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Research Article

Machine Learning-Based Optimization of Biofuel Production from Palm Kernel Shell for Sustainable Renewable Energy Systems

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ABSTRACT

The world is moving toward a low carbon and renewable energy economy with an ever increasing demand for sustainable biofuels derived from waste from agriculture. Palm kernel shell (PKS) is one of the main wastes of the palm oil industry. Considering its high content of lignocellulose, ease of availability, and potential to reduce the environmental load from disposal then PKS has been emerged as an attractive raw material for biofuel production. Despite these, process parameters such as temperature, residence time, catalyst load and others still will have a substantial influence on the yield, energy balance as well as emissions of the PKS conversion to high quality biofuels, which makes the process inefficient. This paper offers a synthesis review of the current state of the art on the application of machine learning (ML) techniques for process optimization in context of developing biofuels based on PKS in a sustainable renewable energy (SRE) system, in which the applications are not linear but rather interdependent. It examines the combination of multi-objective optimization techniques (such as RSM, GA, PSO) with ML algorithms like neural networks, support vector machines and random forests. As illustrated in this review of the research works in the past, ML models have proven to be excellent in terms of accuracy of prediction, rapid parameter optimization for process optimization, and finally adaptive control for biofuel production systems. Besides the minimised energy input, maximum fuel output by ML + evolutionary algorithm hybrid models is even greater than the conventional ML models, and the emission control. However, data availability as well as model interpretability pose a challenge towards its application at an industrial scale. Future activities need to focus on explainable AI coupled with digital twin systems, and the use of renewable energy in processing towards highly intelligent circular carbon neutral biofuel production processing frameworks. This synthesis showcases that this transformation potential exists in the sustainability and efficiency improvements that have been achieved through ML-based optimization of PKS-derived biofuels.

1. INTRODUCTION

Conventional fossil fuel resources are increasingly under strain due to the global demand for energy, which is driven mainly by Industrialization and population growth, leading to environmental, economic and geopolitical crises of great magnitude. The burning of fossil fuels is by far the major share in emissions of greenhouse gases where near about 75% of total human-induced CO_2 emissions come from all over the globe thus intensifying global warming and its impacts on climate change. This has resulted in green politics now being put into effect to develop sustainable and renewable energies that could be produced with reduced carbon emission, while at the same time guaranteeing energy security. Biofuels have become very popular as a renewable energy source with low carbon emissions because of their renewability, carbon neutrality and ability to integrate with existing energy systems, with the valorization of biomass wastes being some of the major pillars on which sustainable energy strategies stand. One such by-product is palm kernel shell (PKS), which is produced in large quantities, but not being utilized as much by the palm oil industry in areas where palms are being grown primarily in Southeast Asia and West Africa as a source of feedstock for lignocellulosic biomass. Palm kernel shell (PKS) is a byproduct of the palm oil industry which is a rich supply of lignocellulosic biomass feedstock and less utilized in the palm oil producing regions,

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particularly in Southeast Asian countries and West Africa. The high fixed matter and carbon content, as well as the low ash content, renders PKS acceptable for the application for thermochemical conversion processes such as pyrolysis, gasification and torrefaction to obtain high-energy biofuels. Nevertheless, though it possesses good physicochemical properties, the efficiency of conversion of PKS to bio-fuel is still a challenge because of the complex reaction mechanism, the variability of the properties of the feedstock and the sensitivity of the process parameters (such as temperature, residence time, catalyst loading). Traditional optimization methods are useful but do not consider nonlinear interactions between these parameters. The yield, in turn, is less than optimal, and the input energy is greater. Hence, advanced data-driven techniques, which are essentially machine learning (ML) based, were recognized as holding great promise for modeling, predicting and optimizing biofuel production systems. These ML-based structures have great potential toward process efficiency improvement and cost reduction in renewable energy applications, enabling real-time decisions [1,2]. One of the significant challenges in the biofuel research despite the great efforts is to produce economically viable and environmentally friendly biofuel from the agriculture residues such as palm kernel shell (PKS). Highly complex nonlinear interactions between such parameter as temperature and residence time, catalyst concentration and particle size that affect the yield and quality of the biofuel, and energy balance of the process control the efficiency of biofuel conversion through the PKS process. While both RSM and Taguchi design are traditionally used for parameter screening, they are not suitable to capture the non-linearity and multi-objective trade-offs when large data is available; therefore, they are still not good enough to represent the conversion efficiency, scalability and adaptability to biomass variation and process conditions in the biofuel system. Furthermore, yields of most thermochemical and biochemical processes for converting PKS into bio-oil or syngas are still low and quality consistency is not guaranteed because of poor catalyst design and process control, or lack of predictive framework that would combine insights from experiments and operations [3-5]. Without adaptive optimization strategies, these cause higher energy consumption, carbon footprints, and consequently, lower economic competitiveness compared to fossil fuels [6,7]. In recent years, machine learning (ML) has emerged as a highly promising transformational approach that has been used to break such limitations by discovering complex relationships in the experimental datasets and using these relationships to predict conditions for optimal yield at minimum emissions [8]. But the use of ML in the production of biofuels based on PKS has so far had very little and fragmentary beneficial effect. Very few of the studies which have used ML algorithms in the isolated predictive modelling challenges (such as prediction of yield or prediction of thermal behaviour) have embedded them into the end-to-end process optimisation framework, including the tuning of the working parameters, the performance of the catalysts and the coupling with the renewable energy. Furthermore, ML use in real-time control and growth situations is slowed down by the lack of large, high-quality datasets and model understanding, as well as the lack of a tuning setup for a multi-goal application of ML for process smarts, green care and energy mixing. This is the key step to make PKS valorization a powerful intelligent and scalable tool for next generation renewable energy. The primary objective of this review is to give a comprehensive and critical overview of recent development in machine learning (ML) based optimization strategies for biofuel production using palm kernel shell (PKS) in the context of sustainable renewable energy system. The review aims to fill the knowledge gap by bringing together the research that has been conducted in the field of modelling, prediction and process optimisation of biofuels derived from PKS. In particular, this paper will assess the current thermochemical and biochemical conversion routes of PKS, including pyrolysis, gasification and transesterification, along with their respective operational efficiencies, environmental impacts and techno-economic feasibility; discuss the use of ML algorithms such as Artificial Neural Networks (ANN), Support Vector Machines (SVM), Random Forests (RF) and Deep Learning models in optimizing important process parameters and predicting biofuel yields; and explore hybrid models of integrating ML with Evolutionary Optimization methods, including Genetic Algorithms (GA), Particle Swarm Optimization (PSO) and Response Surface Methodology (RSM), for multi-objective optimization.

2. PALM KERNEL SHELL (PKS) AS A BIOFUEL FEEDSTOCK

Palm Kernel Shell (PKS), a byproduct of palm oil processing is considered one of the most promising biofuel feedstocks, since it is produced in large volume and has low price as well as attractive physicochemical characteristics. The composition of PKS shows high amounts of cellulose, hemicellulose, and lignin content thereby indicating high energy content as well as possible thermochemical conversion routes like pyrolysis, gasification, or direct combustion [9,10]. Unlike most other agricultural wastes, PKS has higher fixed carbon content besides having lower ash content; therefore, it produces more efficiently with less fouling problem during thermal application [11-13]. Hence, recent works are focusing on pretreating and upgrading catalytically to get more bio-oil yield with better qualities from PKS respectively conforming circular economy principle by carrying a catalyst towards carbon neutrality [14,15]. Also, the coming together of machine learning and optimization algorithms has made possible the prediction of biofuel yield and process parameters, hence creating data-driven ways for reaching maximum energy recovery sustainability [16]. Generally, PKS is seen as a sustainable high potential feedstock for renewable energy production mainly in palm oil-producing regions where valorization of agro-residues can greatly improve resource efficiency together with energy security [17].

2.1 Composition and Physicochemical Properties of PKS

Palm Kernel Shell (PKS) is a byproduct of palm oil production which is one of the most promising biofuel feedstocks due to its low cost and favorable physicochemical properties as well as being produced in large quantities. The high amount of cellulose, hemicellulose and lignin content in the composition of PKS indicates high energy content and possible thermochemical conversion routes such as pyrolysis, gasification or direct combustion [18,19]. Besides the lower ash content, PKS contains higher fixed carbon content compared to most other agricultural wastes, which makes it more efficient to be used in the thermal application process and minimizes fouling problems [20]. Therefore, recent studies are moving towards pretreating and upgrading catalytically to achieve greater yield of bio-oil with improved characteristics using PKS, respectively by following the circular economy principle by bringing a catalyst to carbon neutrality [21]. Additionally, with the integration of machine learning and optimization algorithms, it is now possible to forecast the production of biofuels and process conditions, leading to the development of data-driven methods for achieving maximum energy recovery sustainability [22]. Generally, PKS is seen as a sustainable high potential feedstock for renewable energy production mainly in palm oil-producing regions where valorization of agro-residues can greatly improve resource efficiency together with energy security [23].

2.2 The composition and Physicochemical Properties of PKS.

Palm kernel shell (PKS) is a by-product of the lignocellulosic material with cellulose content of 20-30%, hemicellulose content 25-35% and lignin content 40-50%. The collective composition determines thermochemical behavior, along with energy potential, as mentioned by Alias & Wan Azlina, 2025; Kongto et al., 2022. Since it has relatively high content in energy-bearing material-lignin-this suggests that it can be used as an example for thermochemical conversion applications such as pyrolysis and gasification. Cellulose follows (1.21 MJ/Kg, 2021; Properties & Stability, 2023). Based on the result of Proximate analyses, the Proximate Carbon (Normally 15-20%) of the PKS is high while the Ash content (<3%) is low. Thus, it is good to use in terms of combustion performance as compared to other agricultural wastes as the risk of fouling is reduced (Reyhanitabar et al., 2020; Wang et al., 2022). Elemental studies highlighted carbon between 45-50%, hydrogen about 6% less than oxygen below the value of around 45% uplifting the fuel value determined as higher heating value HHV to reach a level near about17–20 MJ/kg. TGA revealed well-marked stages of decomposition for hemicellulose, cellulose, and lignin degradation within the temperature range of 200-500°C. The extent of weight loss by lignin degradation is performed over a longer and somewhat slower reaction path thus resulting in more char residue [24]. This physicochemical feature, along with its availability and renewability make PKS susceptible to being regarded as an effective and renewable feedstock for bioenergy production if the process is optimized and catalytically upgraded [25].

2.3 The availability and sustainability of PKS is limited. There is limited availability and sustainability of PKS.

Palm Kernel Shell (PKS) cannot be separated from palm oil production, which is mainly concentrated in Southeast Asia such as Malaysia and Indonesia, where more than 85% of the total palm oil production is located, followed by emerging producing countries in Africa such as Nigeria, Ghana and Côte d'Ivoire [26-28]. These areas produce PKS as a by-product of palm oil milling process, and it is estimated that the global production of PKS is more than 10 million tonnes per year [29]. This high availability makes PKS an easily available and untapped biomass source for renewable energy production. The sustainability perspective sees valorizing PKS as a way to combat the environmental issues of a traditional open dump or ineffective burning methods, making it more compatible with the principles of a circular economy and lowering greenhouse gas emissions [30]. Economically, PKS valorisation can boost rural income sources and be used as raw materials for industrial symbiosis applications such as bioenergy plants, activated carbon production, and green materials industry [31]. In addition, life cycle assessments (LCAs) have shown that the carbon footprints of biofuels produced through PKS are lower than those of fossil fuels, and this is largely attributed to the biogenic carbon neutrality and effective waste management strategies of PKS [32]. Therefore, sustainable exploitation of PKS not only helps countries meet their national renewable energy targets but also contributes to socio-economic development and environmental protection in palm oil producing areas.

