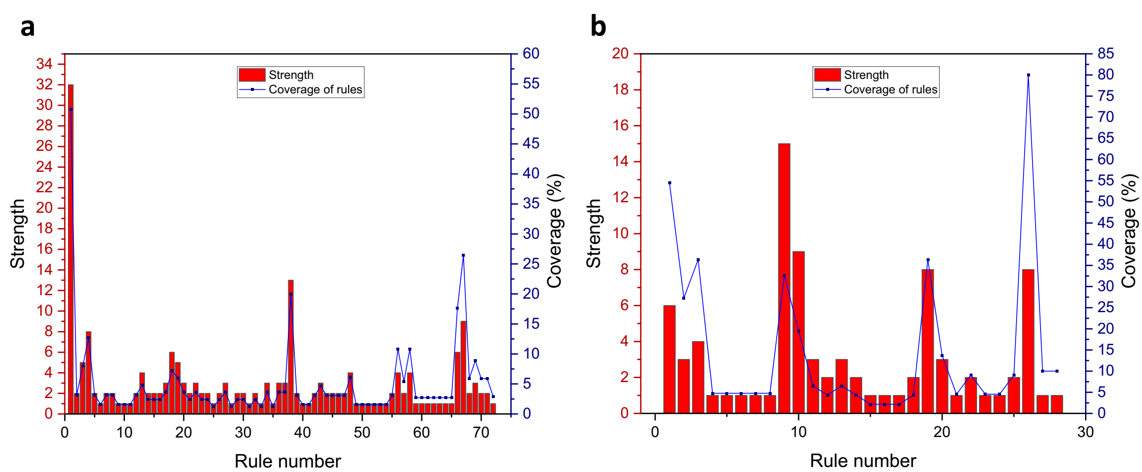

Fig. 5 Validation metrics for rules generated for microwave-derived biochar **a** yield and **b** HHV

Table 5 Confusion matrix generated for rule prediction for microwave-derived biochar yield

	Class	Predicted 1	2	3	4	5	None
Actual	1	42	12	5	2	2	0
	2	10	35	23	10	5	0
	3	5	12	36	10	2	0
	4	1	5	7	19	5	0
	5	0	2	2	8	22	0

Table 6 Validation metrics for rule prediction of microwave-derived biochar yield for each class (The values are represented in %)

Class	Accuracy	Precision	Recall	F1 score
1	86.88	72.41	66.67	69.42
2	71.99	53.03	42.17	46.98
3	76.60	49.32	55.38	52.17
4	82.98	38.78	51.35	44.19
5	90.78	61.11	64.71	62.86

(500<=P<600) to produce HHV corresponding to class 1. With change in nitrogen content of biomass and moderate microwave power (500<=P<600), the class of HHV differs from 1 to 2. However, this contradicts to the finding reported by Qian et al. [49] where the authors did not find any linear or non-linear relationships between nitrogen and HHV. This could be because of the additional role of microwave power that mostly influences the properties of biochar. The required microwave power to produce higher class of HHV of biochar increases with classes and is also correlates with literary studies [46, 50]. The rule 1 of predicting HHV of microwave-derived biochar follows Gautam et al. [51] and Zhou et al. [52]. The rule 3 depicting the range of microwave power and nitrogen content of biomass for obtaining class 1 HHV of biochar is correlated to Gautam et al. [51] and Bowlby et al. [53].

In class 2 of HHV of microwave-derived biochar, the main parameters influencing the characteristic are microwave power in range of 500–600 W and time 10–15 min

Table 7 Selected rules for prediction of HHV of biochar obtained through microwave pyrolysis

Rule no	Reducts	Rule	Strength	Relative strength	Coverage	Certainty
Class 1						
1	2	(FC < 10) & (10 < = Ash < 20)	6	6	54.55%	100.00%
3	12	(1 < = N < 2) & (500 < = P < 600)	4	4	36.36%	100.00%
Class 2						
4	1	(500 < = P < 600) & (10 < T < = 15) & (10 < MWA < = 30)	1	1	4.76%	100.00%
6	8	(0.5 < = N < 1) & (35 < = O < 40) & (500 < = P < 600)	1	1	4.76%	100.00%
8	6	(500 < = P < 600) & (10 < T < = 15) & (MWA = 0)	1	1	4.76%	100.00%
Class 3						
9	10	(500 < = P < 600) & (20 < T < = 30)	15	15	32.61%	100.00%
12	6	(700 < P < = 900) & (30 < MWA < = 50)	2	2	4.35%	100.00%
13	7	(7 < = H < 12) & (600 < = P < = 700)	3	3	6.52%	100.00%
18	2	(700 < P < = 900) & (10 < MWA < = 30)	2	2	4.35%	100.00%
Class 4						
19	4	(woody) & (200 < = P < 400)	8	8	36.36%	100.00%
20	3	(5 < = Ash < 10) & (900 < P < = 1200)	3	3	13.64%	100.00%
25	5	(70 < = VM < 80) & (5.5 < = H < 6) & (10 < MWA < = 30)	2	2	9.09%	100.00%
Class 5						
26	4	(Ash < 2) & (N < 0.5)	8	8	80.00%	100.00%
27	12	(2 < = N < 3) & (30 < = W < 50)	1	1	10.00%	100.00%
28	2	(20 < = FC < 35) & (900 < P < = 1200)	1	1	10.00%	100.00%

