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A Machine Learning Approach for Pyrolysis of Plastic Waste: An Overview of Types, and Applications

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Abstract:

Pyrolysis pathways have emerged as one of the most promising approaches to managing plastic waste (PW). However, the commercial use of pyrolysis is hampered by a number of unresolved blind spots, and the industrial use of such technologies has been limited. Even though global kinetic techniques have been used for many years to explain pyrolysis models, new developments in computational modeling, such machine learning (ML), provide fresh perspectives. An overview of the types and applications of ML techniques for pyrolysis of PW is the main topic of this review. The outcome shown that ML is a potent tool for pyrolysis process improvement, interpretation, and predictive modeling. In addition to enabling reasonably accurate forecasting of product yields and properties, ML algorithms such as artificial neural networks, genetic algorithm-artificial neural networks, support vector machines, and decision tree techniques can also give researchers insights into complex pyrolysis kinetics so that process parameters can be further tuned to achieve desired results. All things considered, pyrolyzing PW using ML approaches can increase product production and quality, reduce environmental effect, and promote sustainable PW management initiatives.

Keywords — Pyrolysis, Plastic Waste, Machine Learning, Artificial Neural Network, Application of Machine Learning

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I. INTRODUCTION

Plastic is essential to modern life and is used extensively in the automobile, electronics, healthcare, construction, and packaging sectors [1–3]. The manufacture of plastics has increased dramatically since their inception due to social needs and the world's expanding population [4]. Polyethylene (PE), polypropylene (PP), polystyrene (PS), polyvinyl chloride (PVC), and polyethylene terephthalate (PET) are among the petroleum-based polymers that make up the majority of plastics [5]. Also, the global capacity of the current waste management systems is insufficient to securely dispose of or recycle daily generated plastic waste (PW). The discharge of PW in the environment inevitably increased as a result of high consumption of plastic materials [6–8]. Besides, eight million metric tons of microplastic and 1.5 million metric tons of primary microplastic are thought to enter the ocean each year, according to earlier studies [9]. It could take billions of years for PW to break down in the environment [10]. However, energy recovery from solid waste management (SWM) techniques, thermochemical recycling, mechanical recycling, and landfilling can be used to manage PW [11]. One promising and appealing technology is the thermochemical conversion of PW into usable bioenergy. This is because of its quick reaction time, wide variety of products, low carbon dioxide (CO_2) emissions, feedback adaptability, low capital and processing costs, and commercialization

possibilities [11, 12]. PW can be converted via a variety of thermochemical processes, such as gasification, pyrolysis, combustion, carbonization/torrefaction, and liquefaction, to produce green fuels, chemicals, and other derived products. While gasification and pyrolysis are used to create green chemicals, charcoal, and liquid fuels for transportation, combustion is usually used to generate direct heat and electricity. Biofuels produced by pyrolysis or gasification methods can be utilized directly or refined to replace transportation fuels made from petroleum. The negative environmental effects linked to the transportation sector's usage of fossil fuels may be successfully mitigated by this alternative [13]. It can help lessen the detrimental environmental effects of fuels sourced from petroleum by using biofuels. One of the most promising methods for extracting minerals and energy from PW, biomass, and organic waste is pyrolysis [14–16].

Additionally, the conventional models are mathematical formulas that are utilized to determine the ideal values for various operating parameters that affect a process's efficacy or the best operational parameters for a process itself [17, 18]. However, these models have certain drawbacks, such as their intricacy and time commitment [19]. Kinetic models, for instance, are restricted to a certain type of reactor but can take reactor design into account [20]. CFD models are also subject to similar restrictions. One disadvantage of the CFD approach is that, in addition to being costly and complex, CFD models are also very demanding. Researchers used reduced response mechanisms in CFD models to alleviate the high computing demands of these models; nevertheless, due to the simplified assumptions used in their creation, these models are less accurate [21]. In a number of domains, machine learning (ML) is a distinct model that provides numerous benefits over conventional approaches [22]. Predicting yields, optimizing parameters, and tracking pyrolytic processes have all seen a surge in research interest in ML in recent years [23]. ML can precisely map inputs to corresponding outputs, in contrast to traditional models that can only depict the chemical and physical events that occur in a reactor. It accomplishes this by figuring out the intricate mathematical link between several variables or parameters in a process utilizing an operational algorithm. Because ML models are inherently uninterpretable, they are frequently referred to as "black-box" models.