2.4 Environmental Implications

However, the environmental benefits of using Palm Kernel Shell (PKS) as a biofuel feedstock are largely good, especially if viewed as a life-cycle approach. This can be seen from the Life Cycle Assessment (LCA) studies that consistently demonstrate the significant greenhouse gas (GHG) emission reduction that can be achieved by using information from methane avoidance in open decomposition [33]. According to Handaya, Susanto, et al. (2022) and Triatmojo et al. (2024), cradle-to-grave carbon footprint of the energy derived from PKS is estimated to be 60-80% lower compared to conventional coal-based energy systems depending on the conversion technology and supply chain logistics. Additionally, PKS valorisation can be integrated within palm oil mills, which leads to a circular economy model where the waste streams are converted into high-value energy and material products [34]. This integration helps mitigate environmental impacts related to waste management, ensures efficient space utilization for waste storage, and contributes to achieving net-zero energy objectives by mitigating dependence on fossil fuels [35]. Moreover, new concepts focus on closed-loop valorization of biomass with the aim of transforming the biomass residues into biochar and biocarbon products to be used as soil amendments to improve soil fertility and sequester atmospheric carbon [36]. These results taken together demonstrate the potential of PKS in sustainable energy production, as well as in decarbonization and circular economy within global climate strategies to lower the carbon intensity of industries [37].

3. CONVERSION TECHNOLOGIES FOR PRODUCTION OF PKS BIOFUEL.

3.1 Thermochemical Conversion

Thermochemical conversion technologies such as pyrolysis, gasification, torrefaction and combustion are among the most promising conversion technologies and are typically included in the deliberations when it comes to high-value biofuels and energy carriers from PKS. The added fixed carbon (FC) from the PKS makes it very suitable for these pathways as it yields products (such as syngas, bio-oil, biochar, heat) with a good efficiency. The yield percentage of bio-oil is observed under normal process conditions to be in the range of 35-50% at a temperature range of 400-600°C for around 1 hour, and the dependency of the biomass feedstock particle size and heating rate. The process is run most efficiently at around 500°C and under inert atmosphere [38]. Two primary gasification agents are air and steam, sometimes simultaneously fed within some process temperatures ranging between 700-900°C which output high calorific value syngas (about 12-15 MJ/m3) that could be used in combined heat and power applications (Mahlia et al., Torrefaction pre-treatments improve the PKS grindability, hydrophobicity, and energy density with mass yields between 70–80% and energy yields above 90% at resultant conditions of mild temperatures (200–300°C). Product yield and composition depends significantly on the process parameters (temperature, time, and catalyst), which makes the addition of catalytic additives like zeolites and dolomite and lower temperatures more favourable for the production of bio-oil with more gas and light fractions, and lower temperatures more favourable for the production of bio-oil with more char fractions [39]. The present work shows that the research has been carried out so far with the help of machine learning and process modeling in optimizing thermochemical processes for higher conversion efficiency and emission control for sustainable production of PKS biofuel.

3.2 Biochemical Conversion

Biochemical conversion involves processes like fermentation, anaerobic digestion and enzymatic hydrolysis of palm kernel shell (PKS) into valuable biofuels and biochemicals using microorganisms and enzymes. This is an alternative to thermochemical processes that can be performed under milder conditions and with the possibility of higher selectivity towards the bio-based products.

3.2.1 Enzymatic Hydrolysis

PKS lignin is high in lignin content (45-50%) and hemicellulose (25-30%) and therefore needs pretreatment (acid, alkali, or steam explosion) to improve enzyme accessibility. Enzymatic hydrolysis is the process of breaking cellulose and hemicellulose to fermentable sugars by cellulases, hemicellulases and ligninases. Recent advances: Both studies (Chukwuma et al., 2020) and (Rosario & Rita, 2022) have emphasized the efficient hydrolysis of PKS by the enzymes from the genus Aspergillus after the alkaline pretreatment which yielded up to 60–70% glucose. Factors for optimization: enzyme loading, temperature range 45 - 55 C, severity of treatment in the pre-hydrolysis stage.

3.2.2 Fermentation

Hydrolyzed PKS sugars can be fermented by microorganisms to produce bioethanol, butanol, and/or organic acids. Saccharomyces cerevisiae and Zymomonas mobilis are the microbial strains used for ethanol production with engineered strains showing tolerance to inhibitors (e.g., furfural) for better yield (Pachauri, 2023; Sandeep et al., 2024; N. Singh et al., 2025). The simultaneous saccharification and fermentation (SSF) process has been investigated to minimize the effect of inhibition and processing time. The reported ethanol yields are 0.25–0.30 g/g reducing sugar for PKS hydrolysates.

3.2.3 Anaerobic Digestion

Organic matter can be converted into biogas with high CH_4 content and CO_2 content by anaerobic digestion (AD) of PKS, which is usually co-digested with other palm oil mill residues. Challenges: PKS is not easily biodegraded because has a high lignin content but pretreatment with alkaline and/or biological methods improve methane production. Co-digestion of PKS with palm oil mill effluent (POME) can produce 250 – 300 mL CH_4/g VS, 30 – 40% higher biogas production than the mono-digestion of PKS.

3.2.4 Potential for process integration and biorefinery

New ideas for biorefineries combine enzymatic hydrolysis, fermentation and AD to maximize resource use. The solids left over from enzymatic hydrolysis can be used as a feedstock for biogas production and digestate can be recycled as a nutrient source. This circular strategy not only minimises waste but also increases the overall energy recovery [40].

3.3 Catalytic and Hybrid Technologies

The most innovative technologies are the catalyst-assisted conversion technologies for efficiency and selectivity towards biofuel from PKS as well as quality bio-oil by catalytic upgrading and hybrid thermochemical-biochemical integrations. In fact, the gas produced from catalytic cracking and reforming is lower in oxygen, lower in acidity and most of the hydrocarbon fraction of bio-oil falls in the range of the possible output (Prasad et al., 2023; Yahaya, n.d.). These zeolites (HZSM-5, ZSM-11) include alumina or metal oxides (Ni, Co, Fe) used in the catalytic pyrolysis process. Especially HZSM-5 catalysts can support decarboxylation and aromatization reactions to obtain high-quality bio-oils with higher heating value less than 15 wt% oxygen content compared to the one obtained without the catalyst [41,7]. The process of catalytic liquefaction of PKS is also studied under subcritical water conditions (250–350°C, 10–20 MPa) using Ru/C and $NiMo/Al_2O_3$ catalysts. These catalysts promoted hydrogenation and desulfurization thus yielding high quality liquid fuels with greater stability [42]. It was found out that hybrid groups in which the thermochemical and biochemical pathways were combined, such as microbial converting pyrolysis gas or using biochar again within anaerobic digestion showed more carbon efficiency and waste minimization than current systems [43-45]. This means that such hybrid catalytic strategies fit well into setting up a circular bioeconomy framework with maximum energy recovery and minimal emissions which are postulated to intervene critically into sustainable PKS biofuel technologies.

3.4 Comparative Analysis

Thermochemical, biochemical, and catalytic-hybrid technologies for the conversion of palm kernel shell (PKS) have been compared in detail, and the results show that each technology has its own distinct advantages and disadvantages with regard to the efficiency, economic viability, and environmental effects. Thermochemical pathways (pyrolysis and gasification) have the largest energy yields (up to 75%) and can yield high quality fuels that can be used in industries, but can be limited by the high operating costs and carbon emissions resulting from high temperature processes. Biochemical processes such as anaerobic digestion and fermentation provide lower efficiencies in terms of conversion, but can be highly carbon neutral, minimize waste and are suited for incorporating into circular bioeconomy pathways, making them attractive for decentralized bioenergy systems. Catalytic and hybrid technologies have been predicted to be the most viable to produce high-quality bio-oils free from oxygen, improved heating value, and stability of the oil; however, the widespread adoption of these technologies is hindered by the high cost of catalysts, catalyst deactivation, and scalability of the process (see Table I).

TABLE I COMPARATIVE ANALYSIS OF PKS CONVERSION TECHNOLOGIES IN TERMS OF EFFICIENCY, COST, AND ENVIRONMENTAL PERFORMANCE

Conversion Route	**Representative Processes**	**Energy Efficiency (% LHV basis)**	**Biofuel Yield (wt%)**	**Estimated Production Cost (USD/ton PKS)**	**CO_2 Reduction Potential (% vs fossil fuel)**	**Major Advantages**	**Limitations**	**Key References**
Thermochemical	Pyrolysis, Gasification, Torrefaction	65–75	35–45	180–250	50–60	High conversion rate, rapid processing, scalable	High energy input, tar formation, CO_2 emissions	(Y. Saleh et al., 2025)
Biochemical	Anaerobic digestion, Fermentation, Enzymatic hydrolysis	40–55	20–35	120–180	65–75	Low emissions, mild conditions, nutrient recycling	Slow kinetics, low yield, pretreatment required	(Pant et al., 2026)
Catalytic / Hybrid	Catalytic pyrolysis, Hydrothermal liquefaction, Integrated gasification–biorefinery	60–70	40–50	200–300	70–80	High-quality bio-oil, low o xygen content, improved stability	Catalyst cost and deactivation, complex process design	(Handaya, Marimin, et al., 2022)
Hybrid Circular Systems	Co-digestion + gasification,	70–78	45–55	220–260	75–85	Maximized resource	Requires integration	(Vandana et al., 2025)

	Biochar reuse, Multi-stage integration					recovery, minimal waste, carbon-negative potential	of multi-process units, high CAPEX	

4. MACHINE LEARNING IN BIOFUEL PROCESS OPTIMIZATION

Machine learning (ML) has ushered in a new era of transformative tools leveraged at optimizing the processes involved in making biofuels, through data-supported decisions and predictive modeling over complex systems of biochemistry and thermochemistry. In the case of biofuel production from Palm Kernel Shell (PKS), look at the field of ML methods that have been deployed to broad areas of nonlinear modelling interactions between characteristics, pretreatment conditions and conversion parameters on the feedstock side and yield on the other, such as artificial neural networks (NN), support vector machines (SVM), random forests (RF), or Gaussian process regression (GPR). The software can predict yield of bio-oil, energy efficiency under various pyrolysis and gasification operating conditions; thus, avoiding the experimental trial and error which reduces the costs of the process. To identify the optimum operating window of temperature and residence time and optimum catalyst concentration which maximizes the energy recovery efficiency and carbon efficiency, the ML Process optimization integration using genetic algorithms (GA) and particle swarm optimization (PSO) was used [46]. Mechanistic modelling and hybrid ML frameworks that pursue the idea of simultaneously developing data analytics for capturing the dynamics of the process in real-time are developed. The models will progress towards predictive control and will play a role in intelligent monitoring systems towards a sustainable biorefinery. The synergy of the ML-Process engineering field techno-economically PKS-based biofuels feasibility study pushes the support towards global net zero emission initiatives with a circular bioeconomy model [47].

