Energy Proceedings
Vol 43, 2024
ISSN 2004-2965

Evaluation of Explainable Deep Learning Models in Predicting Hydrogen Production

Chiagoziem C. Ukwuoma [1,2], Dongsheng Cai [1,2*], Chibueze D. Ukwuoma [3], Favour AB Ekong [4], Emmanuel S.A Gyarteng [5], Chidera O. Ukwuoma [6], Qi Huang [1,2]

1 College of Nuclear Technology and Automation Engineering, Chengdu University of Technology, Sichuan P.R., 610059, China

2 Sichuan Engineering Technology Research Center for Industrial Internet Intelligent Monitoring and Application, Chengdu University of Technology, Sichuan P.R., 610059, China

3 Department of Physics, School of Engineering and Engineering Technology, Federal University of Technology Owerri, Nigeria

4 School of Information and Software Engineering, University of Electronic Science and Technology of China, Chengdu 611731, China

5 School of Computer Science and Engineering, University of Electronic Science and Technology of China, Chengdu 611731, China

6 Department of Prosthetics and Orthotics Technology, Federal University of Technology Owerri, Nigeria
(*Corresponding Author: caidongsheng@cdut.edu.cn)

ABSTRACT

To meet the difficulties of the current energy environment, hydrogen has enormous potential as a clean and sustainable energy source. Utilizing hydrogen's potential requires accurate hydrogen production prediction. Due to its capacity to identify intricate patterns in data, Machine learning alongside deep learning models has attracted considerable interest from a variety of industries, including the energy industry. These algorithms are inherently black boxes, which makes it difficult to comprehend and interpret their predictions, particularly in important sectors like hydrogen generation. First, this study conducted an extensive experiment using 4 machine learning regression models and a novel deep learning model based on Keras API for hydrogen production prediction based on the co-gasification of biomass and plastics datasets. Secondly, this study investigates the application of explainable AI models including Shapley Additive Explanation (SHAP), Local Interpretable Model-Agnostic Explanations (LIME), and Explain Like I'm Five (ELi5) in predicting hydrogen production. We explore the significance of these models in providing insights into the underlying mechanisms and factors influencing hydrogen production processes hence improving our understanding of the relationships between input factors and hydrogen production outputs. This will allow for better-informed decision-making and process optimization in the energy industry. Our results demonstrate the interpretability and transparency of these models, highlighting their potential to raise the accuracy and dependability of forecasts of hydrogen generation. These models provide a useful resource for stakeholders to make informed decisions and enhance the use of hydrogen as a sustainable energy source by bridging the gap between predicted accuracy and interpretability.

Keywords: machine learning, deep learning, explainable artificial intelligence, predicting hydrogen production, co-gasification

NONMENCLATURE

Abbreviations

HDPE	High-Density Polyethylene
RSS	Rubber Seed Shell
RFR	Random Forest Regressor
XGBoost	Extreme Gradient Boosting
SVR	Support Vector Regressor
KNN	K-Nearest Neighbor
RS	Renewable Sources
CO_2	Carbon Dioxide

This is a paper for 15th International Conference on Applied Energy (ICAE2023), Dec. 3-7, 2023, Doha, Qatar.

CH_4	Methane
H_2	Hydrogen Gas
$Ni/CaFe_2O_4$	Nickel/Calcium Ferrite
RBF	Radial Basis Function
MLP	Multi-Layer Perceptron
ANN	Artificial Neural Network
SEE	Standard Error of Estimates
CNN	Convolutional Neural Networks
GA	Genetic Algorithms
DT	Decision Trees
MAE	Mean Absolute Error
MSE	Mean Square Error
RMSE	Root Mean Squared Error
RMSLE	Root Mean Squared Log Error
R^2	R-squared
AI	Artificial Intelligence
XAI	Explainable AI
SHAP	Shapley Additive Explanation
LIME	Local Interpretable Model-Agnostic Explanations
Eli5	Explain Like I'm Five
Symbols	
$	Dollar
£	Pound
mm	Millimeter
C	Centigrade
vol %	Percentage in Volume
wt %	Weight in Volume
kg	Kilogram

1. INTRODUCTION

Conversations regarding the pursuit of environmentally friendly, cost-effective, and enduring energy resources have gained prominence due to the escalating global energy requirements[1][2]. Anticipating a global population of 10 billion by 2050, experts predict a substantial surge in energy consumption, accentuating the need for sustainable solutions. While fossil fuels have driven economic development globally, their ecological toll is evident. Consequently, researchers and scientists are exploring alternative energy production methods with minimal or no adverse environmental consequences[3–6]. As mentioned earlier, substances containing hydrogen, such as carbohydrates or water, are transformed into hydrogen gas. It's worth noting that around 96% of the world's hydrogen production is traditionally derived from fossil fuels. Specifically, 30% comes from naphtha reforming, 48% from natural gas steam reforming, and 18% from coal gasification[7]. However, these conventional hydrogen production methods are linked to the environmental issues currently plaguing the planet. As a result, environmentalists and the energy sector are actively striving to develop more eco-friendly approaches to generate hydrogen RS.

While simultaneously transforming carbon into sustainable energy sources such as hydrogen and syngas, the utilization of plastics and biowastes can reduce the environmental impact of industrial processes found in sectors like iron steel, and cement[8][9]. The co-gasification of plastic and biomass mixtures through dry and steam reforming of CO_2 generates H_2, with factors like feed composition and catalyst type influencing the conversion of waste plastics into fuel products[10][11]. Variables such as temperature, the ratio of polymers to biomass, CO_2/CH_4 ratios, and the choice of catalyst all play a role in the production of H_2[9][12][1]. Waste polymers like polyethylene and polypropylene exhibit low moisture and ash contents but high volatile content, viscosity, and heating value. Among these materials, polypropylene stands out as the most effective for producing hydrogen. However, in comparison to biomass, which contains substantial quantities of hydrogen-rich molecules such as cellulose, hemicellulose, and lignin, polymers demand more energy for gasification and yield less hydrogen[13][14]. While the fossil fuel and renewable energy sectors have been vying for control over the production of green hydrogen crucial for the energy transition, there's now a third contender in the mix. Green hydrogen derived from organic waste has emerged as a significantly more cost-effective alternative to both fossil fuels and renewable energy sources, offering a carbon-negative solution. This type of green hydrogen, produced from various combinations of organic waste, has the potential to power mobile homes and remote hospitals lacking access to electricity. In contrast, the electrochemical method used to produce green hydrogen, which requires substantial amounts of freshwater and renewable energy, is both environmentally friendly and efficient in separating water into hydrogen and oxygen. The cost of producing green hydrogen from waste blends is approximately $3 per kilogram, whereas utilizing solar or wind energy can cost roughly $11 to $16 per kilogram. Moreover, each tonne of dry waste can yield between 40 and 50 kg of green hydrogen, though this amount may vary between 30 kg and 120 kg depending on the moisture content in the waste blends.

Artificial intelligence techniques, which include machine learning and deep learning algorithms, can be employed for clustering, optimization, prediction, and

classification, tasks in the green hydrogen generation process. These AI methods analyze various data streams[14]. For example, in Scotland, a real-time machine learning system is being utilized to enhance the production of green hydrogen using wind and tidal power[13]. To ensure the security and reliability of the system and make informed data-driven decisions, a cloud-based hydrogen management platform has been developed, incorporating machine learning and optimization algorithms. This platform helps determine the most cost-effective times for hydrogen production and storage and has received £494,000 in support from the Department of Business, Energy, and Industrial Strategy. Consequently, the competence and trust of decision-makers in the application of machine learning models within specific domains are paramount[15]. Improving decision-making relies on the ability to detect flaws and concealed biases in these models' operations[16]. However, the intricate nature of machine learning models poses challenges for domain experts in comprehending their intricate structures. This underscores the necessity for tools that address the current demand and provide precise and comprehensible insights. Therefore, AI must emulate human judgment and interpretive abilities to gain acceptance and credibility[17][18]. Explainable AI (XAI), often referred to as "black-box models," strives to elucidate the decision-making process by seeking to understand the internal workings of these AI models, which are challenging due to their inherent complexity and opacity[19]. This has led to a significant increase in the adoption of post hoc approaches designed to render complex models understandable to humans.