Although they are not interpretable, they offer a number of benefits over kinetic/CFD models. These benefits include computing efficiency, flexibility in complicated systems, and the capacity to manage massive amounts of data. Due to its enormous potential, ML may be used to model pyrolysis processes and produce predictions that are on par with those of conventional models [24]. Techno-economic analysis (TEA) and life cycle assessment (LCA) are two methodologies used to investigate and comprehend the economic and environmental elements of biomass pyrolysis processes. LCA focuses on evaluating the environmental effects of the process's whole life cycle, which includes the manufacturing of raw materials, transportation, processing, and disposal at the end of its useful life [25]. Conversely, TEA concentrates on assessing the pyrolysis process's economic feasibility, taking into account variables including capital expenditures, operating costs, revenues, and profitability [26]. The quality and availability of data unique to the pyrolysis process hinder both LCA and TEA evaluations. It can be difficult to directly compare various evaluations because pyrolysis data can be few and inconsistent, and different research may make different assumptions [27, 28]. This may lead to ambiguities in the evaluation results and make it more difficult to make insightful deductions. In comparison to conventional methodologies, ML algorithms can reduce uncertainties and produce more accurate predictions by utilizing their high throughput potential to gather data for LCA and TEA of PW pyrolysis. Prior review articles in the field of thermochemical biomass conversion, like pyrolysis, have mostly concentrated on the application of ML techniques for predicting chemical kinetic parameters and product yield. In a recent review study, Ascher *et al.* [29] described the uses, drawbacks, and advantages of the common ML algorithms used to model pyrolysis processes. A

thorough review of the research and development related to the application of ML in biomass combustion, torrefaction, gasification, and hydrothermal treatment was given by [30]. The literature on the limitations, opportunities, possibilities, and capacities of ML in promoting the uses and sustainable development of carbon-based materials derived from biomass was reviewed by [31]. This study will therefore focus on different ML approaches used in pyrolysis, their advantages and disadvantages, and the possible pyrolysis research areas where these techniques might be implemented.

II. Research Methodology

To demonstrate the use of ML in pyrolysis processes, a comprehensive review of the most recent research was conducted, with an emphasis on a summary of kinds, uses, and difficulties. The review procedure began with locating published works on the topic of interest. This was accomplished by selecting a collection of phrases, such as "application of ML on pyrolysis processes, types, and challenges," and entering them into the search box of scholarly websites like Google Scholar, the Web of Science (WoS), and the Scopus databases. With the document category limited to "Scientific Article" or "Article" and the language limited to "English," the recovered manuscripts were further filtered to exclude only English-language articles. The selected articles were carefully examined in light of the given keywords.

III. Overview of different Types of Machine Learning Approach for Plastic Pyrolysis

In-depth investigations on the mechanisms for plastics pyrolysis are complicated due to the numerous interlinked network reactions that occur simultaneously. Hence, the prediction of product yields and reactor modelling is extremely complex [32]. Based on the documents dataset examined, the landscape of plastic pyrolysis is being transformed by ML-based tools such as artificial neural network (ANN) [33], genetic-algorithm-artificial-neural-network (GA-ANN), and support vector machines (VSM) [33]. The workflow for ML based optimization of pyrolysis products is given in Fig. 1.