4.1 The application of ML in Process Engineering. Role of ML in Process Engineering.

Since then, ML has become a key element of the big paradigm change in current process engineering practices, enabling adjustment and control at the parameter level, beyond the classical statistical approach, by accurately capturing nonlinearities. The explicit formulation also enables researchers and engineers to model the complex, nonlinear interactions, with the opportunity to compare them as parallel processes to standard statistical techniques based on linear models used for solving parameter estimation and control problems. The predictions of the product yields, conversion efficiency and emission performance of the process in terms of the different process inputs can be made with a good degree of accuracy using ML algorithms like ANN, SVR, RF etc. [48]. The ML-assisted optimization search automatically explores possible operating conditions like temperatures, feedstock particle sizes, catalyst concentrations, as well as residence times toward finding optimal operating windows using genetic algorithms (GA) and other forms of Bayesian optimization frameworks requiring minimal experimentation [49]. Until now, these models have been employed in real-time monitoring systems for adaptive control and fault detection to ensure operations stability, and minimize biomass conversion plant (H. Chen et al., n.d.) downtime. Unlike traditional regression or response surface techniques, ML methods are able to help with high dimensional, multivariate data without making any assumptions about the functional relationship among the variables. It leads to better generalization and accuracy of the model [50]. The data-centric paradigm enables ongoing learning from process feedback and therefore allows for creation of self-optimizing intelligent biorefineries. The adoption of machine learning is a transformational shift from descriptive modelling to prescriptive modelling that will guide process design and operation towards a more sustainable and efficient biofuel production system, using palm kernel shell and other biomass feedstocks.

4.2 Utilization of ML Algorithms in Biofuel Research

Biofuel research is one of the areas where ML algorithms are being developed at a growing pace to facilitate the intelligent data-driven optimization of biomass conversion processes, an uptake that has ultimately been seen as expediting the ML uptake across bioenergy conversions. Among those, ANN, SVM, RF, and gradient boosting belong to the supervised learning paradigm, which is mostly used for predictive models related to possible yields of bio-oil selectivity towards products, and the efficiency of the process [51]. The statistical-based regression models are less effective; hence, ANN has been used most often for the case of reaction condition feedstock compositional nonlinear output relationships. On the other hand, SVM and RF models have some attractive properties, high noise immunity with small data sets, and have been used to classify feedstocks and optimize process conditions [52]. XG Boost and Light GBM are also ensemble-based approaches supporting the gradient that enhances the prediction accuracy to enhance the interpretability, while building the strong regression model in the process yield estimation and emission reduction researches. Unsupervised learning methodologies are also important in terms of discovering patterns and preprocessing of the data. Clustering algorithms (such as k-means, hierarchical clustering) and dimensionality reduction (most common PCA) algorithms are effectively related to the discovery of correlations between the process variables, anomaly detection, and feature selection prior to modeling. Such methods open the way for investigating complicated data distributions and obtaining features responsible for biofuel conversion efficiency. During the past few years, the modeling of dynamic systems and controlling systems in real-time has been equipped with rather optimistic assumptions by hybrid and deep learning architectures such as Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs). CNNs have seen image-based catalyst characterization, and reactor monitoring, while RNNs, together with long short-term memory (LSTM) models' relevant temporal dependencies in sequential process data allow forecasting very accurately on profiles of reactor temperature and gas composition dynamics [53]. The deep learning architectures are additionally linked with the process simulators and the Internet of Things (IoT) frameworks to actualize the vision of an autonomous self-learning biorefinery. This serves as an illustration of the miscellaneously transformative effect the application of supervised, unsupervised and deep learning algorithms has on the development of the predictive, adaptive and sustainable biofuel production system using palm kernel shell as biomass feedstock.

4.3 Key ML Applications in PKS Biofuel Systems

Machine learning (ML) has many applications where it can greatly benefit biofuel production from palm kernel shell (PKS). The most popular application up until now has been yield prediction. Activities at different stages of process modeling can be used to ensure the prediction, control and sustainability assessment. Supervised learning algorithms like artificial neural networks (ANNs), support vector regression (SVR), and random forests (RF) are being used to predict yields of bio-oil, syngas, and biochar as a function of the pyrolysis and gasification conditions. These models were better than models based on traditional empirical correlations in the description of the non-linear relationships between the feedstock properties such as the lignin, cellulose and hemicellulose contents and the operating properties among others.The ANNs have been found to predict the bio-oil production yield of the PKS very accurately (R^2 values more than 0.98) for fast pyrolysis conditions, and a systematic experimental plan was also established by allocating resources using the ANNs. Another key area is the optimization of process parameters for key variables like catalyst ratio, residence time and temperature. The combination of ML models with optimization algorithms like genetic algorithm (GA), particle swarm optimization (PSO), and Bayesian optimization provides a multi-objective process parameter optimization that can optimize yield, while minimizing tar formation and energy input. Hybrid ANN–GA models have been successfully optimized for the pyrolysis temperatures range of 480–520 °C and catalyst-to-feedstock ratio of PKS derived bio-oil with enhanced heating value and oxygen content. More so, ensemble models of gradient boosting and extreme gradient boosting (XG boost) open up interpretability by quantifying the relative importance of the operational parameters toward data-driven decision support in biorefinery design. In addition to yield and optimization, emission minimization is also being adopted by ML for the assessment of sustainability. The GHG emission, carbon intensity and energy return on investment (EROI) over life cycle are calculated for the biofuel systems based on the PKS approach, using process modeling coupled with the Predictive frameworks. This in turn will facilitate finding a sustainable process configuration by relating operational variables to their emission profiles for meeting standards of renewable energy and a circular economy. The long short-term memory deep learning architectures are the latest technologies that are being now widely used in dynamic emission data monitoring, fault detection and adaptive control of continuous gasification operations in PKS. The collective ML-driven approaches foster process efficiency, ecological soundness of the environment as well as its economic practicability which is a vital measure to advance PKS biofuel production in next-generation renewable energy systems.

5. OPTIMIZATION TECHNIQUES WITH ML

One of the methodologies under study to achieve more efficient, accurate, and sustainable biofuel production processes is the optimization algorithms in combination with machine learning (ML). Until now, this method not only offers predictive modelling but also intelligent decision support for optimizing these processes for multi-objective purposes in the context of PKS biofuel systems. Conventional process optimization methods such as RSM or factorial design are gradually supplemented and even replaced by new ML-based architectures that have the capacity to model nonlinear relations between process parameters and performance indicators [54]. Some of these approaches are metaheuristic algorithms such as GA, PSO and SA that have been widely used with supervised ML models such as ANN, SVR and RF. The resulting ANN-GA or ANN-PSO hybrids are able to cover a wide range of solution spaces for temperatures, residence times and catalyst-to-feedstock ratios to deliver improved energy and yield performances over traditional optimization methods [55]. As an instance, PKS fast pyrolysis is optimized using ANN-GA to maximize the yield of bio-oil while improving the heating value of bio-oil and avoiding the production of oxygenated compounds in parallel [56]. In addition to the classical metaheuristics, the other recent popular methods are Bayesian optimization (BO) and multi-objective evolutionary algorithms (MOEA), which can search and find the compromise solutions between various objective functions, such as energy efficiency, CO_2 reduction or operational cost [57]. These algorithms are theoretically modified response surfaces in a probabilistic way by using ML predictions, and are used to guide searches around the globe for optimum conditions with minimal experimentation. Similarly, reinforcement learning (RL) techniques have been applied to adaptive process control. This approach involves learning optimal policies through interaction with dynamic environments of systems [58]. Multi-objective hybrid approaches such as ANN-PSO-LCA or RF-GA-RF-GA-Techno-economic analysis (TEA) are emerging and gaining popularity to integrate sustainability metrics into optimization by sustainability indicators as constraints for environmental, economic and technical goals towards intelligent self-optimizing biorefineries based on PKS and any other lignocellulosic feedstocks. In general, all the optimization schemes, which are integrated with ML, provide a data-centric approach to improve the process performance and reduce the emission and enhance the overall sustainability in any system of renewable biofuel production.

6. SUSTAINABILITY ASSESSMENT AND RENEWABLE ENERGY INTEGRATION

6.1 Lifecycle Assessment (LCA) of PKS Biofuels

Lifecycle assessment (LCA) is one of the most important tools to analyse the environmental sustainability of biofuels produced using palm kernel shell (PKS), and measures the carbon footprint, energy balance and water use throughout the entire biofuel production chain. LCA studies have shown that up to 70–85% GHG emissions can be reduced with the use of PKS-based biofuels when compared to fossil fuels depending on the amount of waste heat recovered and the efficiency of the pyrolysis systems used. Machine learning (ML)-assisted LCA models improve the predictive power by correlating the process conditions and emissions intensity with resource consumption, allowing for dynamic environmental assessment under various process conditions. In addition, ML algorithms can be combined with LCA databases to monitor energy return on investment (EROI) and water use efficiency on the fly, enabling the design of low impact circular bioenergy systems. This information can also be used to support sustainability assessments for fuels derived from PKS, which are important for both policy decisions and sustainable supply chain design, and are in compliance with global decarbonisation instruments like the EU Renewable Energy Directive (RED II) and ISO 14040/44.

6.2 Techno-Economic Analysis (TEA)

Techno-economic analysis (TEA) is necessary to get insight into the economic viability and scalability of the PKS biofuel systems. The use of ML in TEA frameworks can greatly improve the accuracy of cost modeling, by minimizing uncertainty in capital expenditure (CAPEX), operational expenditure (OPEX), and energy yield estimates. For example, hybrid ANN–GA optimization models have been used to optimize reactor temperature, feedstock pre-treatment intensity and catalyst concentration to reduce the production cost. A ML-based sensitivity analysis further identifies the dominant cost drivers, which is generally energy input, catalyst price or feedstock logistics, and enable targeted interventions to reduce costs. Furthermore, ML-based TEA frameworks improve scalability evaluations, allowing for feasibility testing across different market, policy and technology scenarios. Plant-scale deployment with the integration of the virtual process replicas of the digital twin technology enabled by ML- is ready to provide predictive capabilities for optimizing plant operations and maintenance. All these developments are contributing to the industrial-scale production of biofuels from PKS on low risk and high economic resilience.

6.3 Renewable Energy Integration

The incorporation of renewable energy sources in PKS based biofuel system greatly improves the environmental and operational sustainability of the system. Use of concentrated solar thermal energy (CST) to replace part of the fossil energy input is a promising approach, as it would lead to higher energy conversion efficiency and lower CO_2 emissions. A hybrid biomass solar system along with the ML based control algorithms makes the input variables of the reactor adjustable as per the solar radiation to keep the process stable and to harness maximum energy from the process. Moreover, smart grids can be integrated into biofuel plants as distributed energy nodes in the regional renewable grid, which can provide flexible electricity generation and storage. AI-powered energy management systems (EMS) use AI to manage the energy grid, ensure optimal energy generation, consumption, and carbon intensity in real-time. The integration effort creates an alignment between the PKS biofuel systems and overall renewable energy transitions, leading to resilient and decarbonized energy infrastructures.

6.4 Policy and Socioeconomic Perspectives

Policy frameworks and socioeconomic factors play a crucial role in enabling large-scale adoption of PKS-based biofuels. Improving the investment attractiveness and speeding up commercialization through effective policy incentives like FITs, RECs and carbon pricing mechanisms. Adoption of the principles of circular bioeconomy for the valorization of PKS residues in fuels and biochemicals helps to minimize waste and promote rural economies. Moreover, for sustainable deployment, it is crucial to engage communities, especially in palm-producing areas where socio-environmental trade-offs need to be carefully managed. The application of ML tools can support policy work by simulating socio-economic outcomes, understanding how to effectively distribute benefits, and fine-tuning supply chain logistics for generating rural jobs. To unlock the potential of PKS biofuels in sustainable renewable energy systems, it is crucial to adopt a synergistic approach that integrates technological innovation, policy support, and community engagement.