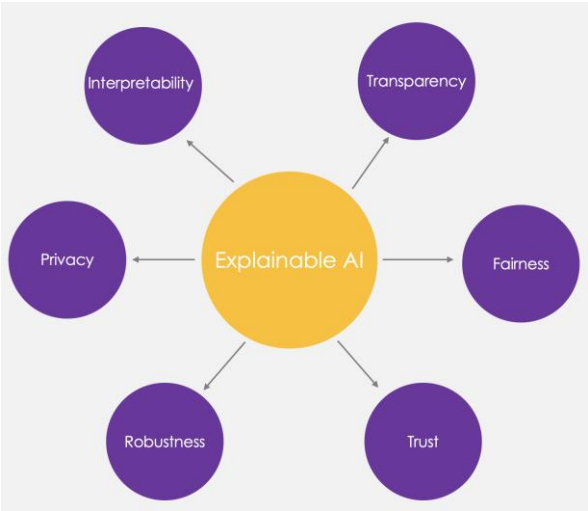

Fig. 1 Principles of explainable AI

Motivation: The intricate nature of cutting-edge machine learning algorithms poses significant challenges in the field of Hydrogen production prediction. Emphasizing the critical importance of accurate and reliable Hydrogen production prediction models cannot be overstated, as they play a pivotal role in enabling well-informed decisions. Nevertheless, as AI models become more complex, transparency often diminishes, making it increasingly challenging to comprehend the rationale behind specific predictions and any potential associated shortcomings[18]. Conventional black-box machine learning algorithms cannot typically elucidate their predictions, creating a trust and acceptance hurdle for end-users and regulatory bodies[20]. In response to these pressing issues, researchers have diligently worked on developing Explainable AI (XAI) solutions (Fig. 1). These approaches offer coherent explanations for the outcomes generated by AI models, serving as guiding lights of understanding within their inherent opacity.

The goal of the study is to make useful resources for stakeholders to make informed decisions and enhance the use of hydrogen as a sustainable energy source by bridging the gap between predicted accuracy and interpretability. The following are the main objectives of this study;

- Use SHAP, LIME, and Eli5 to evaluate the transparency and explainability of machine learning models.
- Showcase the ability of explainable machine learning to produce an explicit understanding of how models create predictions, intending to boost acceptance and trust in cutting-edge ML methods in hydrogen production prediction and the Energy sector.
- Evaluate and contrast the benefits and drawbacks of LIME, ELi5, and SHAP in providing clear explanations of hydrogen production prediction.
- Add to the corpus of current knowledge by emphasizing the practical consequences

This paper is divided into the following sections; The second section contains the related studies. The third section details the comprehensive working processes and our proposed model. The experimental results, discussion, and future works are presented in section 4 while our conclusion is found in 5.

2. RELATED WORKS

The scientific research on the topic of predicting hydrogen generation has only produced a few numbers of answers. The research community has undergone some thorough studies of the problems relating to hydrogen generation[20–22]. Additionally, several

techniques and fixes for creating green hydrogen that utilize biological, chemical, or physical processes have been suggested. For example, Nicolas et al's[23] investigation on the potential for creating green hydrogen via bioethanol using nanocatalyst design. To create green hydrogen from seawater, Rafaeld'Amore-Domenech et al[24] used and contrasted four electrolysis techniques. Few works focus on the aspect of predicting hydrogen generation. In Islamabad, Haider et al[25] looked into a machine-learning algorithm to forecast hydrogen generation from solar energy. One of the green technology tools, AI may help produce green hydrogen using a variety of methods and resources. Methane drying and reforming is one of the popular techniques that uses machine and deep learning models to forecast the generation of green hydrogen based on diverse catalysts. The Bayesian regularization algorithm, the Leven-Marquardt algorithm, and a scaled conjugate gradient algorithm were examined by Ayodele et al[26] for their suitability as training algorithms for an ANN prediction model to predict the quantity of CO and H_2 production by the methane drying and reforming technique. In comparison to the two used methods, the empirical findings demonstrated the overpowering advantage of the Bayesian regularization technique with the lowest SEE. The effectiveness of two ANN models to forecast the generation of hydrogen-rich syngas from the drying and reforming of methane over cutting-edge $Ni/CaFe_2O_4$ catalysts was examined by Hossain et al[27]. The results of the experiments from the methane drying and reforming cycle over innovative $Ni/CaFe_2O_4$ catalysts were trained and validated using RBF and MLP neural network models. The assessment findings demonstrated that, in predicting the generation of hydrogen-rich syngas from drying and reforming of methane over new $Ni/CaFe_2O_4$ catalysts, the ANN-MLP-based approach outperformed the ANN-RBF-based approach.

To anticipate the overall hydrogen output resulting from thermo-catalytic methane reforming, May et al[28] investigated the performance of two deep learning models: one utilizing Bayesian regularization and another trained with the Levenberg-Marquardt method for a multilayer perceptron neural network. The experimental findings indicated that the Levenberg-Marquardt-trained neural network, with a model architecture of 7-16-1, outperformed the Bayesian regularization-trained network in predicting the green hydrogen production rate. This was demonstrated by a coefficient of determination (R^2) of 0.953 and a MSE of 0.03. Additional ANN models were employed, assessed, and compared to forecast green hydrogen production[29]. Alternatively, an alternative approach involves generating green hydrogen through oxygen injection and hydrocarbon tanks submerged in water. Klemens et al[30] introduced a data-centric AI system in their work aimed at enhancing the production of green hydrogen within hydrocarbon reservoirs submerged in water. Their study marks a pioneering effort in the realm of improving oxygen injection techniques while simultaneously optimizing hydrogen generation through the utilization of an AI-based genetic optimization framework. Generating hydrogen from organic waste is regarded as one of the foremost and cost-effective methods[30–34]. Nonetheless, the existing body of literature does contain a limited number of AI models designed to strategize and enhance the production of green hydrogen from waste sources. More recent investigations[35][36] have focused on harnessing machine learning algorithms to maximize hydrogen generation from wastewater and sewage sludge. Five uses of machine learning methods for forecasting the treatment and recycling of organic solid waste were examined by Hao-nan et al[37]. Their research primarily focused on the use of ANN, SVM, GA, DT and RF for forecasting organic solid waste treatment. Their analysis was based on examining published papers from 2003 to 2020. It's important to note that the study did not address the application of these machine-learning methods for generating hydrogen from organic solid waste. This research holds significance due to the identified gap in knowledge within this particular domain.

Accurate predictions often require testing a limited and unrepresentative sample from the initial dataset, which can lead to increased accuracy but often at the cost of model representativeness. These neural network models exhibit three notable flaws. First, different approaches vary in the type of input data used for predictions; experimental data-based hydrogen descriptors may not always contain all the necessary information to predict a specific attribute accurately. These descriptors are not easily transferable and tend to perform poorly when applied to another machine learning-based approach with a different test set, as each model possesses unique characteristics. Secondly, the limited availability of data poses a challenge to constructing models, as it confines the models to specific estimations of free hydrogen generation, omitting significant variations in aqueous or organic solvents. Lastly, most of these models do not provide explanations

for their statistical forecasts, reinforcing the "black-box" nature of machine learning-based predictions. Previous models, except for Low et al[38], which still employ quantum mechanics calculations, fail to elucidate the physical significance of each prediction[39].

3. MATERIALS AND METHODS

3.1 Explainable Models

The goal of XAI is to provide users with clear explanations. These explanations have a crucial use in assisting domain specialists in exposing biased biases concealed inside these black box models[40]. The relevance of features for machine learning predictions is determined in this work using XAI approaches including SHAP, LIME and ELi5. These techniques modify a given data instance and track the impact on the black-box classifier's output to determine the role of certain characteristics in a given prediction[41].

- LIME: LIME is a method created to use interpretable surrogate models to describe the behavior of any base estimator. By fitting local surrogate models, such as linear classifiers or decision trees, to explain individual predictions, it produces locally true explanations[42]. Instead of attempting to fit a global surrogate model, LIME concentrates on the local behavior of the model. This method enables a thorough analysis and comprehension of the behavior of the model, but the explanations might not be consistent with the overall behavior.
- ELi5: Since ELI5 is based on LIME, it uses a straightforward method to interpret predictions. It accomplishes this by assessing the significance of various traits in a random forest[43]. Following the decisions made in the tree structure allows for the determination of this importance. The influence of a feature is determined by how much the score shifts from a parent node to a child node at each point in the tree, where each point has a score.
- SHAP**:** Game theory is used by SHAP to explain predictions made by machine learning[44]. The model's inputs are viewed as participants in a game, and the prediction result is the reward. SHAP measures how each input affects the forecast. By decomposing the impact of a model's attributes, SHAP, an explicable AI method, enables us to comprehend how a model decides[45]. For different kinds of models, such as decision trees and deep learning models, many techniques are used to estimate SHAP values, including kernel SHAP, Gradient SHAP, and TreeSHAP.