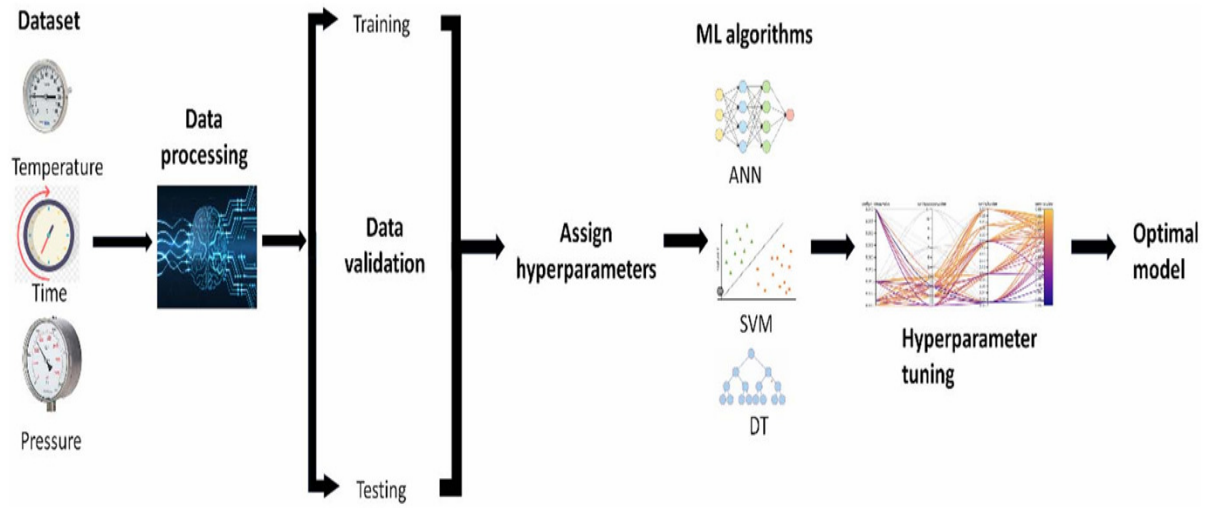

Fig. 1 Machine learning workflow for optimizing plastic waste pyrolysis

A. Genetic Algorithm-Artificial Neural Network (GA-ANN)

New methods that concentrate on the mechanics of natural selection and natural genetics, including GA-ANN, have been used to study and optimize the plastic pyrolysis reactions as machine power has increased. Though in distinct ways, ANN and GA-ANN both strive for the greatest outcomes. Genetic algorithms (GA) are heavily focused on issue optimization, even though ANNs are used to anticipate the answer for the given inputs. Numerous genetic algorithm-based applications have demonstrated their usefulness in a variety of domains,

including engineering [34]. A genetic algorithm was used by [35] to assess fifteen distinct decomposition models that were published in the literature. Support for the ANN on the genetic algorithm and the use of ML to model the data from the catalytic pyrolysis reaction of PP (based on Al-MCM41) are the two main pillars upon which this study is built. According to the authors' findings, once the weak connections are eaten, the PP degradation process shifts from initiation-propagation to random scission. Accordingly, by investigating parallel methods based on GA, comparable outcomes for PP pyrolysis employing HZSM-5 as a catalyst have been reported by [35]. When comparing this work to the one before it, it can be shown that GA is able to forecast changes in the kinetic parameters based on the catalyst (128 kJ/mol for Al-MCM41 and 92 kJ/mol for HZSM-5, respectively). Despite the accuracy achieved by using the GA to compare multiple kinetic models at the same time, the models are so similar that additional tools, like "operando," must be used to track and analyze the reaction in order to identify the precise decomposition model and the rate-limiting step. With a high degree of certainty, several recent GA investigations of virgin polymers like polystyrene, polyurethane, or PW [36] have been highlighted. The ability of hybrid GA-ANN to forecast the change in liquid yields during the catalytic conversion of PP/PE was demonstrated by [37]. In order to obtain the highest production of C_4–C_{13} liquids with a comparatively high degree of precision, the authors adjusted the reactor settings. The modeling results show that catalyst properties have a major impact on product yields, even if the calculated kinetic parameters are not shown in this work. One of the main responsibilities in the scaling process is to comprehend and forecast the reactor's behavior. In order to simulate the normal composition of PW, [38] tested various types of plastic feedstock. Based on the catalyst/feedstock ratio, reaction temperature, and reaction time data, the authors simulated the product yields with a high degree of confidence. The modeling result indicates that each design is statistically adequate in terms of R^2 and MSE, making both highly accurate and dependable tools. The authors assessed the ability of the ANN and least square support vector machine to predict the gas and liquid products.

B. Decision Tree (DT)

Pyrolysis benefits greatly from the use of Decision Trees (DTs), a potent ML method that makes it possible to analyze and forecast results based on a variety of process variables. For problems involving regression and classification, DTs are a popular and effective technique [22]. By choosing split points, they divide the feature space into several sections. Each region that is produced is subjected to the splitting process recursively, which at first produces a big tree structure that could be prone to overfitting. This is addressed by pruning procedures, which frequently use a cost-complexity criterion that strikes a compromise between the tree's goodness of fit and generalization ability, guaranteeing the model's correctness while adapting to new, unknown data. Fig. 2 illustrates the process of decision tree decision making.