VM, volatile matter; *FC*, fixed carbon; *AC*, ash content; *C*, carbon content; *H*, hydrogen content; *O*, oxygen content; *N*, nitrogen content; *W*, weight of feedstock; *P*, microwave power; *T*, retention time; *MWA%*, microwave absorber percentage used

Table 8 Confusion matrix generated for rule prediction for microwave-derived biochar HHV

		Predicted					
	Class	1	2	3	4	5	None
Actual	1	9	0	1	0	1	0
	2	1	15	2	1	2	0
	3	4	4	31	7	0	0
	4	2	0	6	13	0	1
	5	0	1	1	0	8	0

with absence or addition of microwave absorber. The rules 4 and 8 are supported by Fodah et al. [36]. The study by Foong et al. [46] supports the rule 6 and rule 8. The rule 9 of class 3 of microwave-derived biochar's HHV depicts the microwave power range of 500–600 W and reaction time of 20–30 min. This condition is supported by study of Kuan et al. [43] where the pyrolysis at 500 W for 30 min with different absorber dosage resulted in 22.8–24.4 MJ kg^{-1}. Liew et al. [54] have produced biochar with 23–24 MJ kg^{-1} through microwave pyrolysis under 500–600 W for 25 min. The produced biochar possessed higher surface area, carbon content, and porosity in addition to calorific value of class 3 (rules 9 and 13). The rules 12 and 18 are correlated to results reported by Fodah et al. [36]. The microwave pyrolysis of woody biomass like *Leucaena* wood [39], *Quercus ilex*, and *Cistus ladanifer* [55] under microwave power of 200–400 W results in class 4 HHV (25–30 MJ kg^{-1}). These entries support the rule 19 for prediction of microwave biochar's HHV. The study by Fodah et al. [36] supports the rules 20 and 25 for prediction of HHV of microwave-derived biochar.

Since most biomass has low dielectric power, the addition of microwave absorber is essential to increase the heating rate and to attain maximum temperature. Different types of microwave absorber like activated carbon, biochar, and silicon carbide are being used in various studies that determine the product distribution of microwave pyrolysis. Most of the microwave pyrolysis research has used microwave absorber ranging from 10 to 30% and few studies have reported higher percentage based on the process requirements. From Table 7, the addition of microwave absorber of 10–30% has contributed to class 2 and the dosage increased in few rules corresponding to class 3 and 4. The confusion matrix for prediction of HHV of microwave produced biochar is given in Table 8. The average accuracy of the classifier is of 87.82% and the precision of the classifier is also higher than that determined for yield of microwave produced biochar for classes 2, 3, 4, and 5 (Table 9).

The comprehensive rules obtained for the class 5 yield and HHV of microwave-derived biochar are given in Table 10. These rules define specific quality and composition standards for biochar, ensuring it to meet desired specifications for efficient combustion or industrial processes, minimizing environmental impact, and optimizing energy production. Compliance with these criteria is critical for product consistency and performance in various industries.

4 Conclusions and prospects

Rough set-based machine learning predictive models were used to predict the range of operational variables to achieve biochar with high yield and properties. The rules framed showed promising scientific coherence and logical certainty. The study would assist in making clarified decisions on feedstock selection to achieve the desired yield and properties, while scaling up and commercializing microwave pyrolysis.

Table 9 Validation metrics for rule prediction of microwave-derived biochar HHV for each class (The values are represented in %)

Class	Accuracy	Precision	Recall	F1 score
1	91.82	56.52	81.82	66.67
2	90.00	75.00	71.43	73.17
3	77.27	75.61	68.39	71.26
4	84.55	61.90	59.09	60.47
5	95.45	72.73	80.00	76.19

Table 10 Optimal rules obtained for prediction of class 5 yield and HHV of microwave-derived biochar

Parameters	Optimal rules
Yield	5 < = Ash < 10/20 < = Ash < 55, N < 0.5/2 < = N < 3, 600 < P < 900, 40 < = O < 45, 10 < = w < 20/100 < w < = 500, 10 < T < = 15,C < 40/45 < = C < 50
HHV	Ash < 2, N < 0.5/2 < = N < 3, 20 < = FC < 35, 30 < = w < 50, 900 < P < = 1200

Ash, ash content; *N*, nitrogen content; *P*, microwave power; *O*, oxygen; *w*, weight of biomass; *T*, time; *C*, carbon content

The prediction accuracy for determining classes for biochar yield is lower and this could be resolved by processing more datasets. To overcome the limitations, integration of rough set analysis with other machine learning models such as regression or random forest could be adopted which might be effective in capturing the complex relationships and improve prediction accuracy. The scientific accuracy of the model could be increased by including other process parameters like feedstock particle size and environmental atmosphere. The present study could also be extrapolated to classify surface characteristics, and functional groups of biochar produced through microwave pyrolysis for different applications. The practical implications of using rough set analysis for predicting the yield and HHV of microwave-derived biochar include data-driven decision-making in process optimization, ensuring of consistent quality, and adaptability in the biochar production process. This leads to the ultimate benefit of both producers and consumers of biochar products.

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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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