3.2 Deployed Models

Four regression machine learning models including the SVR, XGBoost Regressor, RFR, KNN Regressor and a novel ANN model based on Keras API were deployed in this study for hydrogen production prediction[46][47].

- RFR: RFR is an estimation method that employs averaging to increase predicted accuracy and reduce overfitting after fitting many classification decision trees to different dataset subsamples. If bootstrap is set to default (i.e., True) the size of the sub-sample is determined by the max_samples argument; otherwise, each tree is constructed using the whole dataset. In this study, only the Nos. of estimators = 30 and random state = 100 were set based on the Grid search analysis. Fig. 2 depicts the basic structure of the RL Algorithm.

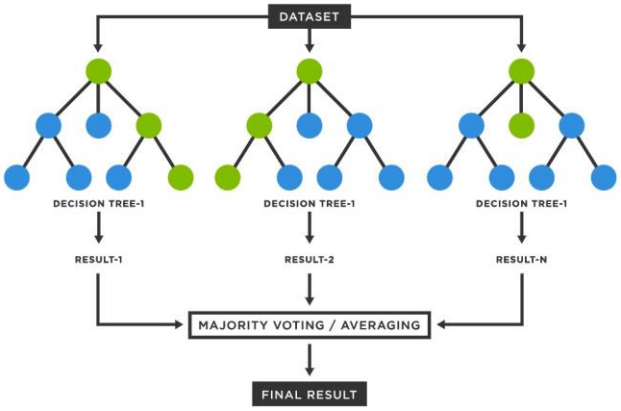

Fig. 2 Basic structure of the RF algorithm

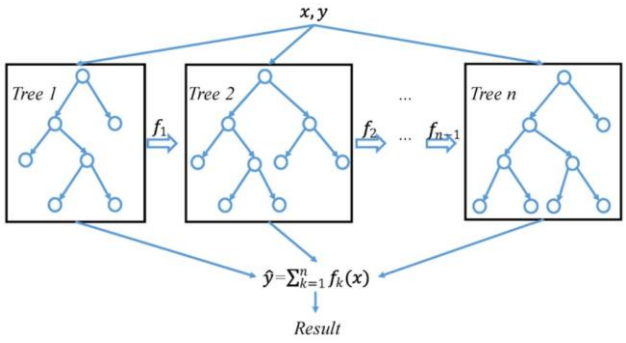

Fig. 3 XGBoost architecture

- XGBoost Regressor**:** This is a machine learning model used for supervised learning tasks, in which the training data is used to predict a target/response variable. It is used for regression (continuous response variable) and classification (qualitative response variable). In this study we used it for

regression analysis i.e., to create a prediction for a quantitative response variable based on explanatory factors that can be quantitative and/or qualitative as shown in Fig 3. The optimal training parameter used in this study includes Base score = 0.5, learning rate = 0.200, nos. of estimators = 50, max depth = 12, gamma = 0.7, alpha = 0.7, random state = 42, and was based on the Grid search method.

- SVR: Regression analysis is carried out using this particular kind of machine learning technique. Finding a function that minimizes the prediction error and roughly approximates the connection between the input variables and a continuous target variable is the aim of SVR. SVR looks for a hyperplane in a continuous space that best matches the data points. As seen in Fig. 4, this is accomplished by projecting the input variables into a high-dimensional feature space and identifying the hyperplane that minimizes the distance (margin) between the hyperplane and the nearest data points while also reducing the prediction error. By applying a kernel function to translate the data to a higher-dimensional space, SVR can manage connections that are not linear between the input variables and the target variable. The training parameters were set using the Grid search algorithm (Kernel = 'rbf', random seed = 42).

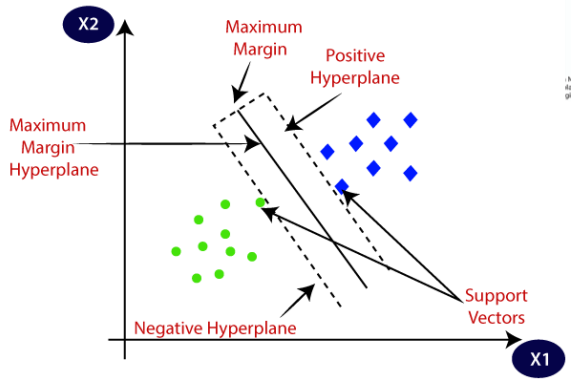

Fig. 4 Basic structure SVR algorithm

- K-NN Regressor: a supervised learning classifier that employs proximity to produce classifications or predictions about the grouping of a single data point. It can be applied to classification or regression issues. Here, the average of the k nearest neighbors is used to predict a classification (continuous values) because it is being used in a regression task as shown in Fig 5. During training, the Grid search algorithm was used to set the optimal hyperparameter (Nos. neighbors = 4) of the model.

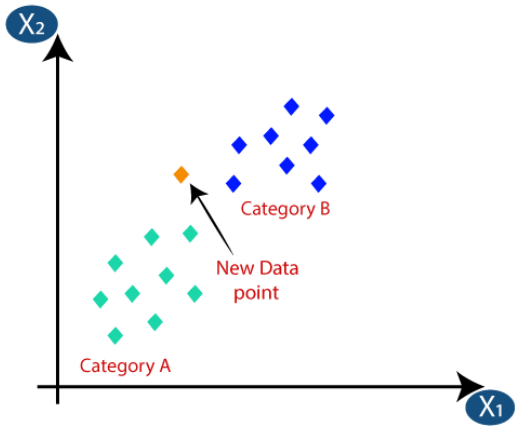

Fig. 5 Basic structure KNN algorithm

- Proposed Model Based on Keras API: The model is composed of interconnected nodes organized into layers. Information flows through these layers, starting with an input layer, passing through hidden layers, and concluding with an output layer as shown in Fig 6. The model's input layer comprises a [16, 3, 1] architecture, 30 rows of data, and 4 independent variables. Given that the regression issue is intended to provide an exact prediction of numerical values, the output layer does not receive an activation function. The L2 regularization is used to avoid overfitting by encouraging weight decay toward zero. The model is constructed using the Adam optimizer, mean squared error loss, mean absolute error, and other measures. During training, a batch size of 2, 3000 epochs, and a verbose output setting of 1 are employed.

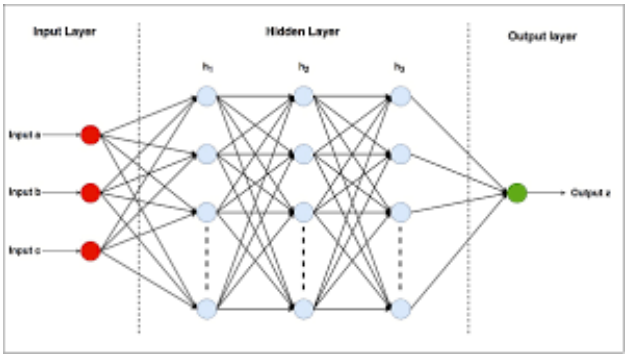

Fig. 6 Basic structure of an ANN model

3.3 Dataset

The study's dataset was based on Chin et al.[48] research. In statistics, a sample size of 30 is typical. A population data set's confidence interval can be increased by a factor of 30 to support claims that the result is false[49].