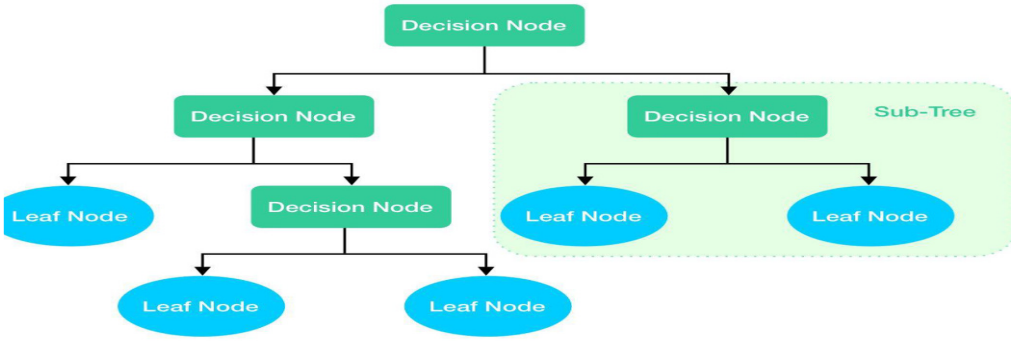

Fig. 2 Decision Trees (DT) and decision-making capabilities

C. Ensemble Methods

Several DTs are used in the ensemble learning technique known as random forest (RF) to produce reliable and accurate predictions. Using random selections of training data and covariates, each DT is built separately. In contrast to RF, which combines several DTs in parallel, Gradient Boosting (GB) constructs an ensemble of trees one after the other, fixing the mistakes of the earlier trees. GB is able to capture intricate linkages in the pyrolysis process and progressively improve predictions because to this iterative method. Generally speaking, an RF model performs worse than a well-tuned GB model. However, GB models are prone to overfitting, and GB model fine-tuning can be difficult [39]. On the other hand, RF models have fewer hyperparameters and can still produce good results even when the hyperparameters are not chosen optimally. By modifying variables such as learning rate, number of trees, and maximum tree depth, hyperparameter tuning is essential for maximizing the performance of DT-based models and improving their accuracy and generalization. By combining predictions from several trees, these ensemble approaches have an advantage over a single DT in that they can decrease overfitting and enhance generalization [40]. This ensemble approach is a useful tool for yield prediction and optimization because it allows RF and GB to manage intricate interactions in the pyrolysis process. The capacity of DTs and its variations to manage complex interactions between process variables and output reactions is one of their advantages in pyrolysis. To attain the intended results, process optimization activities are guided by this knowledge. These techniques also have the benefit of not requiring a lot of data preprocessing and being robust against noise and anomalies in pyrolysis data. By combining predictions from several trees, RF and GB lessen the effect of individual noisy samples or variables, which are inherent in experimental or simulated data from various sources. This combination guarantees more precise forecasts and offers trustworthy information about the pyrolysis process. These techniques are used in the context of pyrolysis to forecast the yield and caliber of pyrolysis products by taking into account various process variables. These models help choose the best circumstances by estimating predicted results based on inputs such as temperature, heating rate, and feedstock composition [29]. Additionally, by measuring the relative significance of each process variable, RF and GB make sensitivity analysis easier. With this knowledge, researchers can concentrate on enhancing the intended product qualities and process effectiveness while also comprehending which variables have a major influence on the pyrolysis process.

D. Support Vector Machines (SVM)

Pyrolysis makes use of the Support Vector Machine (SVM), a potent ML method that makes it possible to analyze and forecast results based on a variety of process variables. The goal of the supervised learning technique SVM is to identify the best hyperplane for dividing the data into distinct groups. Fig. 3 provides an illustration of this. SVM has several benefits, including the capacity to manage intricate relationships, resilience to noise, and adaptability when working with both linear and non-linear data. When dealing with noisy or uncertain data, which is a feature of all pyrolysis data, whether it be simulation or experimental, SVM is incredibly resilient. However, SVM can handle noisy data because it can find the best hyperplane to maximally separate classes. By concentrating on the most relevant samples, SVM reduces the impact of noise and outliers, resulting in more accurate predictions and useful insights into the pyrolysis process [41]. However, SVM has drawbacks, including computational complexity, especially when working with large data sets. It can take a lot of time and resources to train an SVM model, especially when there are a lot of process variables, which can be a major problem as pyrolysis data becomes more accessible. Careful feature selection and suitable preprocessing methods are needed to overcome these obstacles. SVM can be applied to regression as well as classification. SVM, on the

other hand, is frequently used in pyrolysis, mostly for regression tasks that predict continuous output variables, including forecasting the yield or composition of pyrolysis products based on what influences them. Selecting an appropriate kernel function is essential to building a model that works as intended. By determining the ideal values for parameters like the regularization parameter (C) and the kernel parameters to attain the best trade-off between model complexity and generalization ability, hyperparameter tweaking is essential to maximizing the performance of SVM [30].

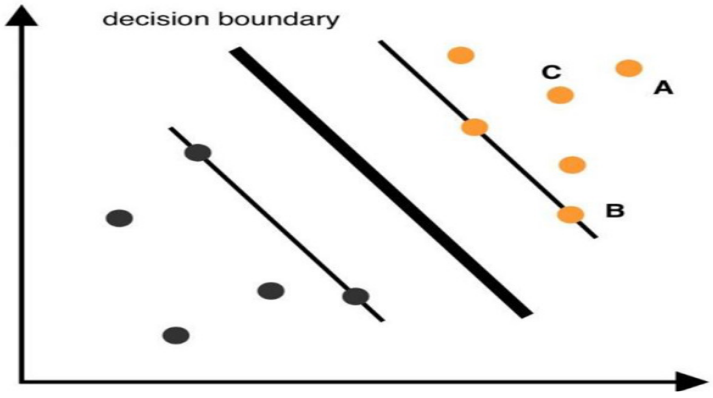

Fig 3. Pictorial view of the supporting vectors, decision boundary (boldened) and the points in the feature space