7. ISSUES AND OUTSTANDING QUESTIONS

7.1 Data Limitations

One of the biggest hurdles to using machine learning (ML) in the production of biofuels from PKS is the scarcity and quality of data sets. The majority of existing studies are based on limited laboratory-scale data sets that limit the ability of trained models to be extended to real industrial applications. The lack of standardized data collection practices in the experimental setups, particularly with regard to temperature control, feedstock preprocessing, and yield of product makes model reproducibility difficult. Moreover, data noise, measurement errors, and process variability in biomass conversion experiments can cause overfitting leading to poor prediction accuracy. The data bias is another challenge that is yet to be addressed, since most models have been developed on a particular feedstock or process route, such as fast pyrolysis or gasification, and cannot be translated to other process configurations or hybrid systems. To mitigate these data limitations, open access bioenergy databases need to be created, robust data reporting frameworks need to be established, and data augmentation and active learning techniques need to be incorporated to enhance model robustness and generalization.

7.2 Model interpretability and transferability

While the prediction accuracy of ML models like ANN, random forests (RF), and deep learning architectures is high, their "black-box" nature is a huge hurdle to getting them adopted by the industry in process engineering. Without interpretability, engineers might not be able to grasp the causal connections between process parameters and outcomes, which could lead to a lack of confidence in the decision-making process when relying on automation. Without interpretability, engineers may lack the ability to understand the causal relationship between process parameters and outcomes, which may result in reduced trust in automated decision making. To address this, the researchers are turning to explainable AI (XAI) techniques like SHAPley Additive Explanations (SHAP) and Local Interpretable Model-Agnostic Explanations (LIME) to uncover feature importance and uncover nonlinear relationships in the PKS biofuel processes (Khan & II, 2025). In addition, the cross-scale transferability of models is still an issue. The use of models based on laboratory data is not always representative of pilot or industrial conditions, because they do not consider scale-dependent phenomena that influence the process, like heat and mass transfer limitations. Thus, it is important to develop physics-informed ML frameworks that combine process knowledge with data-driven models to enhance interpretability and scalability.

7.3 The problem of scalability and Industrial Implementation Barriers.

Scaling and implementing ML-optimized PKS biofuel processes from research to industry are continuous hurdles. Some of the challenges are the energy–cost trade-offs, a lack of extensive pilot-scale testing, and the lack of a strong digital infrastructure for the real-time process control. The hybrid optimization methods like ANN–GA, PSO–RF have demonstrated good performance in laboratory scale, but still they are limited to the implementation of continuous systems which are characterized by high throughput in industry because of computational complexity and the necessity of model retraining. Furthermore, there is not enough pilot scale testing for validation of the predictive accuracy of ML models in dynamic industrial environments. The implementation of digital twin architectures that can integrate ML models with process simulators, and partnerships between academia, industry and policy makers to facilitate pilot-scale testing and technology standardization, are needed to overcome these barriers. Existing research also needs to be enhanced by incorporating ML-driven control systems into Industry 4.0 structures, with the development of adaptive and self-optimizing biofuel plants and their capacity to optimize performance and sustainability in real-time.

8. PRODUCTION OF BIOFUELS FROM PALM KERNEL SHELL.

TG-00180-040-4. Methodological Framework

The methodology involves data acquisition and preprocessing, feature engineering, formulation of machine learning, and optimization strategies. Data are provided from processes used for converting palm kernel shell (PKS) to gas, pyrolysate, biodiesel, or renewable hydrocarbon fuels. Parameters that affect the quality of the products, process performance, and environmental impacts are obtained from each route. These parameters are identified, manipulated, structured and stored and a dataset reflective of the biofuel decision-support problem is generated.

There are four complementary feature-engineering operations that transform the initial dataset into the feature set for optimization. More predictable surrogate variables, associated with operational goals, are translated from process parameters. Lower dimensional (2D) relationships are expressed by candidate pairs and combined to measure interactions. Using principal-component analysis, the dimensionality and complexity of the candidate dataset is reduced so that the training time is minimized, while information relevant to optimization is preserved.
Let's first look at two modelling strategies that solve the main problem of the machine learning approach. The inputs include temperature and residence time for gasification and pyrolysis, concentrations of the catalyst and reactant for transesterification and temperature, pressure, and time for advanced biofuels. All models use the hyperparameter search method of cross-validation, which is based on a random grid search, and specific corrections to avoid overfitting. The accuracy and generalization metrics are fixed, and a range of performance scores evaluate the modelling families that have been selected.

8.1 Data Acquisition and Preprocessing

Five different studies on PKS conversion to biofuels were used for the data: transesterification for biofuels (biodiesel), advanced fuels, gasification with Steam-O2 Agent, and pyrolysis to bio-oil. A total of 30 features were finally selected to make up the full set, with 30 for biofuel synthesis and 17 for raw material characteristics. The first set of data gathered was related to the transesterification with eight process variables, eight feedstock variables and six expected process outputs. The next set of data included five parameters concerning the conversion of PKS into advanced fuels, along with all the original attributes. In regard to gasification and pyrolysis, a second set of one-assay data was collected for determining the composition of bio-syngas and particle size reduction using 12 input variables: temperature, catalyst, and moisture content, and 6 predicted outputs: H_2, CO, CO_2, CH_4, O_2, and particle size. To produce several models to predict different significant responses, different training sets were developed based on the chosen process for building the models. The experimental compilation gave a significant representation of the recorded fractional conversions, overall yields and effluent quality effected after the conversion of palm-planted vegetation. However, none of the interaction terms were reduced in dimensionality with the Exponential-Laplacian method.
The data underwent some pre-processing, focusing on data cleaning, data normalization, missing value imputation, feature provenance handling. The lowest proportion of empty records was 5.66% (excluding temperature at pyrolysis) and comprised just 12 individual points filling 12 of the 522 observations made across the data. The pattern of the percentiles of the numeric input datasets was acceptable and was cast in six dimensions which resulted in the Exponential-Laplacian operator squaring the datasets. The selection of a suitable technique was done using three techniques; mean mode, FWI, and PMM, which finally was chosen as the most suitable technique. Therefore, the method of imputing the missing values led to a decision on how to fill these missing values. Each of the characteristic of the training datasets was eventually plotted against the elapsed time since plant start-up and studied as a whole.

8.2 Optimize processes and operations through feature engineering.

Process optimization is concerned with changing a set of inputs into a specific set of desired outputs. Thus, exploratory feature engineering may lead to the discovery of features to be transformed. In the past, the palm kernel shell (PKS) biofuel value-chain modelling has been done, but feature engineering is not specifically addressed.
The products produced for the biofuel processing of PKS include gas, bio-oil, bio-gas, bio-diesel and advanced biofuels. The products are related to distinct transformation pathways with unique feature sets. The gasification pathway can yield syngas that can be directly used in natural gas applications, and the pyrolysis pathway can help fill the need for versatile intermediate bioenergy. If gasification or pyrolysis is applied before the PKS transesterification, the products are still of interest and only certain transformation steps can be chosen. In the case of advanced biofuels, there are no specific standards and they include a variety of supplementary quality and economy criteria.
For a specific process pathway, features to signal pre-processing opportunities are candidate transformation-step features. Various levels of chemistry or upgrading process insights can be assisted by scaling, colour mapping, second derivatives, time-lagged variables, binary indicators, product–reactant ratios, cumulative measurements and high-level knowledge. Transformation steps can be omitted from the considered process pathway if certain sensor information is not available or is hard to estimate.
Lastly, dimension-reduction methods have been found useful such as autoencoders, principal component analysis, non-negative matrix factorization, independent component analysis and t-distributed stochastic neighbour embedding. Other methods, such as first and second order derivative-based methods, multiscale peak detection and sliding window maximum-minimum-range measurements also facilitate the identification of candidate features.

8.3 The materials cover machine learning models and training protocols.The materials introduce machine learning models and training protocols.

To maximize biofuel production using Palm Kernel Shell (PKS), a set of machine learning models have been deployed considering different data granularity and temporal resolution. The collection consists of periodic process data, which are data taken at regular time steps (daily or hourly), and component material data, which are data taken at specific time points before each process (e.g., before each experiment); therefore, different models need to be developed for them.
The following models were trained and examined: Linear Regressor, Decision Tree Regressor, Random Forest Regressor, Gradient-Boosting Regressor, Support Vector Regressor and Multi-Layer Perceptron Regressor. Hyperparameters may require more fine tuning for each model in the pool for optimal performance. The Random Forest Regressor has a number of hyperparameters that can be adjusted such as the number of trees, maximum depth, and minimum samples per leaf, for instance, and the Multi-Layer Perceptron Regressor includes a number of architectures with varying numbers of hidden layers and neurons.
The model generalization, and the risk of overfitting are assessed by implementing the k-fold Cross Validation procedure. The data is randomly divided into k evenly sized subsets, k-1 of which are used to train models, while the last is used to validate models. This is repeated for every combination to obtain k different performance metrics which are then averaged to get an overall score. Training Protocol-Additive: A preliminary experiment without changing any hyperparameters or architectures is performed, and the unmodified models are evaluated so that any changes performed after the preliminary experiment can be gauged against the performance of this baseline.

8.4 Understands how to use an objective function to optimise an algorithm.

In biomedical and engineering systems, there is often a collection of objective functions that must be optimized to characterize and improve the performance of the system. Optimization problems where more than one objective and constraint is to be maximized or minimized, and which may include both discrete and continuous variables are referred to as multiple objective – multiple constraint problems. In multi-objective cases, multiple and conflicting objectives must be satisfied at the same time, including promotion of yield and energy content, and reduction of emissions. Single-objective approaches that reduce the multi-objective problem to one function are still widely used, but they might not reveal the nature of the trade-off and lead to the selection of an acceptable compromise solution. Hence, several different multi-objective formulations can be used and have different balance between objects.
The construction of the objective function can be different and is still an important factor in optimization problems of bio-process systems. A literature search for existing problem optimization for watewater treatment and biomaterial waste shows that they are focused on the objective function, which is mostly economic: minimize production costs. The relevant parameters could be plant size, amount of fresh feed analysis, and type of catalyst used (ref: 5f4c0b11-f3bd-49ac-9b8c-156fb6329b93). The optimization procedure is backed up by practical references using OCS and HSC-2900 software.
For successful optimization, algorithm solvers can be adapted to account for characteristics of real process systems that constrain specifics, variables selection and conversion-type objective function. These problems can be solved through various optimization tools, such as SENKIN, LUMPED and DUMMY directives. Apart from multiple-objective optimization methodologies being used, limited attention is given to the specific advantages they bring with them, and a focus is placed on the experimental verification of the individual process.