Table 1. Description of the Hydrogen Production Data

Temperature (C)	RSS Particle Size (mm)	HDPE Particle Size (mm)	Percentage of Plastics in Mixture (wt%)	H2 (vol %)
800	0.25	0.25	10	46.676
700	0.125	0.375	20	50.123
600	0.5	0.25	30	47.751
800	0.5	0.25	10	45.952
500	0.375	0.375	20	44.781
700	0.375	0.625	20	43.031
600	0.5	0.25	10	45.324
900	0.375	0.375	20	49.23
800	0.5	0.5	30	44.355
600	0.5	0.5	30	44.208
700	0.375	0.375	0	44.466
700	0.375	0.375	40	46.603
700	0.625	0.375	20	43.072
800	0.25	0.5	30	47.396
700	0.375	0.375	20	39.98
800	0.25	0.25	10	46.338
700	0.375	0.375	20	38.569
700	0.375	0.375	20	49.868
800	0.25	0.25	30	46.545
700	0.375	0.375	20	38.612
600	0.5	0.5	10	41.032
700	0.375	0.375	20	38.625
600	0.25	0.5	30	47.123
700	0.375	0.375	20	38.621
600	0.25	0.25	10	48.634
800	0.5	0.25	30	48.475
600	0.25	0.5	10	48.132
700	0.375	0.375	20	39.262
600	0.25	0.25	30	46.502
800	0.5	0.5	10	41.93

The dataset consists of 30 experimental runs, with gasification temperature, rubber seed shell (RSS), and high-density polyethylene (HDPE) particle size, the volume of plastic in the mixture acting as independent variables, and the volume of hydrogen produced acting as the dependent variable (Table 1). A larger sample size, however, has a better likelihood of being representative of the population at hand. According to statisticians, a sample size of 30 is enough for the majority of distributions.

3.4 Evaluation Metrics

This paper made use 5 evaluation metrics namely the MAE, MSE, RMSE, RMSLE and R^2. By dividing the total number of observations by the sum of all errors, the MAE determines the exact difference between the actual and anticipated values mathematically represented as

$$\mathrm{MAE} = \frac{1}{\mathrm{n}}\sum_{\mathrm{i}=1}^{\mathrm{n}}\left(\mathrm{Y_i} - \widehat{\mathrm{Y}}_\mathrm{i}\right) \quad (1)$$

where n = number of samples, Y_i = observed values and $\widehat{Y}_i$= predicted values. The squared variation in the actual and anticipated value is known as the mean squared error mathematically represented as;

$$\mathrm{MSE} = \frac{1}{\mathrm{n}}\sum_{\mathrm{i}=1}^{\mathrm{n}}\left(\mathrm{Y_i} - \widehat{\mathrm{Y}}_\mathrm{i}\right)^2 \quad (2)$$

The RMSE corresponds to the square root of the average squared error, and its measurement unit aligns with that of the dependent variable.

$$\mathrm{RMSE} = \sqrt{\frac{1}{\mathrm{n}}\sum_{\mathrm{i}=1}^{\mathrm{n}}\left(\mathrm{Y_i} - \widehat{\mathrm{Y}}_\mathrm{i}\right)^2} \quad (3)$$

$$\mathrm{RMSLE} = \sqrt{\frac{1}{\mathrm{n}}\sum_{\mathrm{i}=1}^{\mathrm{n}}\left(\log(\mathrm{Y_i}+1) - \log\left(\widehat{\mathrm{Y}}_\mathrm{i}+1\right)\right)^2} \quad (4)$$

R-squared (R^2) also known as the Coefficient of Determination or Fit Quality, measures how much better the performance of the regression line is than a simple mean line. It is dimensionless, analyzes model performance in every situation, and consistently produces numbers below one. it is mathematically represented below as;

$$\mathrm{R}^2 = 1 - \frac{\text{sum squared regression (SSR)}}{\text{total sum of squares (SST)}} = 1 - \frac{\sum\left(\mathrm{Y_i} - \widehat{\mathrm{Y}}_\mathrm{i}\right)^2}{\sum(\mathrm{Y_i} - \overline{\mathrm{Y}})^2} \quad (5)$$

4. RESULTS AND ANALYSIS

The descriptive statistics for the used dataset are displayed in Table 2. We used boxplots to show the data distribution, identify probable outliers, and determine the range of values in each of the indicated columns. The most crucial statistical information about a dataset, such as the median, quartiles, and any potential outliers, are concisely displayed in boxplots. Additionally, we displayed the intrinsic characteristics of the dataset's features using the boxplot as shown from Fig. 7 to Fig. 10.

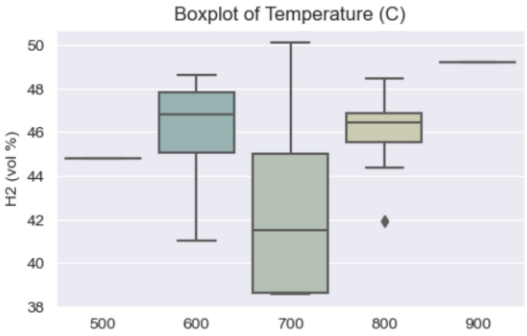

Fig. 7 Temperature vs. H_2

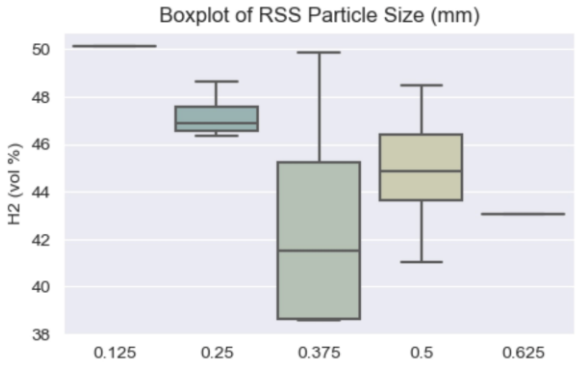

Fig. 8 RSS Particle Size vs. H_2

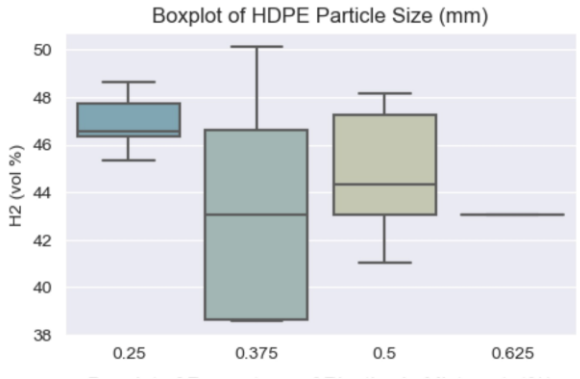

Fig. 9 HDPE Particle Size vs. H_2

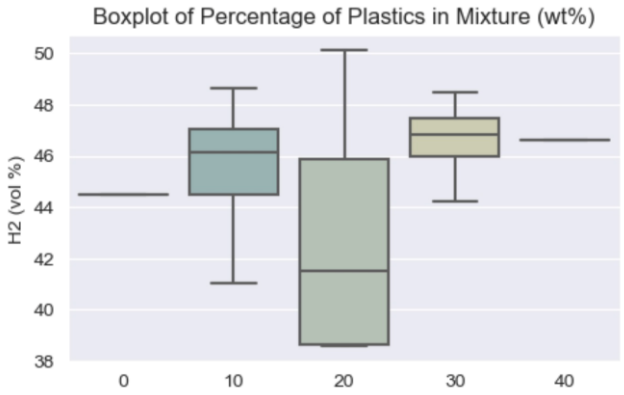

Fig. 10 % of Plastics in Mixture vs. H_2

Table 2. Descriptive Statistics Hydrogen Production Data

	Temperature (C)	RSS Particle Size (mm)	HDPE Particle Size (mm)	% of Plastics in Mixture (wt%)	H2 (vol %)
count	30.0000	30.0000	30.0000	30.0000	30.0000
mean	0.7778	0.6000	0.6000	0.5000	44.7072
std	0.1011	0.1819	0.1661	0.2274	3.6519
min	0.555556	0.2000	0.4000	0.0000	38.5690
25%	0.666667	0.4000	0.4000	0.2500	42.2053
50%	0.777778	0.6000	0.6000	0.5000	45.6380
75%	0.888889	0.8000	0.7500	0.7500	47.3278
max	1.000000	1.0000	1.0000	1.0000	50.1230

4.1 Results

We give the findings from our analysis in this section. According to Table 3, RFR performs the best in terms of accuracy and error metrics since it has the lowest MAE, MSE, and RMSE of all the models. The fact that its R^2 is so low, though, indicates that it doesn't adequately account for the data's variation. XGBoost performs worse than RFR due to larger errors (MAE, MSE, RMSE) and a very low R^2. SVM has a negative R^2, performing marginally worse than XGBoost in terms of error metrics, indicating that it does not well match the data. R^2 and error metrics place KNN between RFR and XGBoost.