E. Artificial Neural Networks

In the realm of pyrolysis, artificial neural networks (ANNs) have become a potent tool for assessing and forecasting different process elements. The structure and operation of the human brain served as the inspiration for the ANN, a computational model made up of interconnected nodes known as neurons. Based on the relationships discovered from the input-output data, these networks are able to learn from data, spot intricate patterns, and generate predictions [42, 43]. According to Fig. 4, an ANN is made up of three layers: (i) an input layer that receives input data; (ii) an output layer that makes predictions; and (iii) a hidden layer that sits between the input and output levels and handles the majority of the network's tasks. An ANN typically arranges data, "learns" to identify patterns, and then forecasts the results for a fresh batch of comparable data. The central processing unit of an ANN is made up of neuron layers with less than two hidden layers. A deep neural network (DNN) is defined as one that has more than two hidden layers [44]. The literature provides a thorough analysis of the specifics of the underlying algorithms and architecture, as well as the "forward" and "backward" propagation strategies employed to train the networks [45–47]. Over the past ten years, there has been a steady increase in the use of ML and its representative subset in engineering and other subfields, as discussed by [48]. Drugs, materials design, and "in silico" catalyst creation are some of the key areas with noteworthy advancements in this field [49]. The number of new applications to comprehend the connection between catalyst characteristics and reaction performance is growing quickly. Additionally, the ability to screen various reaction paths with non-linear correlations and get past conventional bottlenecks has improved with the present advancement of ML. A novel and more computationally viable method for predicting reaction yields, processes, and kinetic parameters is represented by the recent use of ML in plastic pyrolysis. The aforementioned elements are essential to scaling-up procedures, particularly those that conventional kinetic models are unable to monitor. It has been shown that ML can be used in plastic pyrolysis [50]. One of the earliest attempts to train an ANN to examine the kinetic parameters of the heat degradation of PE and other natural polymers is this study. Through the use of 20 input data points from each experimental TGA curve at varying

heating rates, along with 20 input neurons, 10 hidden layer neurons, and 3 output layer neurons (ANN-20-10-3), the authors were able to accurately predict the kinetic parameters (activation energy Ea, reaction order n, and the pre-exponential factor k_0) within the range previously reported by model-free or model-fitting approaches.

Similarly, Fazilat *et al.* [51] were able to determine the kinetic parameters for the thermal degradation of Nylon 6 (also known as polycaprolactam) with a high degree of accuracy. This was accomplished by combining ANN with fuzzy interference-based adaptive networks to uncover the nature of the relationships the ANN formed. This work marks a significant advancement in the use of ANN for plastic pyrolysis, even though the number of neuron layers is unknown. The authors' modeling tool produced results that closely matched the Friedman or KAS model and the experimental data. The results indicate that it may be possible to incorporate decision-making tools and predictive models into the plastic pyrolysis process. In order to estimate the composition yield for the pyrolysis of PW including HDPE, LDPE, PP, and PS in a fixed-bed reactor, Abnisa *et al.* [52] used ANN. In addition, the authors trained the ANN using a combination of pyrolysis products and PW as input and output data. With a very low mean square error (MSE < 2.6×10^{-4}) and a high coefficient of determination ($R^2 > 0.9$), the authors were able to accurately and successfully predict the experimental and reported data using an ANN architecture consisting of four neurons for the input layer, ten in the hidden layer, and the remaining three for the output layer (ANN-4-10-3). Nonetheless, Abnisa's work was founded on architecture that was comparable to that employed by [50]. The scientists employed data from a batch reactor, which is a more accurate scale than that used in earlier thermogravimetric analysis investigations. In order to create a highly effective kinetic model for LDPE pyrolysis, Al-Yaari & Dubdub [53] examined the effects of several neural network designs and transfer functions [54]. Based on two distinct designs (ANN-2 10-10-1 or ANN 3-10-10-1), the results validate the adaptability of the ANN and the ability of the two transfer functions (Tan-sig-Logsig or Logsig-Logsig) to mimic the catalytic pyrolysis reaction of HDPE and LDPE, respectively. The ANN-3-10-10-1 and Logsig–Logsig are the best architecture and transfer functions, respectively, according to the MSE and R^2 achieved, even if the authors did not draw a conclusion favoring a particular strategy. In terms of MSE and R^2, the results offer more proof that ML applications work. The analysis also indicates that one or two hidden layers with ten neurons each are the optimal designs for plastic pyrolysis [50, 52]. However, it takes some trial and error to figure out how many neurons or hidden layers to use for data modeling. Stathakis promotes the employment of a genetic algorithm [55], although this is merely a broad concept, and as [53] shows, neuron layers need to be shaped according to certain parameters.