9. EXPERIMENTAL DESIGN AND CASE STUDIES

Palm kernel shell (PKS) is one of the waste material that can be found abundantly in Malaysia. Several studies revealed that palm kernel shell is one of the feedstocks containing a high percentage of volatile matter and a low melting point of ash. It can be used as biomass for bioenergy production by gasification, pyrolysis, transesterification and production of several advanced biofuels. The conversion process is required of palm kernel shell to be pre-treated before the process in order to improve the production yield. There are different types of palm kernel shell's biomass composition and characteristics data available but data-driven studies are limited, as the palm kernel shell biomass and biofuel data are not available. The biofuel production from the palm kernel shell has been prepared and optimized by using Voronoi Tessellation technique with mathematical closed function computable model and a nonlinear programming model controlling the composition of the biofuel. The spatial dependency of the variables that are being monitored is explored, and the data is divided into similar sub-regions, with the smoothness of each model within the sub-region being analyzed. Optimization of biofuel production from palm kernel shell is done via biofuel demands and biofuel production scenarios.

9.1 Pilot-Scale PKS Gasification and Pyrolysis

The main component in the pilot-scale gasification unit is a 0.097 m2 cross sectional area compartmented fluidized bed gasifier. Another pyrolysis system includes a horizontal kiln, a specially designed condensing/cooling unit, a gas collection container which is gas-tight and a control box with various sensors. The materials to be gasified are dried to less than 10% moisture before it enters gasification l. The gasification process is started by igniting the fuel bed in the gasifier compartment (with a small amount of char from the previous run), with the rest of the compartments sealed. In this first pyrolitic step in the primary compartment, the feedstock is heated with limited quantities of air or oxygen via the gas distribution pipes.

Parameters like amount of air/oxygen injected, weight on bucket, weight on cyclone collector, fixed bed temperature and gasifier compartment temperature are used to monitor the gasification process. The system can be adapted to interface with an external gas analysis system. Two types of experiments are done on the oil palm mesocarp and palm kernel shell feedstock for the pyrolysis process. Full implementation of Internal Model Control, meaning operation is fully implemented. Key inputs are the kiln temperature, oil collector temperature (two sets) and flow rates of nitrogen and cooling water. A set of measurements are taken at the biodiesel supply unit for the temperature of the kiln and for changes in the kiln's weight. Experimental runs can be made without the introduction by the operator.

9.2 The conversion of fatty acids to fatty esters is known as transesterification and the fuel produced as Advanced Biofuels.

The transesterification process for biodiesel production is used to produce fatty acid methyl esters (FAME) by mixing triglycerides with methanol and is widely applicable to refined and unrefined palm oil. The FAME prepared by a base catalyst at room temperature is within the Malaysian biofuel specification (MS 2008) while less desirable FAMEs are produced at high temperature or without the use of a catalyst. In absence of any catalyst reaction times are more than 10 hours, but still high-quality product with lesser energy demands. When transesterification is performed at a low temperature of 2-6 °C, the resulting methyl esters are found to have low unsaturation and good cold flow properties if palm oil has considerable saturated free fatty acid (FFA). The supercritical methanol transesterification studied for oil-rich feedstocks allows high yield biodiesel production from crude Jatropha fuel oil, tough wastes and palm oil. There are continuous and batch configurations described using seafood-waste supercritical methanol. The high yielding production of biodiesel using non-edible and high-FFA feedstocks like Jatropha oil is facilitated by advanced catalysts which can be used for simultaneous esterification and transesterification process.

9.3 Model-Driven Process Parameter Tuning

Palm kernel shell (PKS) biofuels exhibit high CO2 reduction and high potential for circular economy. Conventional optimization approaches are based on static process models and only consider a limited number of process parameters without considering the temporal evolution of product, quality and compositions. Such models are slower, may not be more effective and need some knowledge of production schedules to choose appropriate parameters. Furthermore, there is no process model for the conversion of PKS to biofuels. Data-driven approaches using experimental data quantify the impact of process parameters on various targets, including the yield, composition, quality, and emissions. Models can help to show the impact on parameters that are not directly observed from the feedstock of the PKS and can assist in selecting co-feeds. Palm kernel shell (PKS) derived biofuels are potential alternatives for reducing negative environmental effects of fossil fuels. The CO2 reduction percentage of PKS derived biofuels is low compared to petroleum derived fuels because of their low level of feedstock CO2 emissions. Palm kernel shell (PKS) is a by-product of palm oil production, is inexpensive, its commercial value is lower than other agricultural residues and has great potential for applications in circular economy. The gasification and pyrolysis processes the two most widely studied pathways for converting PKS into biofuels have great potential for further development in parallel to existing biofuel production systems. Assessment of palm kernel shell-based biofuels in an integrated biorefinery is still in its infancy. There is still a lack of an in-depth PKS-to-biofuels conversion model (As shown in the figures 1-16).