Table 3. Results

Model	MAE	MSE	RMSE	R^2	MSLE	RMSLE
RF	2.516	8.946	2.991	0.285	0.004	0.066
XGBoost	2.880	12.266	3.502	0.020	0.006	0.077
SVM	3.361	12.809	3.579	-0.024	0..006	0.080
KNN	3.266	11.564	3.401	0.076	0.006	0.075
Proposed Model	1.775	5.488	2.323	0.459	0.003	0.053

In terms of MAE, MSE, RMSE, and R^2, the Proposed Model performs better than any other model. It makes the most precise predictions and accounts for a significant proportion of the variation in the data since it has the lowest error values and greatest R^2. Furthermore, it has the lowest MSLE and RMSLE, indicating that it effectively manages the large range and probable skewness of the data. Fig. 11 to Fig. 14 illustrates the machine learning model prediction vs. actual result. The proposed model result is shown in Figure 15.

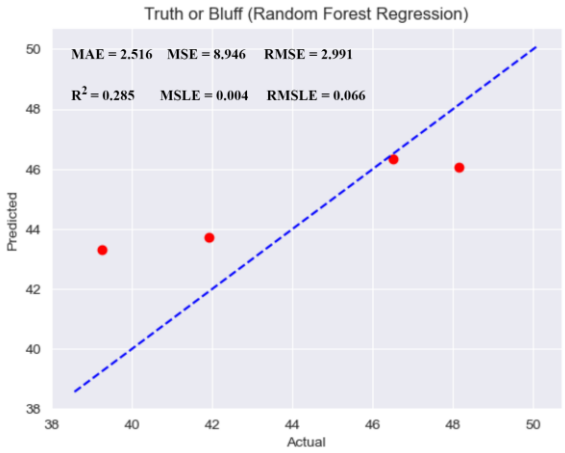

Fig. 11 RFR prediction

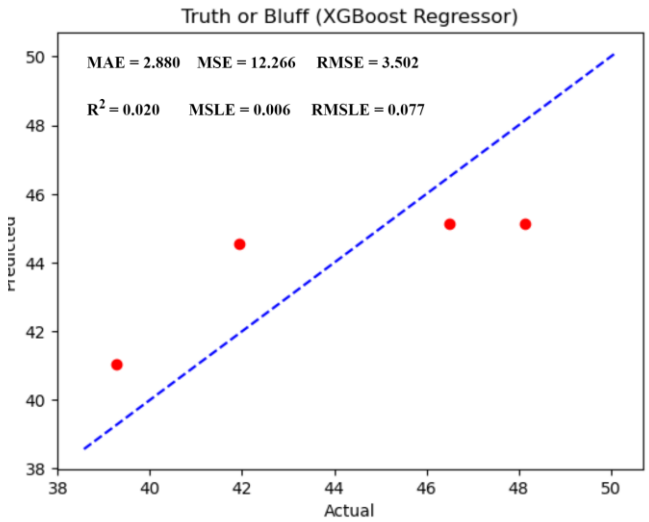

Fig. 12 XGBoost regressor prediction

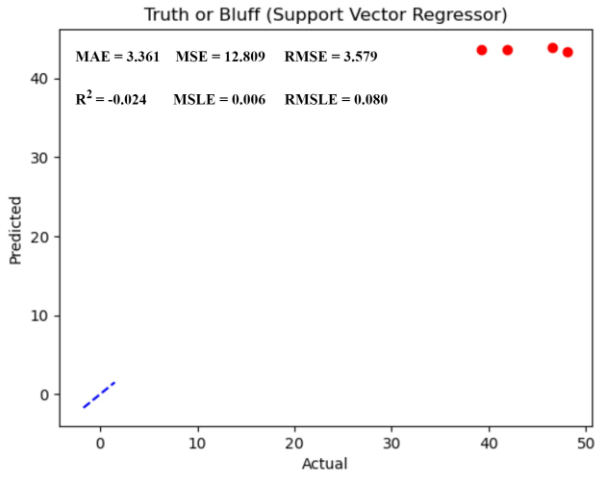

Fig. 13 SVR prediction

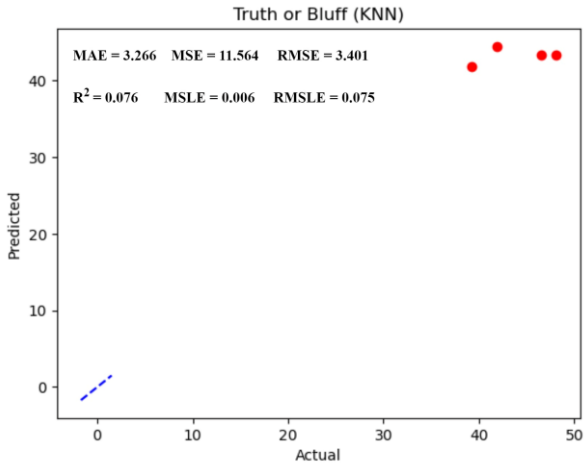

Fig. 14 K-NN regressor prediction

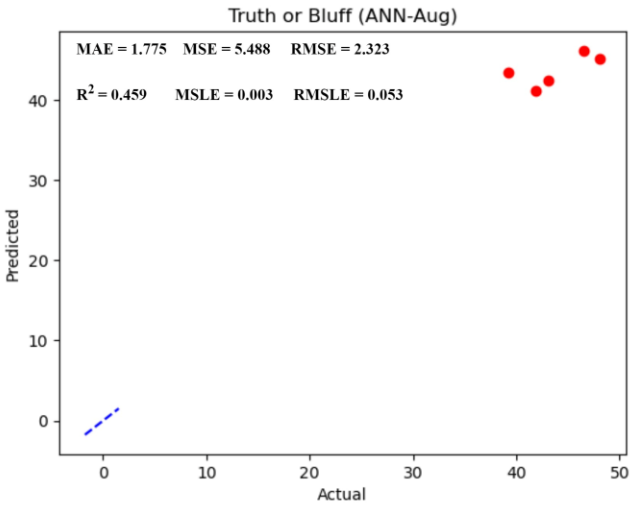

Fig. 15 Proposed model prediction

4.2 Result Explanation Using Explainable AI Models

A description that is simple and easy for a human to grasp for the judgments made by AI and machine learning models is referred to as explainable AI. The SHAP Interpreter, LIME Explainer, and Eli-5 were used in this investigation.

4.2.1 SHAP

By calculating the contribution of each attribute to the forecast, this technique seeks to explain the prediction of an instance or observation. We provided two reasons using the SHAP; variable significance and a defined goal. The variable relevance for the suggested model prediction is shown in Fig. 16. The characteristics are sorted in this plot according to their average SHAP values, with the most significant features appearing at the top and the least significant ones at the bottom. This makes it easier to comprehend how each attribute affects the predictions made by the model. However, the first two parameters with the highest predictive power are HDPE particle size and RSS particle size. % of plastics in the mixture, however, do not contribute as much as the first three characteristics. A more detailed breakdown of the effect of each attribute on a particular result is shown in Figs. 17 to 21. The characteristics are shown on the Y-axis in order of their average absolute SHAP values. Values on the X-axis are SHAP values. Positive values for a particular characteristic move the prediction of the model closer to the label being looked at. Negative values, on the other hand, tend to favor the opposing class. those with red dots are more likely to contribute significantly to the hydrogen prediction (positive result), whereas those with blue dots do not.