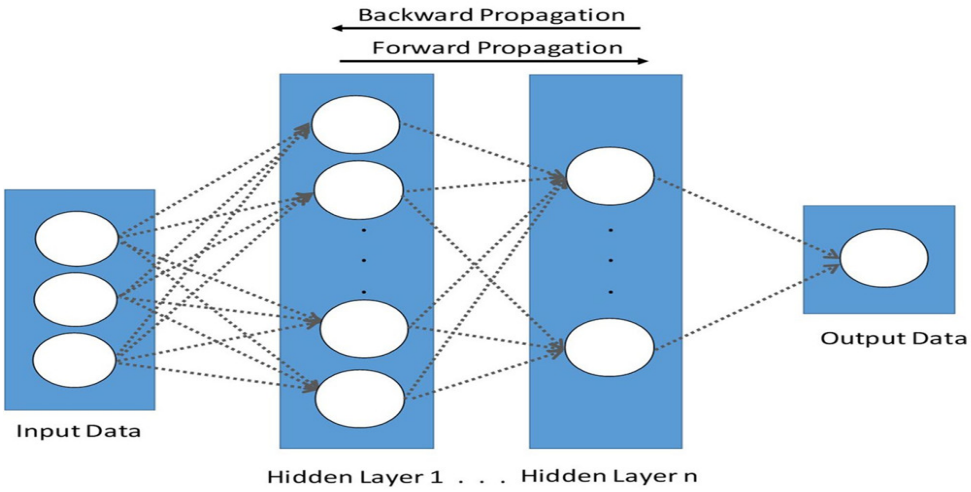

Fig. 4. Schematic representation of a typical artificial neural network (ANN)

IV. APPLICATIONS OF MACHINE LEARNING FOR OPTIMAL REACTOR PERFORMANCE

Through implicit and automated learning that develops on its own without the need for explicit pre-programming, Industry 4.0 uses ML to handle complex queries [56]. In the context of pyrolysis, ML algorithms predict the quantities of different pyrolysis products, such as gas, char, and pyrolysis oil, as well as their physical and chemical makeup. These predictions can help scientists and business experts improve pyrolysis processes to achieve the necessary product yields and compositions and adjust process parameters to meet requirements. The ANN and SVR techniques have been extensively employed in the field of ML model construction to model PW pyrolysis [57, 58]. Determining the input and output variables is crucial for building ML models. Different input variables related to PW pyrolysis have been investigated in a number of ML research [59, 60]. In order to forecast the weight loss and ascertain the activation energy of PW during pyrolysis, ML modeling research focuses on examining pyrolysis kinetics. Typically, time, temperature, and pressure are set as the input parameters, while yield is the outcome. The distribution of liquid and gas generated by plastic pyrolysis has been predicted using the SVR, ANN, GA-ANN, and DT. With a test of $R^2 > 0.85$ for liquid yield, it was found that DT performed better than the others. Additional training improved the prognosis of other items' attributes, with R^2 values ranging from 0.61 to 0.94124. The impact of varying PW to biomass ratios on yield and conversion was also examined using ML, which produced a noteworthy R^2 that ranged from 0.81 to 0.94128. The kind of PW, temperature, heating rate, and quantity and type of catalyst were among the variables used by SVR and GP models to predict the amount of gas produced during the pyrolysis of packaging waste. The R^2 score for the SVR model was 0.89. The ML model interpretation was enhanced by the Shapley additive explanations approach, which demonstrated that the biomass to plastic ratio and pyrolysis temperature were important determinants of oil output [61]. Additionally, at 525 °C with 10 weight percent, the highest oil yield of 82.3 weight percent and the highest styrene to aromatics ratio of 55.2 weight percent were achieved using ANN-genetic algorithm optimization.

In another study, the co-pyrolysis of oily sludge and HDPE on conversion and degradation reactions was examined, which indicated synergistic effects between the two, enhancing the conversion, and accelerating the degradation reactions due to significant CH_3 radicals generated by HDPE