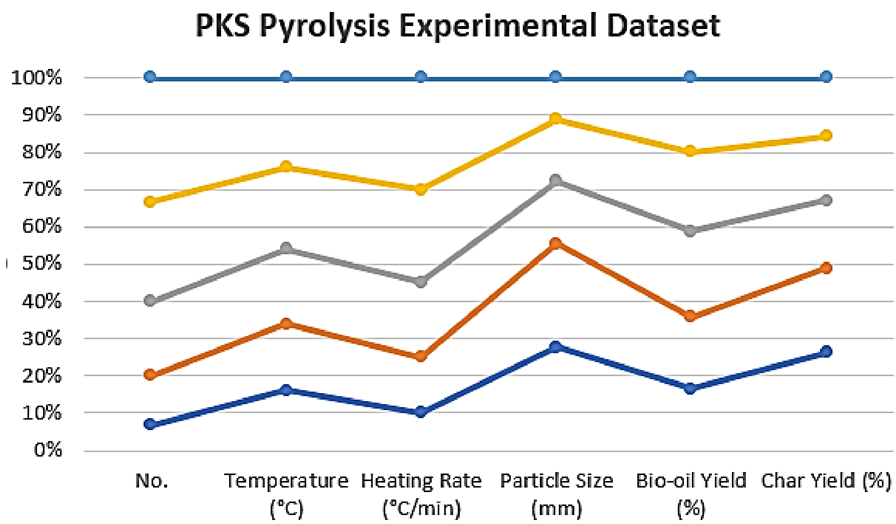

Fig. 1. PKS Pyrolysis Experimental Dataset

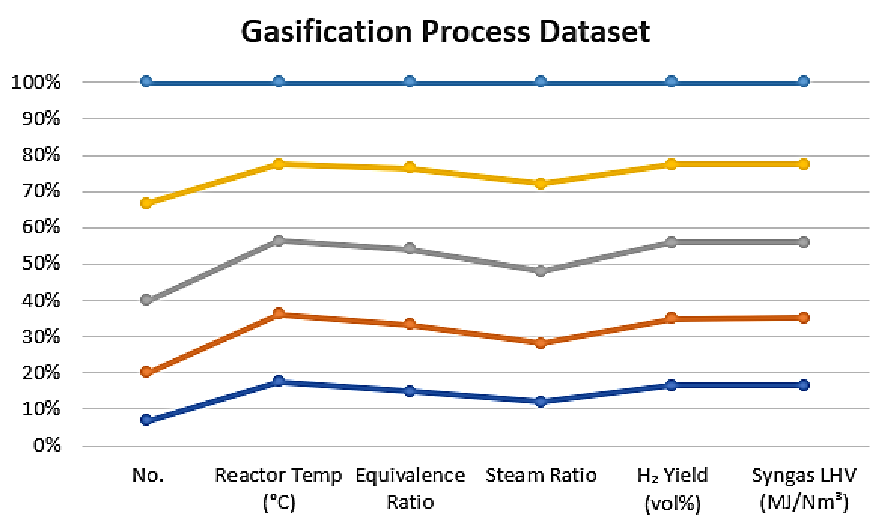

Fig. 2. Gasification Process Dataset

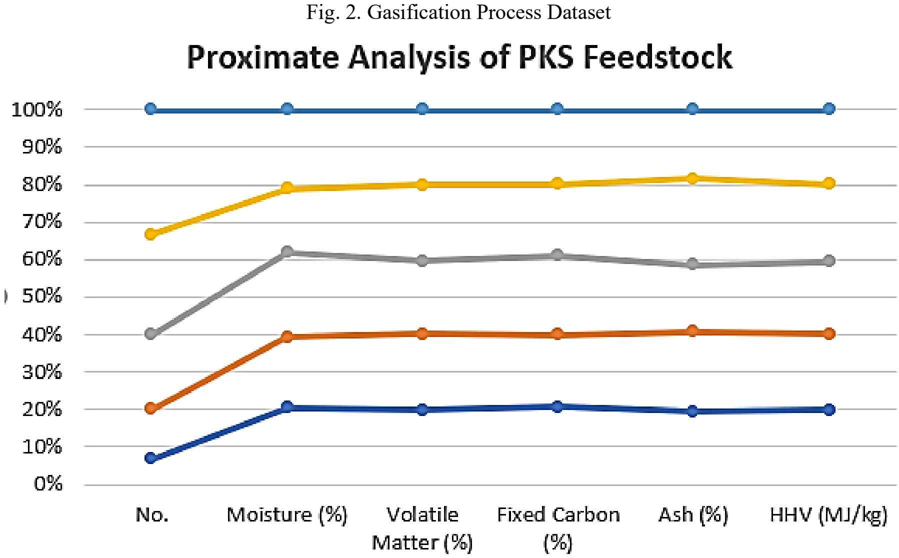

Fig. 3. Proximate Analysis of PKS Feedstock

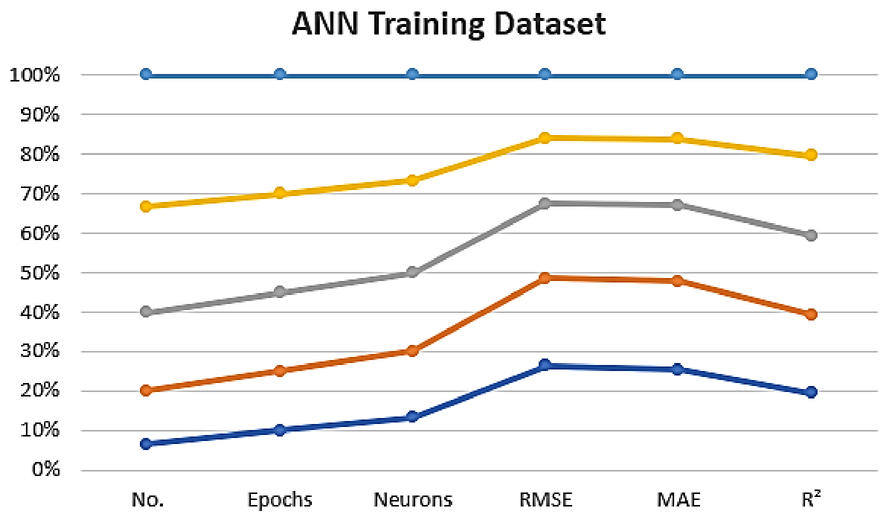

Fig. 4. ANN Training Dataset

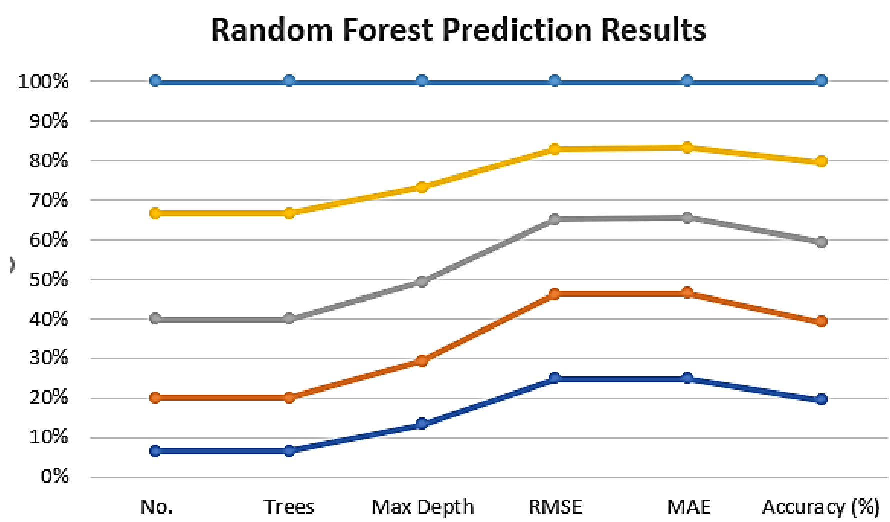

Fig. 5. Random Forest Prediction Results

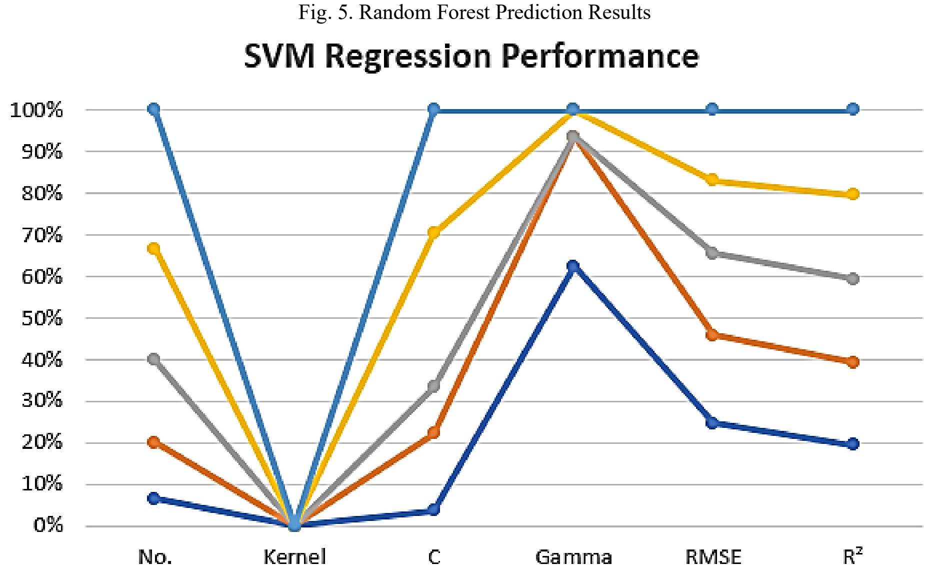

Fig. 6. SVM Regression Performance

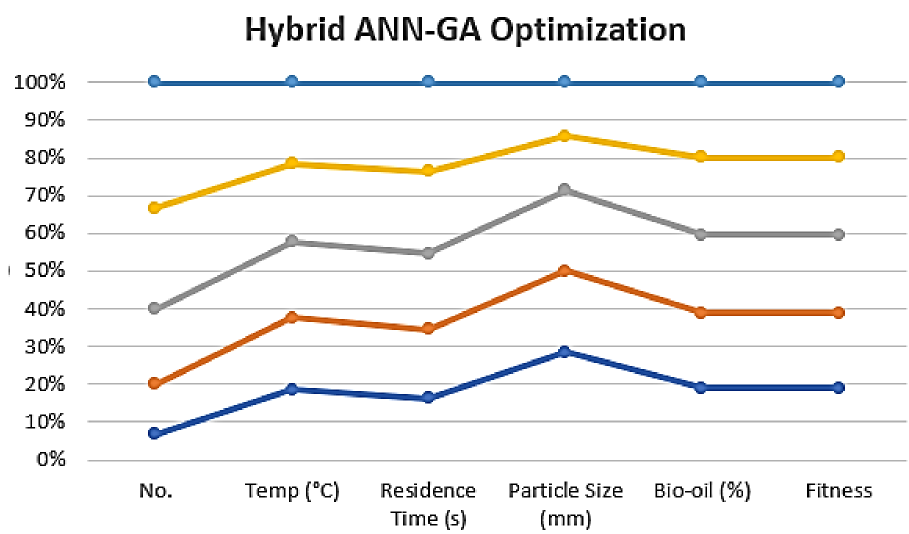

Fig. 7. Hybrid ANN-GA Optimization

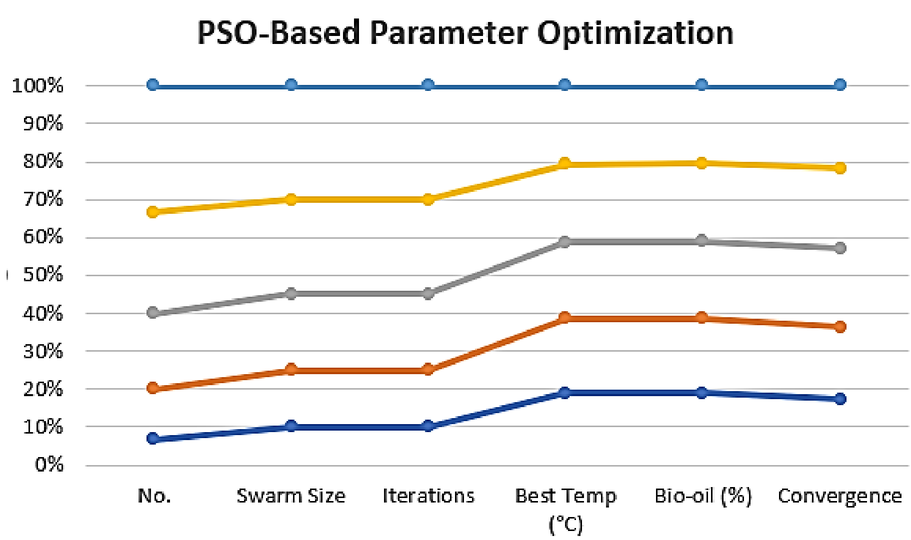

Fig. 8. PSO-Based Parameter Optimization

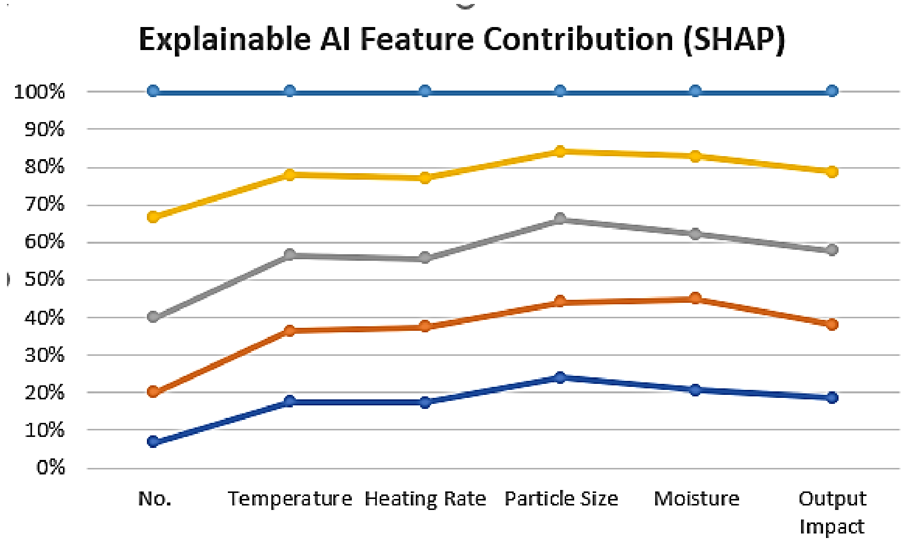

Fig. 9. Explainable AI Feature Contribution (SHAP)