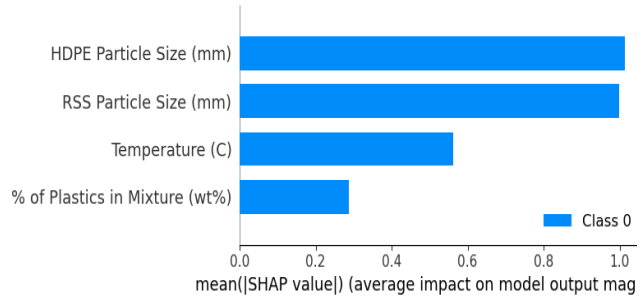

Fig. 16 Variable importance plot - global interpretation of the proposed model

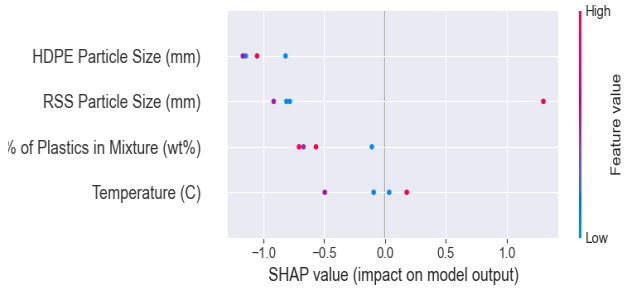

Fig. 17 RL prediction interpretation using SHAP

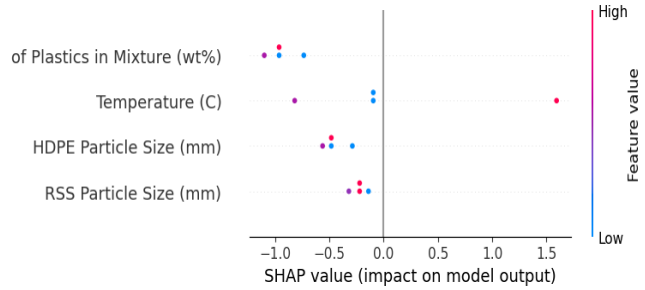

Fig. 18 XGBoost prediction interpretation using SHAP

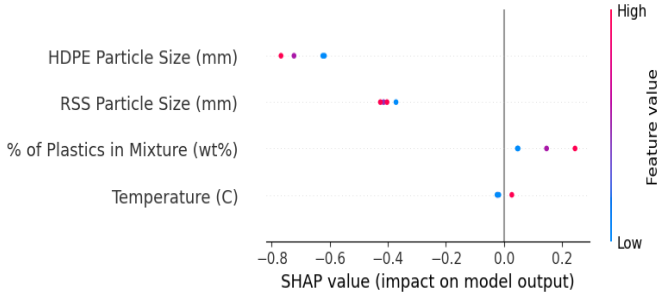

Fig. 19 SVR prediction interpretation using SHAP

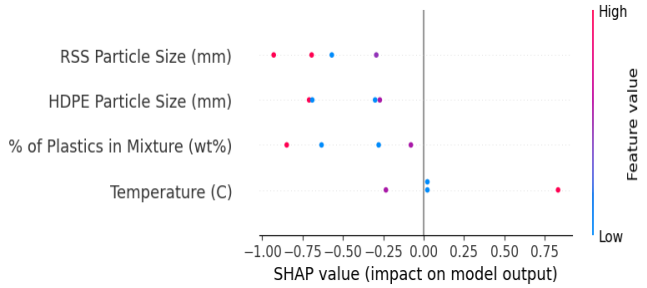

Fig. 20 K-NN prediction interpretation using SHAP

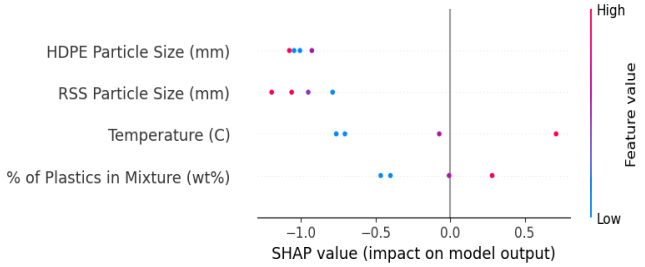

Fig. 21 Proposed model prediction interpretation using SHAP

4.2.2 LIME

LIME focuses on describing the model's prediction for specific occurrences rather than giving a broad knowledge of the model on the full dataset. The suggested model based on Keras API and the LIME explanation for the first instance in the test data are shown in Fig. 22 together with the final feature contribution in a tabular fashion. From left to right, the result includes three key pieces of information: (1) the model's predictions, (2) the contributions of the features, and (3) the actual value of each feature. From Fig 22, the proposed model's predicted value for hydrogen production is 39.12. The variables RSS Particle size, Temperature and Percentage of the mixture have a positive influence while HDPE Particle size has a negative influence on predicted hydrogen production. All the values are in thousands of dollars. The same explanation goes for other employed models.

***4.2.3** ELI5*

This paper tends to explain the result of the implemented Tree-based models we (RFR and XGBoost) as shown in Fig 23 to Fig. 26. The weights assigned to each characteristic as seen in Figs. 23 and 25, indicates the average influence of a characteristic on the predictions, while the sign indicates the direction of that impact. For the Random Forest regressor, we suspect that the Temperature will contribute highly to the production of hydrogen. However, Fig 24 says otherwise

as our model indicated that the prediction made by the random forest regressor was biased.

Weight	Feature
0.3812 ± 0.4405	HDPE Particle Size (mm)
0.2601 ± 0.3864	Temperature (C)
0.1960 ± 0.3046	RSS Particle Size (mm)
0.1627 ± 0.3085	% of Plastics in Mixture (wt%

Fig. 23 RF weight and feature identification using ELI-5

	0	1	2	3
1	0.5	0.777778	0.6	0.6

	0
1	39.262

y (score **42.522**) top features

Contribution?	Feature	Value
+44.669	<BIAS>	1.000
+0.251	RSS Particle Size (mm)	0.778
-0.489	% of Plastics in Mixture (wt%)	0.600
-0.940	Temperature (C)	0.500
-0.970	HDPE Particle Size (mm)	0.600