pyrolysis. Additionally, the researchers developed two ANN models to anticipate the interactive impact and activation energy, achieving high testing R^2 values of 0.99 and 0.92, respectively. The ANN model was later developed to optimize pyrolysis conditions, to achieve highest synergistic effect and reduce the activation energy. The model determined that the optimal conditions for the highest synergistic effect of 90.6% at 480 °C, a heating rate of 10°C per minute, and biomass to plastic ratio of 0.7, with the experimental validation error of 6%. The tree-based kinetic Monte Carlo model was made using parameters regulating Bayesian optimization to simulate the pyrolysis routes. The research revealed that styrene monomer might be recovered as feedstock for styrene polymerization by improving its yield and selectivity during pyrolysis, with peak styrene yield of 77.3 wt% attained at 600 °C [64]. It was also underlined that in order to create light oil from co-pyrolysis, lower temperatures, higher plastic mass fractions, and lower carrier gas flow rates were preferred. ML approaches have been used to explore the pyrolysis kinetics and forecast, analyze, and improve the output of desired products with outstanding quality in PW pyrolysis [62]. The weight loss, activation energy, and pre-exponential factor could all be precisely predicted with an R^2 of greater than 0.99 and a relative error of 6.8% in a study that used thermogravimetric measurements and ANN modeling to investigate the thermal pyrolysis behavior of HDPE [63]. Additionally, ML approaches are useful tools that can support the investigation of PW pyrolysis products, especially when working with complicated compositions of bio-oil. By creating an ANN model and using spectral data of polar and non-polar phases as inputs to predict the fuse index, gas chromatography-mass spectrometry and ML techniques were successfully used to predict and analyze the liquid products, such as hydrocarbons resulting from plastic pyrolysis post-ozone treatment [65]. Furthermore, ML techniques are helpful resources that can aid in the study of PW pyrolysis products, particularly when dealing with complex bio-oil compositions. Gas chromatography-mass spectrometry and ML techniques were successfully used to combine plastic pyrolysis oil and coconut oil with diesel to assess their potential use in a diesel engine. An ANN model was created to forecast the fuel performance and emission parameters, and the fuse index was predicted using spectral data of polar and non-polar phases as inputs. After adjusting the hyperparameters, the study demonstrated that the ANN model could predict the experimental results with an accuracy of 90% to 93.5% [67].

V. OUTLOOK ON PLASTIC PYROLYSIS MODELS

One of the best methods for managing PW is plastic pyrolysis. The procedure can promote the shift to a circular carbon economy and lessen the carbon footprint of plastic. However, the kinetic modeling and reaction processes of the pyrolysis of PW do have certain blind spots. Scientists can learn the fundamentals of pyrolysis through the conventional method, which is based on the kinetic analysis of global models. Scientists have developed interatomic potentials and estimated energy exchanges using ML to get around the limitations of these models. Quantum mechanical (QM) data, also known as machine-learned interatomic potentials (MLPs), are used to train the ML [68]. Chemical equilibrium and solid-gas interaction can be explained by these novel techniques, which may also aid in forecasting how catalysts would change under reaction circumstances [69]. In recent years, [70] and [71] have highlighted the progress made in this approach. Recently, [72] demonstrated advancements in MLP by the pyrolysis of glucose as a probe molecule. The authors were able to conduct a thorough investigation of the evolution of glucose breakdown by utilizing the capability of global neural networks. The final reaction database was depurated to yield 6000 reaction pairs and 4000 distinct molecules after 1.2 million minima and 150,000 reaction pairs were managed. The most significant mechanisms for the synthesis of 5-hydroxymethylfurfural (HMF) were revealed by the authors' findings. The MLP combined with the global neural network offers a powerful tool to

investigate the intricate paths of chemical reactions, as evidenced by the HMF product being the most valued product seen throughout experiments. These models are limited to narrow ranges of reaction parameters and disregard the effects of mass transport, heat, and catalysts, among other features. These limitations aid in the explanation of why more complex kinetic models is needed to accurately predict and track the final products of plastic pyrolysis across a wide range of conditions and feedstocks at high temporal and geographical scales. Gaining this insight can help reduce the primary bottlenecks and close the loop around PW. One of the main goals of computational chemistry is to unravel and enhance the ability to anticipate new stable structures or possible reaction pathways in order to produce desired molecules. Finding the matching structure of the transition state (TS) in terms of heterogeneous catalysis, however, requires a thorough and in-depth understanding of the basic steps and the numerous intermediate species. During plastic pyrolysis, ML and QM could be useful in forecasting the energy levels and kinetic parameters in the degenerated or transition state. Although this "strange couple" may sound like science fiction, their collaboration is growing and should culminate in major successes in the years ahead [73]. An interdisciplinary team from the Technical University of Berlin, the University of Warwick, and the University of Luxembourg have developed an ML technique to predict the electrical characteristics and molecular wave function of molecules. The tool captures the degree of freedom in molecules, which is essential to quantum chemistry, and offers access to the chemical interpretation of processes, bond order, and charge density without requiring additional machine learning models for each characteristic [74]. It will be necessary to broaden the focus beyond plastic pyrolysis problems and provide a thorough examination of static, stochastic, and quantum knowledge in order to address the vast array of information covered by this process. Nonetheless, the comprehensive reviews in this area published by [75,76] have demonstrated the key benefits of combining various models and the ways in which novel neural network topologies might enhance quantum computation, particularly for large-molecule reactions. As mentioned, the majority of the studies compiled in this study demonstrate that ML offer substantial benefits for data modeling and learning about kinetic triplets. However, in order to have a substantial global impact on plastic recycling technology, some gaps must be filled. Among the difficulties are;

i. *Feedstocks Main Composition:* To enhance the artificial networks' current capabilities, a thorough examination of actual PW is necessary.

ii. *Additives and Impurities:* There are a lot of impurities or other inorganic compounds in PW.