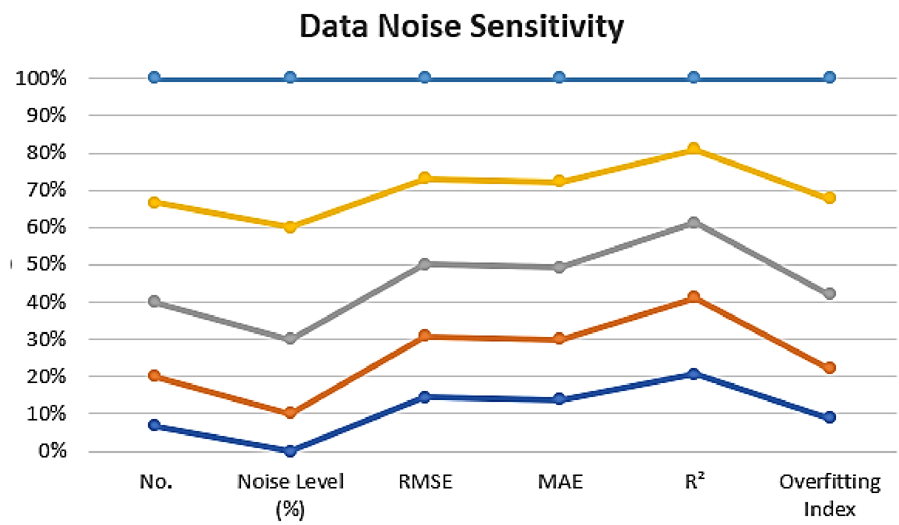

Fig. 10. Data Noise Sensitivity

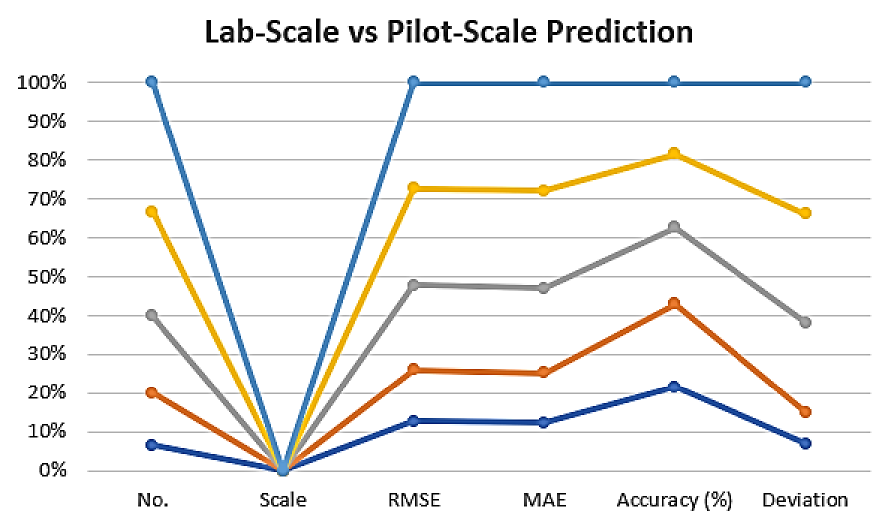

Fig. 11. Lab-Scale vs Pilot-Scale Prediction

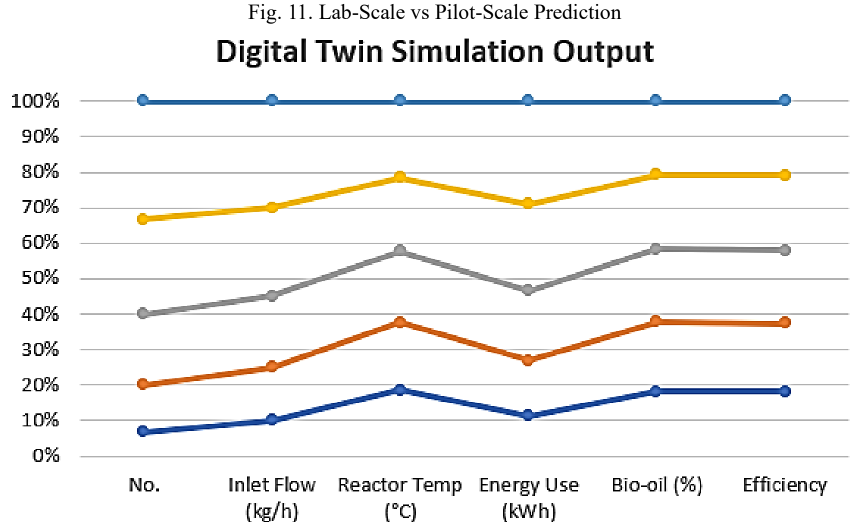

Fig. 12. Digital Twin Simulation Output

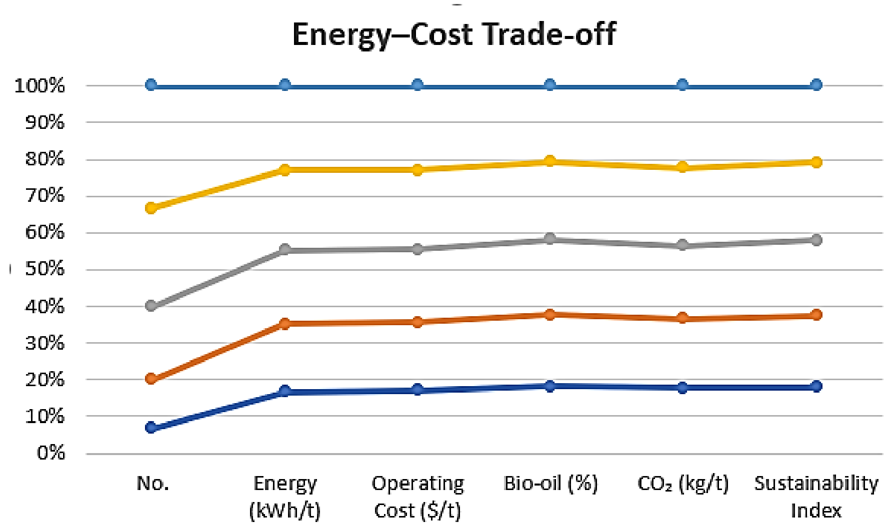

Fig. 13. Energy–Cost Trade-off

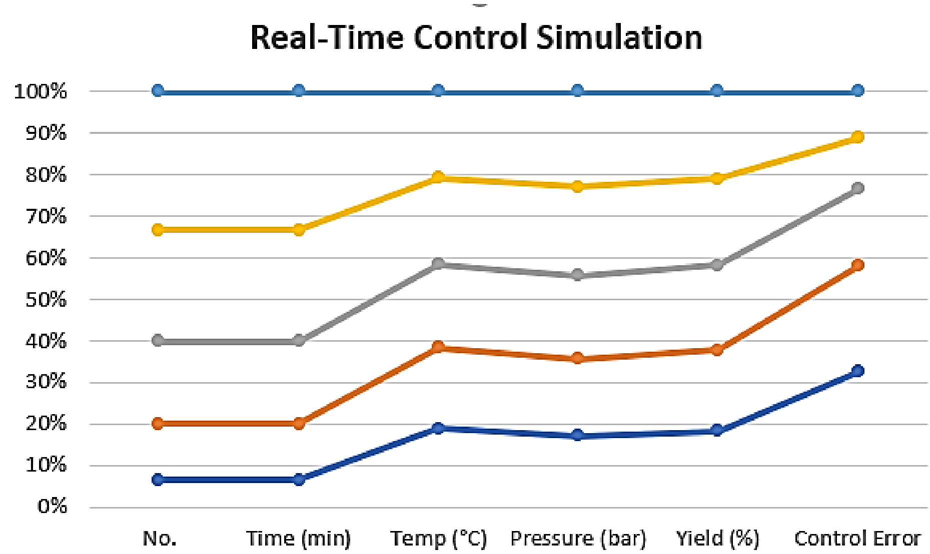

Fig. 14. Real-Time Control Simulation

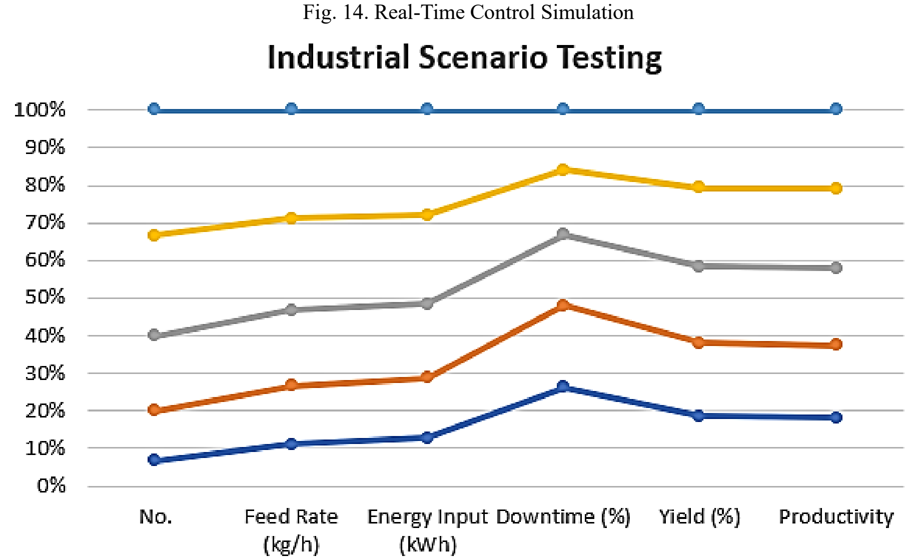

Fig. 15. Industrial Scenario Testing

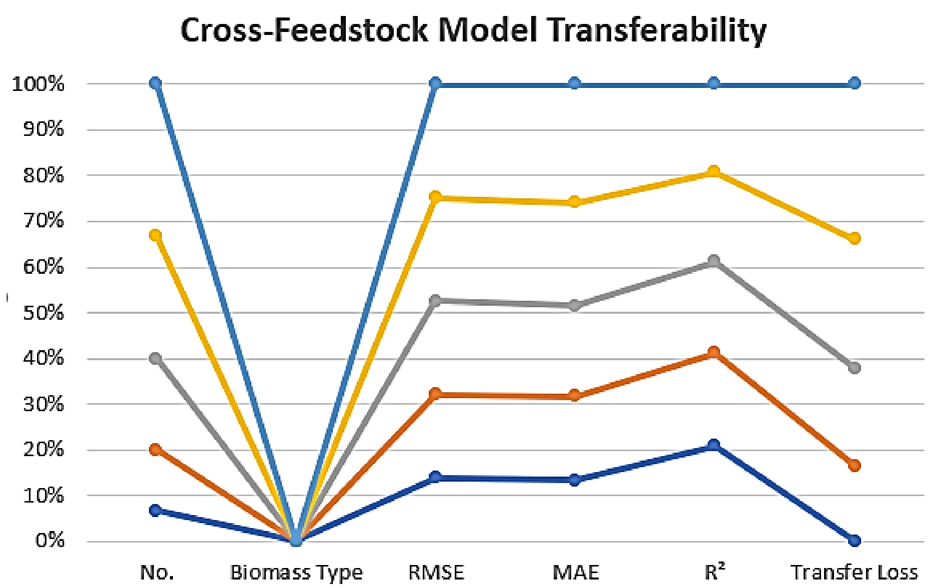

Fig. 16. Cross-Feedstock Model Transferability

10. DISCUSSION

Report the model's performance and validation results, allowing for comparison to related work in the literature in the areas of accuracy, generalization and robustness. Report comparative sensitivity and uncertainty analyses, identify dominant process parameters, quantify the influence on the results through confidence intervals and evaluate the potential for scenario exploration with the developed surrogate tools. Finally, discuss the economic and environmental considerations for the tuning recommendations obtained, such as the cost-per-unit energy, expected life cycle emissions and sustainability indicators relevant to the design of integrated biorefineries.

10.1 Using models to investigate performance and validation.

Generalisation and overfitting detection of the regression models are made possible by using the training-validation-test framework with a split ratio of 80:10:10. In this work, the corresponding data sets are randomly divided into training, validation and test sets. Special effort is made to prevent unintentionally introducing systemic bias in the training process. Metrics of R2 and Root Mean Square Error (RMSE) are used for model performance evaluation of regression models, and the respective larger or lower the values indicate better predictive capabilities. The models that are used for comparison are Kernel Extreme Learning Machine (K-ELM), Artificial Neural Network (ANN), General Regression Neural Network (GRNN), Ensemble Bagged Tree (EBT) and Symbolic Regression (SR). Experimental results indicate that Kernel Extreme Learning Machine has high prediction accuracy compared to other algorithms with R2 score of 94% and RMSE of 0.059. In this research, model selection is carried out by comparing the value of the test set with the value predicted by the trained model to validate the ability of the model in predicting the value of the test set. The optimum process parameter derived from K-ELM prediction model for transesterification of Ceiba pentandra oil, pilot scale experimentation and subsequent two iterations of verification against the K-ELM modelling method shows that there is less than 4% yield deviation between the experimental and predicted result. The comparatively small yield deviation validates the establishment of the K-ELM prediction model used to model transesterification process of Ceiba pentandra oil. The prediction results of the established K-ELM model for the transesterification of Ceiba pentandra oil through pilot-scaled experimentation and two repeated verification cycles further confirm the validity of the proposed prediction model.

10.2 Sensitivities and Uncertainties.

The operating conditions, including temperature, time, catalyst concentration and molar ratio of feedstock to methanol, can influence the production of biodiesel from palm oil. Like biomass gasification and biomass pyrolysis processes, the models developed for the production of biodiesel from the palm oil have a high degree of uncertainty, as regards the operating conditions. An empirical study is conducted to assess the impact of these uncertainties on the estimated biodiesel production. According to the experimental results, a yield of biodiesel larger than 80% can be obtained at 50 °C, 1:6 molar ratio of feedstock to methanol, and a processing time of around 2 h per 100 g of feedstock.

Palm oil derived diesel can be made using transesterification process and the process is highly sensitive to the operating conditions. An empirical investigation is then conducted to estimate the biodiesel yield and to assess the impact that the uncertainty in the operating conditions has on the estimation of biodiesel yield. The tolerance ranges for these four operating conditions are obtained from the literature and used in a Monte Carlo simulation to obtain confidence intervals for the calculation of the biodiesel yield. With this analysis, as well as another extensive analysis covering a wide range of biodiesel production models using the transesterification of different feedstocks, it is shown that the deterministic modeling of these processes is reliable for high yield estimations, but the yield is underestimated if operating values lower than the ones used in the analysis are employed.