Fig. 24 RF prediction explanations using ELI-5

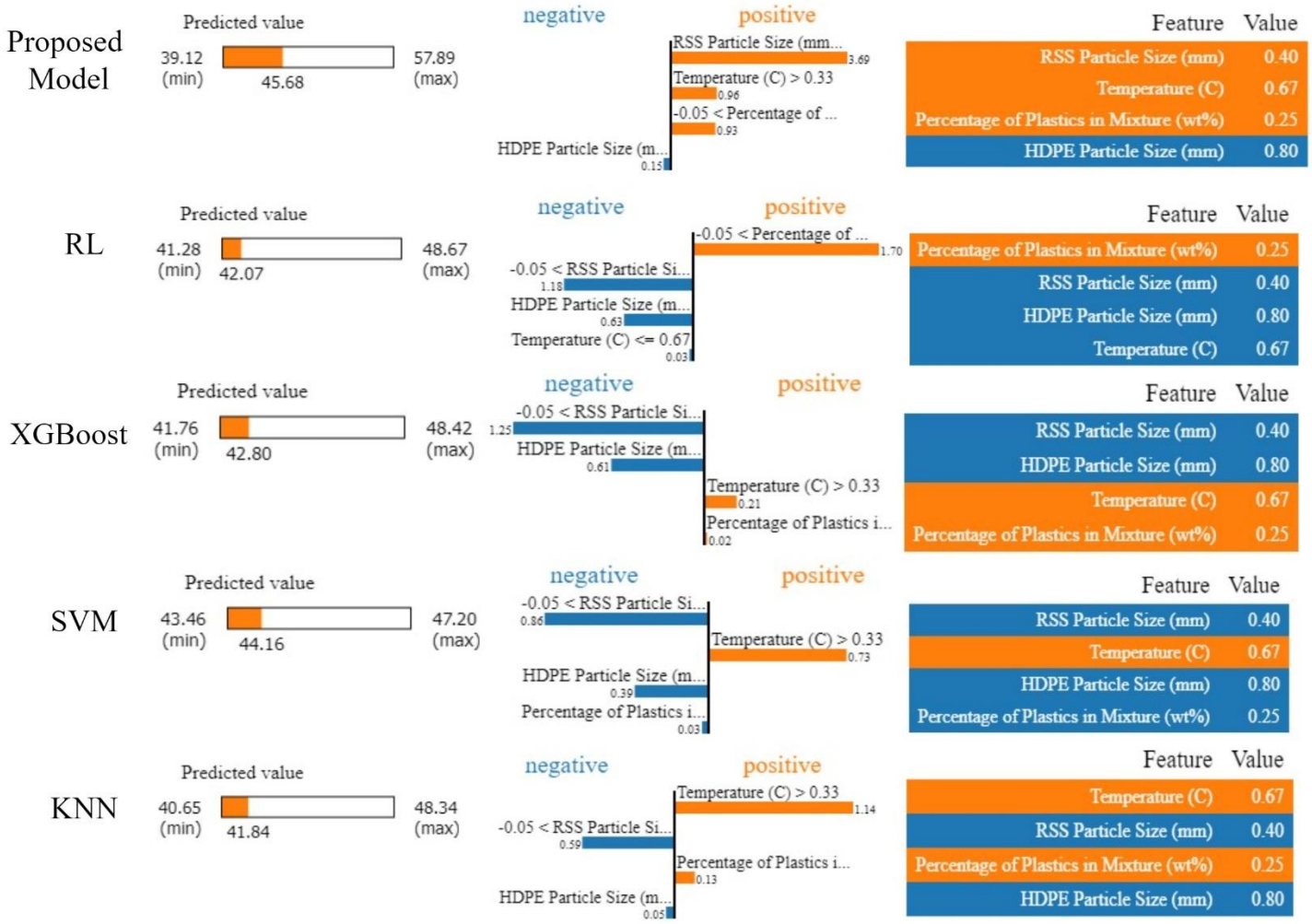

Fig. 22 Proposed model prediction interpretation using LIM

The result shows that the most important factor was that the prospect sees the combination of the features to be important ranking RSS Particle Size first followed by % of Plastic in the mixture, temperature, and lastly HDPE Particle size. For the XGBoost model as seen in Fig. 25. we suspect that the Temperature will contribute highly to the production of hydrogen. However, Fig 26 says otherwise as our model indicated that the prediction made by the XGBoost was biased. The result shows that the most important factor was that the prospect sees the combination of the features to be important in ranking HDPE Particle size. followed by temperature, % of Plastic in the mixture, and lastly RSS Particle Size.

Weight	Feature
0.3232	RSS Particle Size (mm)
0.2954	% of Plastics in Mixture (wt%)
0.2238	HDPE Particle Size (mm)
0.1575	Temperature (C)

Fig. 25 XGBoost weight and feature identification using ELI-5

	0	1	2	3
1	0.777778	0.6	0.6	0.5

	0
1	39.262

y (score **41.261**) top features

Contribution[?]	Feature	Value
+44.060	<BIAS>	1.000
-0.373	HDPE Particle Size (mm)	0.600
-0.556	Temperature (C)	0.778
-0.779	% of Plastics in Mixture (wt%)	0.500
-1.091	RSS Particle Size (mm)	0.600

Fig. 26 XGBoost prediction explanations using ELI-5

4.3 Discussions

The majority of machine learning models are still black boxes despite their broad deployment. Understanding the rationale behind certain forecasts is crucial for determining one's level of trust, which is crucial if one intends to act on a prediction. At the moment, models are assessed using accuracy measures on a validating dataset. However, actual data is frequently vastly different, and the assessment score could not accurately reflect the objective of the product. In addition to such measurements, it is useful to examine specific forecasts and their justifications. In many businesses, machine learning models are utilized because biased data might result in judgments that have a significant negative effect.

From the recorded results, RFR outperforms other models in terms of accuracy and error metrics, with the lowest MAE, MSE, and RMSE. XGBoost performs worse than RFR, with larger errors and a very low R2 score. SVM has a negative R^2 score, indicating poor model fit. KNN falls between RFR and XGBoost in terms of error metrics and R^2. The Proposed Model performs the best, with the lowest error values (MAE, MSE, RMSE) and the highest R^2. It also effectively handles data range and skewness, as shown by low MSLE and RMSLE. Figures 11 to 14 illustrate machine learning model predictions vs. actual results, with the Proposed Model's result shown in Figure 15. SHAP values are used to assess variable significance. HDPE particle size and RSS particle size are the most significant features, while the percentage of plastics in the mixture has less influence. Figures 16 to 21 provide a detailed breakdown of the effect of each attribute on specific results. LIME is used to describe the model's prediction for specific instances. It shows feature contributions to a prediction. An example for the Proposed Model shows that HDPE Particle Size has a negative influence on predicted hydrogen production, while RSS Particle Size, Temperature, and Percentage of Mixture have positive influences. ELI5 is used for global interpretation and understanding of model parameters. The Tree-based models (Random Forest and XGBoost) are explained in Figs. 23 to 26, indicating the influence of features on predictions. Overall, the Proposed Model appears to be the best-performing model for the given task, with comprehensive explanations of feature importance and model predictions provided through various techniques, including SHAP, LIME, and ELI5.

4.4 Limitations and Future Works

This study identified a few data instances as a major drawback to ascertaining the evaluation of Machine learning predictions for hydrogen production. Thus, data augmentation will be looked into in our next study. Secondly, the proposed model-sensitive parameter analysis was not included in this study to show the various effects of different hyperparameters in the model predictions. For the explainable AI models, only one instance was used for illustration due to the limited number of pages required for this conference. Experimenting with various test instances will show more insights to the readers and research community.

5. CONCLUSION

This study aimed to predict hydrogen production in the context of co-gasification of biomass and plastics using machine learning and deep learning models while emphasizing interpretability through explainable AI methods. Among the machine learning models tested, RFR exhibited the best performance in terms of accuracy and error metrics. The Proposed Model based on Keras API outperformed all models, providing the most precise predictions and accounting for a significant proportion of data variation. Explainable AI techniques, such as SHAP, LIME, and ELI5, were employed to shed light on the black-box nature of machine learning models. SHAP values identified HDPE particle size and RSS particle size as the most significant factors influencing hydrogen production. LIME was used to provide detailed explanations for individual predictions, highlighting the impact of specific features on hydrogen production. For instance, HDPE Particle Size had a negative influence, while RSS Particle Size, Temperature, and Percentage of

Mixture had positive influences. ELI5 was utilized for global interpretation, revealing the importance of different features in the Tree-based models (Random Forest and XGBoost). While this study has made significant progress in predicting hydrogen production and enhancing interpretability, there are several avenues for future research including Ensemble Models, Feature Engineering, Real-Time Predictions, Data Collection, Optimization Strategies, and Cost-Benefit Analysis: Evaluate the cost-effectiveness of implementing these predictive models and the potential impact on the energy industry

This study has demonstrated the potential of machine learning models and explainable AI techniques in predicting hydrogen production. Future research should aim to refine and expand upon these findings to contribute further to the sustainable energy sector and bridge the gap between accuracy and interpretability in predictive models.

ACKNOWLEDGEMENT

The authors gratefully acknowledge the support of the National Natural Science Foundation of China (NFSC, Grant No. 52007025) and the Science and Technology Support Program of Sichuan Province (2022JDRC0025).

DECLARATION OF INTEREST STATEMENT

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

REFERENCE

[1] Agyekum E B, Velkin V I. Optimization and techno-economic assessment of concentrated solar power (csp) in south-western africa: a case study on ghana[J]. Sustainable Energy Technologies and Assessments, 2020, 40:100763.

[2] Gyamfi B A, Adebayo T S, Bekun F V, et al. Beyond environmental kuznets curve and policy implications to promote sustainable development in mediterranean[J]. Energy Reports, 2021, 7:6119–6129.

[3] Tarhan C, Çil M A. A study on hydrogen, the clean energy of the future: hydrogen storage methods[J]. Journal of Energy Storage, 2021, 40:102676.

[4] Zhao Y, Ramzan M, Adebayo T S, et al. Role of renewable energy consumption and technological innovation to achieve carbon neutrality in spain: fresh insights from wavelet coherence and spectral causality approaches[J]. Frontiers in Environmental Science, 2021, 9:769067.

[5] Yaqoob S J, Motahhir S, Agyekum E B. A new model for a photovoltaic panel using proteus software tool under arbitrary environmental conditions[J]. Journal of Cleaner Production, 2022, 333:130074.

[6] Adebayo T S, Awosusi A A, Oladipupo S D, et al. Dominance of fossil fuels in japan's national energy mix and implications for environmental sustainability[J]. International Journal of Environmental Research and Public Health, 2021, 18(14):7347.

[7] da Silva Veras T, Mozer T S, da Silva César A, et al. Hydrogen: trends, production and characterization of the main process worldwide[J]. International journal of hydrogen energy, 2017, 42(4):2018–2033.

[8] Devasahayam S, Raju G B, Hussain C M. Utilization and recycling of end of life plastics for sustainable and clean industrial processes including the iron and steel industry[J]. Materials Science for Energy Technologies, 2019, 2(3):634–646.

[9] Devasahayam S. Decarbonising the portland and other cements—via simultaneous feedstock recycling and carbon conversions sans external catalysts[J]. Polymers, 2021, 13(15):2462.