These are theoretically endless and difficult to analyze in depth. "Back-engineering exercises" could be used as a starting point to determine what the industries do not require. What amount of additives or contaminants, for instance, are theoretically acceptable for industrial use without resulting in harm or raising environmental concerns? Because it requires establishing a link between two lowest-energy paths on the potential energy surface in high-dimensional space, more research on the effects of bromine, chlorine, and other contaminants is extremely difficult. The important thing here is that by using information from quantum data, ML can speed up the process of determining the minimal energy paths. Although chemical reaction prediction using ML and QM is still in its infancy, this "strange couple" could be generalized in two ways: First, ML can characterize molecular properties by learning from quantum chemistry (Fig. 5a). Second, the Schrödinger equation-derived ground-state wave function (Fig. 5b) might be predicted by the ML model. A thorough examination of these methods for the plastic pyrolysis process is necessary; lastly, (iii) a "bridge" between ML and QM tools so that researchers from other fields may identify the essential elements for creating accurate kinetic models and effective reactor and product mapping. Finally, in order to enhance effective catalyst

prototyping and parameter optimization processes, scientists and engineers will keep working to integrate ML and QM modeling as a standard tool. For ML applications, more systematic experiments and large data sets with improved accuracy, validity, and curation methods will be needed. The process for this "exotic mixture" calls for (i) databases that can store the operational conditions and catalysts that are ready to use; (ii) each catalyst and product must be identified by its representation, or fingerprint, which includes its atomic and physical properties as well as its electronic structure (this is where QM comes in); and (iii) ML will be used to identify patterns, find descriptors, and find models.

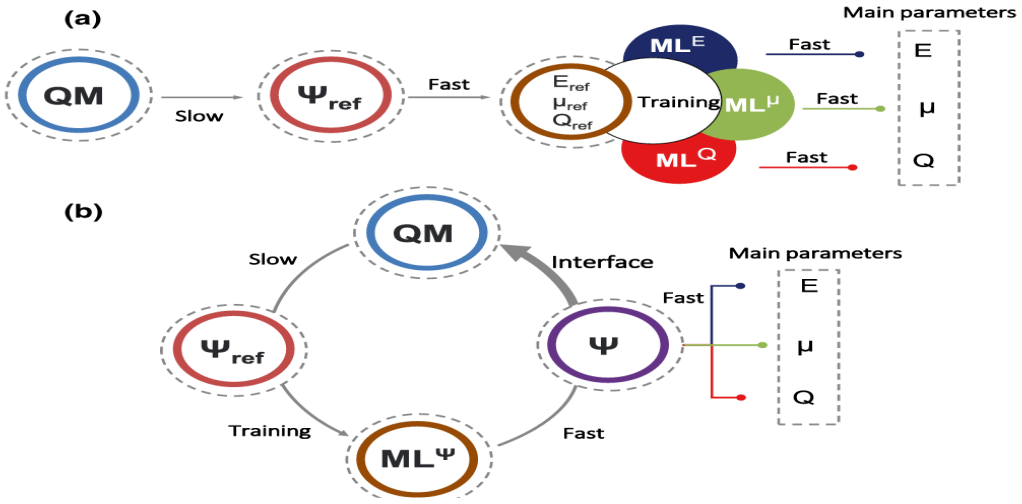

Fig. 5 Integration of machine learning and quantum mechanics adapted from [74]: (a) Representative for ward ML model, (b) ML predict the wavefunction, which acts as an interface between ML and QM

VI. CONCLUSIONS

In conclusion, ML has shown itself to be an effective tool for identifying the kinetic mechanisms and deciphering the kinetic triplets of PW pyrolysis. Additionally, "black-box" solutions based on the link between input data and output data can be provided using data science methods like ML. Furthermore, "first-principle knowledge," which is comparable to quantum mechanics (QM), should be the foundation of ML in the future for forecasting and deciphering the physicochemical nature of processes. This paper also notes that by deciphering intricate reaction networks like PW pyrolysis, computational methods based on ML and QM have the potential to significantly contribute in the years to come. Additionally, the ML algorithms are able to predict the quantities of different pyrolysis products, such as gas, char, and pyrolysis oil, as well as their physical and chemical makeup.

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