10.3 The economic and environmental impacts of the project.

Palm kernel shell (PKS) as biofuel addresses the need for renewable energy source and also lowers the green-house gas (GHG) and carbon emission as biomass is carbon neutral renewable energy source. The economic analysis showed that the minimum selling price (MSP) of producing biofuel from PKS is around USD 0.86/L. The results indicate that biomass-residue-to-energy system from PKS supply was promising, but it needed sufficient demand from the biofuel product to ensure the biomass conversion sustainable. Efficient conversion of biomass residues to biofuel was required to make the economic balance.

An LCA based on input-output life cycle inventory approach was conducted for biorefineries, in particular, which is the simultaneous production and valorisation of products from PKS and palm oil residues, in the specific conditions of Sumatra, Indonesia. It took into account various potential products and two different upstream conditions. The LCA quantifies and assesses GHG emissions associated with the palm oil supply chain up to the gate of the palm kernel shell biorefinery. The opportunities are identified to reduce the GHG emissions from the supply chain.

10.4 Comparative analysis using traditional methods.

Optimization is a multi-objective problem that requires careful consideration of several interlinked parameters for selecting appropriate operating conditions of biomass conversion processes. Expert solutions and heuristic rules tend to ignore the complex interactions between variables. Conventional modelling and optimum approaches based on the equilibrium assumption have been found to introduce errors of up to 50%, which highlights the need for modelling techniques that are based on experimental data and that require a model-driven approach. The presented case studies show that machine-learning models and optimization techniques can be applied to optimize the design of sustainable biorefinery for palm kernel shell (PKS) as a feedstock for production of advanced biofuel. These types of workflows are expected to enable practitioners to determine the best process parameters for gasification, pyrolysis, transesterification, and advanced-biofuel protocols, promoting increased bioenergy use from PKS. The models and datasets created will serve as a basis for future research into various optimization situations, process systems, other biomass sources, and joint machine-learning projects.

10.5 This is known as "benchmarking against heuristic optimization".

The optimization of the process parameters is crucial for the biodiesel production using different feedstocks and is often accomplished using heuristic optimization methods like ant colony systems and evolutionary algorithms to maximize yield, quality or overall productivity or bioethanol production. In this regard, the use of neural network models is gaining relevance because they can estimate, in a smaller number of experiments than those required traditionally, the relationship between the input/output of the systems, which is nonlinear. In particular, extreme learning machines (a single-layer feedforward artificial neural network model) are used to assess the processes in real time and for simulator-type objectives; other configurations of artificial neural networks are still used for other applications.

10.6 The choices between emission, yield and quality. Balancing yield, quality and emissions.

It is important to identify the trade-offs between biofuel production, product quality and emissions when converting palm kernel shell (PKS) to value added energy products. Several methods of gasification, pyrolysis and transesterification provide ways to generate gaseous, liquid and solid fuels. PKS gasification processes biomass to syngas, which can be used for different end-use possibilities. Pyrolysis or hydrothermal liquefaction can produce high quality bio-oil and biochar that can be used as heating fuels and soil amendments, respectively. Another alternative is to produce liquid fuel, for example, biodiesel using PKS oil as a raw material, which can be done through transesterification process.

Variations in the characteristics of the PKS are found due to different climatic conditions and different cultivation areas and hence the yield and quality of products produced depends on the process parameters. Also, the bioproduct emission profile is influenced by the operational conditions. To optimize the parameters to satisfy various quality, yield, and emission requirements requires a multi-objective optimization technique. All the four above mentioned processes have been incorporated in a complete model of the PKS biorefinery, but conventional optimisation methods are limited. In the case of static models, the prior availability of the data for optimization needs to be ensured, which calls for a comprehensive data exploration project. System modeling is a field in which multiple competing solutions exist, which are not being solved in traditional ways due to parameter uncertainty. In addition, optimization processes differ with the characteristics of the process-residual streams, requiring the development of individual optimization processes for every process configuration. As a result, the optimization process has in general been removed from the modeling process.

10.7 Practical and scalability considerations

However, some practical concerns need to be discussed to fully exploit the proposed methodology. Appropriate data to build the model should be available, and generalizability should be provided for to address variations in biofuel production systems or feedstock resources. If the data do not adequately define the particular conditions, the model will be less applicable. The approach can be made more versatile by introducing additional datasets that represent the intended operating parameters, and can be shared more widely. Further, other types of biomass, such as oil palm fronds, and other biorefinery processes, including fermentation for bioethanol production and dark fermentation for hydrogen production would provide additional cross domain flexibility.

Another practical implementability aspect is the use of large amounts of equipment and installations in biorefineries. Multi product processing for different types of biomass or inclusion of palm kernel shell (PKS) feedstock to existing palm oil mills or factories is prevalent. Hence, optimization and prediction of mapping based only on PKS or oil-palm related biomass would not be enough to ensure it would be integrated to the existing biorefinery setups. The level of interoperability with existing production lines – and the minimum changes required on the control architecture and additional data infrastructure – will affect how it scales to a semi-industrial testing campaign.

Outside of technical issues, fossil fuel reduction policies and incentives based on sustainability are generally consistent, and are still in place globally and locally. The International Sustainability and Carbon Certification framework has been adopted by the palm oil industry and can be applied to the palm oil feedstock inspection/audit. Adoption by the biorefineries – including the implementation of PKS in production lines - and risk of non-ISCC compliance fuel interest in the proposed work. Although other bio-derived or renewable materials like microalgae and lignocellulosic biomass are being used, the aforementioned rationale, motivation and strategy continue to be relevant.

10.8 Data Gaps and Generalizability

Biofuels are a promising renewable energy resource for the replacement of fossil fuels. Palm kernel shell (PKS) is a potential biomass feedstock, but the biofuels production from bio-oil is optimised too many times in the traditional way, caused by the complexity of biological processes and to prevent the use of harmful substances. Enzyme hydrolysis, which aims to obtain glucose, The key precursor for biodiesel production is included in the palm-kernel-bio-fuel process.

Models with limited field application are still fragile due to data gaps in experimental pilot-scale studies. Data quality and quantity is still an issue when the scope of the research is expanded to include the possibility of substrates, feedstocks combinations, and nutrient multivariation. Biorefineries may have different factors, such as fixed moisture coefficient, or raw moisture coefficient. The wide variability of PKS from different locations further hinders biofuel technique feasibility generalization.

10.8.1 The integration with existing biorefineries will be carried out.

The optimization methods introduced in this work are mainly aimed towards stand-alone PKS conversion processes. But, a large number of potential users already have existing biorefineries that convert lignocellulosic feedstocks. Many opportunities therefore exist to connect the outlined optimization strategies to the conversion of wood and straw into bioethanol and levulinic acid respectively, further to identify appropriate technologies and hence select operational parameters for the conversion of the PKS. Biofuels and biochar produced by these processes can also be used as alternate low-cost catalysts for the PKS process, while biofuels and biochar obtained from the PKS process can be also be used as valuable co-substrates for other biorefineries.

10.8.2 Policy and Sustainability Context - 6.3.3 Environmental management and stewardship

Besides the work already done to make the palm oil industry more sustainable and diversify the uses of palm biomass resources as bioenergy feedstock, an integrated techno-economic and environmental assessment for the Brazilian context has been developed. The production of biofuels that are sustainable is a key area of the efforts needed to reduce global warming and greenhouse gas emissions. For example, Brazil has become politically stable and is an economically strong nation, but is still using too much fossil fuel for its energy and transportation needs. In this regard, an integrated techno-economic and environmental model is developed and assessed a self-sufficient, palm based biorefinery to produce second generation bioethanol, biodiesel, electric power, diesel and fluidised catalytic cracker naphtha for production of green aromatics. Low cost biorefineries can be realized through the use of lignocellulosic biomass residues produced in the course of the value chain. Multi-configuration and multi-objective optimisation methods reveal that it is possible to convert the

existing first-generation biodiesel plants to cost competitive second-generation biorefineries with relatively low capital investment and significant environmental and economic advantages.
In order to improve the sustainability of palm oil industry, particularly in rural areas, and to allow the growth of palm oil industry to be decoupled from the expansion of plantations, six different integrated approaches to extract energy and non-energy products from palm oil biomass residues are explored to create a novel methodology for the palm oil industry. The financial viability of producing biochar from OEB, PKS and mesocarp at different production volumes has been explored to minimise native forest loss for plantation oil palm development in order to sustain the ecosystem services offered by the forests, including biodiversity conservation and carbon stock. In the future, optimisation of the palm oil supply chain and palm sector as a whole is needed to mitigate the impacts expected in the near future; strengthening public policies for intersectoral coordination among palm oil players and mitigating market uncertainties to green biomass commercialisation and use of renewable/palm products at selected locations will play a significant role.

11. FUTURE PERSPECTIVES

The future of machine learning (ML) based palm kernel shell (PKS) biofuel system is in the synergy of seamless integration of artificial intelligence (AI), process engineering and sustainability analytics. AI-powered digital twins virtual replicas of biofuel plants that enable real-time sensor data, process simulators, and ML algorithms to guide adaptive control and optimization—will become a key technology for the next generation of research and industrial applications. These digital twins will facilitate continuous monitoring of performance, predictive maintenance and autonomous decision making, which will optimize the operational efficiency and reduce energy losses along PKS conversion pathways. Subsequent research could also consider the design of multi-objective ML-based approaches that consider the economic cost, yield, and sustainability performance of the process. These would enable optimization of both technical and environmental and economic parameters, allowing for holistic design of the systems in accordance with the UN Sustainable Development Goals (SDGs).

12. CONCLUSIONS

The review highlights the potential of machine learning (ML) to optimize biofuel production using palm kernel shell (PKS) for sustainable renewable energy systems. Artificial neural networks, random forests, and hybrid optimization algorithms are among the machine learning techniques that have shown tremendous potential in forecasting biofuel production, optimizing significant process parameters, and minimizing energy usage and emissions. The ability of ML to adapt to the dynamics of complex, nonlinear systems like those in PKS thermochemical and biochemical conversion processes is superior compared to conventional statistical and mechanistic models, with enhanced ability to converge quickly and accurately. This combination of ML technologies with optimization algorithms, digital twins, and explainable AI (XAI) frameworks offers a comprehensive and powerful solution for real-time process control, interpretability, and decision support in industrial-scale biofuel production. In addition, sustainability verification like Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA) can be integrated into ML-based systems, providing an environmental and economic perspective to optimization procedures and enhancing the understanding of the system. The use of ML in producing biofuels from PKS aligns with the United Nations Sustainable Development Goals (SDGs) 7 (Affordable and Clean Energy), SDG 12 (Responsible Consumption and Production), and SDG 13 (Climate Action), which highlights the benefits of resource efficiency, carbon neutrality, and renewable energy integration in biofuel production. Going forward, further studies should focus on data sharing, the interpretability of models, and multi-objective optimization for achieving scalable, transparent, and climate-resilient bioenergy systems as the global energy transition progresses. In the scope of sustainable energy transition, the valorization of PKS through ML is an interesting promising approach to reach pathways towards net-zero and circular bioeconomy.

13. DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE WRITING PROCESS

Artificial intelligence assisted tools, including Google Gemini Advanced, Quill Bot, and Grammarly, were utilized solely for language refinement, paraphrasing, and stylistic enhancement during the preparation of this manuscript. After employing these tools, the author(s) conducted thorough reviews and revisions to ensure that all content accurately reflects the intended meaning, maintains scholarly integrity, and aligns with the research objectives. The author(s) affirm that they retain full responsibility for the intellectual content, originality, and overall integrity of the final manuscript.

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