[10] Sepe A M, Li J, Paul M C. Assessing biomass steam gasification technologies using a multi-purpose model[J]. Energy Conversion and Management, 2016, 129:216–226.

[11] Devasahayam S. Opportunities for simultaneous energy/materials conversion of carbon dioxide and plastics in metallurgical processes[J]. Sustainable Materials and Technologies, 2019, 22:e00119.

[12] Devasahayam S. Catalytic actions of mgco3/mgo system for efficient carbon reforming processes[J]. Sustainable Materials and Technologies, 2019, 22:e00122.

[13] Wang Z, Burra K G, Lei T, et al. Co-pyrolysis of waste plastic and solid biomass for synergistic production of biofuels and chemicals-a review[J]. Progress in Energy and Combustion Science, 2021, 84:100899.

[14] Block C, Ephraim A, Weiss-Hortala E, et al. Co-pyrogasification of plastics and biomass, a review[J]. Waste and Biomass Valorization, 2019, 10:483–509.

[15] Guleria P, Naga Srinivasu P, Ahmed S, et al. Xai framework for cardiovascular disease prediction using classification techniques[J]. Electronics, 2022, 11(24):4086.

[16] Ravegnini G, Ferioli M, Morganti A G, et al. Radiomics and artificial intelligence in uterine sarcomas: a systematic review[J]. Journal of Personalized Medicine, 2021, 11(11):1179.

[17] Pappada S M. Machine learning in medicine: it has arrived, let's embrace it[J]. Journal of Cardiac Surgery, 2021, 36(11):4121–4124.

[18] Carvalho D V, Pereira E M, Cardoso J S. Machine learning interpretability: a survey on methods and metrics[J]. Electronics, 2019, 8(8):832.

[19] Yao Y. Explanatory pluralism in explainable ai[C]. In: *Machine Learning and Knowledge Extraction: 5th IFIP TC 5, TC 12, WG 8.4, WG 8.9, WG 12.9 International Cross-Domain Conference, CD-MAKE 2021, Virtual Event, August 17–20, 2021, Proceedings 5*. Springer, 2021: 275–292.

[20] Gerlings J, Jensen M S, Shollo A. Explainable ai, but explainable to whom? an exploratory case study of xai in healthcare[J]. Handbook of Artificial Intelligence in Healthcare: Vol 2: Practicalities and Prospects, 2022, :169–198.
[21] Vidas L, Castro R. Recent developments on hydrogen production technologies: state-of-the-art review with a focus on green-electrolysis[J]. Applied Sciences, 2021, 11(23):11363.
[22] Ishaq H, Dincer I, Crawford C. A review on hydrogen production and utilization: challenges and opportunities[J]. International Journal of Hydrogen Energy, 2022, 47(62):26238–26264.
[23] Bion N, Duprez D, Epron F. Design of nanocatalysts for green hydrogen production from bioethanol[J]. ChemSusChem, 2012, 5(1):76–84.
[24] d'Amore-Domenech R, Santiago O, Leo T J. Multicriteria analysis of seawater electrolysis technologies for green hydrogen production at sea[J]. Renewable and Sustainable Energy Reviews, 2020, 133:110166.
[25] Haider S A, Sajid M, Iqbal S. Forecasting hydrogen production potential in islamabad from solar energy using water electrolysis[J]. International Journal of Hydrogen Energy, 2021, 46(2):1671–1681.
[26] Ayodele B V, Mustapa S I, Alsaffar M A, et al. Artificial intelligence modelling approach for the prediction of co-rich hydrogen production rate from methane dry reforming[J]. Catalysts, 2019, 9(9):738.
[27] Hossain M A, Ayodele B V, Cheng C K, et al. Artificial neural network modeling of hydrogen-rich syngas production from methane dry reforming over novel ni/cafe2o4 catalysts[J]. International Journal of Hydrogen Energy, 2016, 41(26):11119–11130.
[28] Alsaffar M A, Ghany M A R A, Ali J M, et al. Artificial neural network modeling of thermo-catalytic methane decomposition for hydrogen production[J]. Topics in Catalysis, 2021, 64:456–464.
[29] Abdelkareem M A, Soudan B, Mahmoud M S, et al. Progress of artificial neural networks applications in hydrogen production[J]. Chemical Engineering Research and Design, 2022, 182:66–86.
[30] Katterbauer K, Qasim A, Marsala A, et al. A data driven artificial intelligence framework for hydrogen production optimization in waterflooded hydrocarbon reservoir[C]. In: *Abu Dhabi International Petroleum Exhibition and Conference*. 2021: D041S123R003.
[31] Santhosh J, Sarkar O, Mohan S V. Green hydrogen-compressed natural gas (bio-h-cng) production from food waste: organic load influence on hydrogen and methane fusion[J]. Bioresource Technology, 2021, 340:125643.
[32] Soler Crespo V E, Linares Hurtado J I, Arenas Pinilla E M, et al. Hydrogen from municipal solid waste as a tool to compensate unavoidable ghg emissions[J]. 2022.
[33] Yadav V S, Vinoth R, Yadav D. Bio-hydrogen production from waste materials: a review[C]. In: *MATEC Web of Conferences*. 2018: 2020.
[34] Rezaeitavabe F, Saadat S, Talebbeydokhti N, et al. Enhancing bio-hydrogen production from food waste in single-stage hybrid dark-photo fermentation by addition of two waste materials (exhausted resin and biochar)[J]. Biomass and Bioenergy, 2020, 143:105846.
[35] Hosseinzadeh A, Zhou J L, Altaee A, et al. Machine learning modeling and analysis of biohydrogen production from wastewater by dark fermentation process[J]. Bioresource technology, 2022, 343:126111.
[36] Haq Z U, Ullah H, Khan M N A, et al. Hydrogen production optimization from sewage sludge supercritical gasification process using machine learning methods integrated with genetic algorithm[J]. Chemical Engineering Research and Design, 2022, 184:614–626.
[37] Guo H, Wu S, Tian Y, et al. Application of machine learning methods for the prediction of organic solid waste treatment and recycling processes: a review[J]. Bioresource technology, 2021, 319:124114.
[38] Low K, Coote M L, Izgorodina E I. Explainable solvation free energy prediction combining graph neural networks with chemical intuition[J]. Journal of Chemical Information and Modeling, 2022, 62(22):5457–5470.
[39] Liao M, Wu F, Yu X, et al. Random forest algorithm-based prediction of solvation gibbs energies[J]. Journal of Solution Chemistry, 2023, 52(4):487–498.
[40] Guidotti R, Monreale A, Ruggieri S, et al. A survey of methods for explaining black box models[J]. ACM computing surveys (CSUR), 2018, 51(5):1–42.
[41] Shi S, Zhang X, Fan W. A modified perturbed sampling method for local interpretable model-agnostic explanation[J]. arXiv preprint arXiv:2002.07434, 2020.
[42] Angiulli F, Fassetti F, Nisticò S. Local interpretable classifier explanations with self-generated semantic features[C]. In: *International Conference on Discovery Science*. Springer, 2021: 401–410.
[43] Kuzlu M, Cali U, Sharma V, et al. Gaining insight into solar photovoltaic power generation forecasting utilizing explainable artificial intelligence tools[J]. IEEE Access, 2020, 8:187814–187823.
[44] Lundberg S M, Lee S-I. A unified approach to interpreting model predictions[J]. Advances in neural information processing systems, 2017, 30.
[45] Ekanayake I, Meddage D, Rathnayake U. A novel approach to explain the black-box nature of machine learning in compressive strength predictions of concrete using shapley additive explanations (shap)[J]. Case Studies in Construction Materials, 2022, 16:e01059.
[46] Mahesh B. Machine learning algorithms-a review[J]. International Journal of Science and Research (IJSR).[Internet], 2020, 9(1):381–386.
[47] Zhou Z-H. Machine learning[J]. 2021.
[48] Chin B L F, Yusup S, Al Shoaibi A, et al. Optimization

study of catalytic co-gasification of rubber seed shell and high density polyethylene waste for hydrogen production using response surface methodology[J]. Advances in bioprocess technology, 2015, :209–223.
[49] Chang H J, Huang K, Wu C. Determination of sample size in using central limit theorem for weibull distribution[J]. International journal of information and management sciences, 2006, 17(3):31.