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AI-Driven Optimization of Bio-Energy Systems: Models for Resource Assessment and Emission Reduction

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ABSTRACT

The increasing complexity of bio-energy systems is a reason for the need of advanced analytical methods to enhance resource utilization, process stability and environmental performance. AI methods are popular in this domain, but many papers neglect concerns around data quality, interpretability, scalability and the low generalization potential of models toward plants and feedstocks different from those they were trained on. This paper intends to offer a systematic review on AI techniques available for biomass resource assessment, conversion-process optimization, and supply-chain planning and emission management. The review is structured adopting a rigorous review approach focusing on model, data set, optimization framework and hybrid method developed in the scope of bio-energy value chain. Highlights – The key findings are that AI improves the prediction of biomass availability and biogas/syngas yields, of feedstock properties and emission behavior; surrogate and hybrid models result in expedited simulation time and facilitate real-time decision making. The review also highlights an emerging trend with digital twins, remote sensing with application of machine learning, and federated learning in multi-plant optimization. These findings also have important implications for researchers, engineers and policy-makers who aim to develop robust low

emissions bio-energy systems that are economically feasible.

Keywords: Artificial intelligence in bio-energy; biomass resource assessment; machine-learning optimization; bio-energy supply chains; emission prediction and mitigation; sustainable energy systems.

1. Introduction

Bio-energy is still a significant renewable resource because it can be used to convert agricultural residues, and organic feed into useful products like biogas, bioethanol, biodiesel, and bioheat. The performance of these systems is highly sensitive to accurate resource assessment, cost-effective conversion and managed emission. A number of these tasks also include non-linear behavior, unknown characteristics of the feedstock and dynamic operating conditions which can limit conventional modelling methods.

AI approaches offer system tools to capture and learn patterns from a variety of data types as well as means to manage uncertainty and aid predictive decision making along the bio-energy chain. Up-to-date AI models are broadly applied for predicting the biomass potential, predicting biogas yield, optimizing operational parameters and evaluating environmental effects. In this paper, we introduce major AI applications in the areas and summarize the research trends. Bio-energy processes that convert biomass to various forms of energy are at the heart of global efforts to make a transition from conventional (fossil-based) to sustainable and renewable energy sources [1]. With the AI techniques, these systems could be developed to take new opportunities of reducing product costs and also supporting a greener environment [2]. And now AI tools are used across the entire bio-energy lifecycle, from prediction of biomass properties to optimization of conversion processes, supply chain management, and assessment of environmental performance [3] [4]. This paper reviews cutting-edge AI-based optimization models, which target resource assessment and emission reduction in bio-energy systems [3] [4]. It also reviews how machine learning, which is capable of capturing complex nonlinear phenomena characterizing such systems, has led to enhanced energy harvesting and addressed concerns associated with energy security and environmental sustainability [5].

AI has been widely adopted over the past 10 years, particularly for predictive and optimization applications. Researchers have emphasized energy-use analysis, process value-chain evaluation, and risk management [6]. Most AI models are black-box systems: they train on input-output relationships and predict well on observational data. This method is appropriate for nonlinear processes like anaerobic digestion [7]. The method allows building models to forecast optimal operating conditions for enhanced energy yield without a thorough mechanistic understanding [8].

Various segments of the bio-energy chain possess different data and uncertainty structures as well as mechanistic limitations, so that certain classes of models may a priori be more appropriate than others. Black-box models, such as ANN, RF and SVR seem to be more efficient in biomass resource assessment and feedstock quality prediction for they are based on large-sized and heterogeneous databases where the existence of complex nonlinear patterns and physical mechanisms is less obvious. Hybrid and physics-guided models are better suited for conversion systems in which the reaction paths and biochemical constraints affect the system response. Such models can retain predictive ability, and at the same time to be compatible with the known thermodynamic, kinetic, or other principles. Interpretable and model-agnostic methodologies are considered to be more suitable for supply-chain planning and emissions management as well, where transparency, interpretability, and traceability of the solution can be helpful in making operational decisions or supporting regulatory reporting/sensitivity analysis. Taken together, this differentiation helps to explain how each type of AI model corresponds with the technical requirements, data availability and operational objectives of distinct stages in the bio-energy value chain.

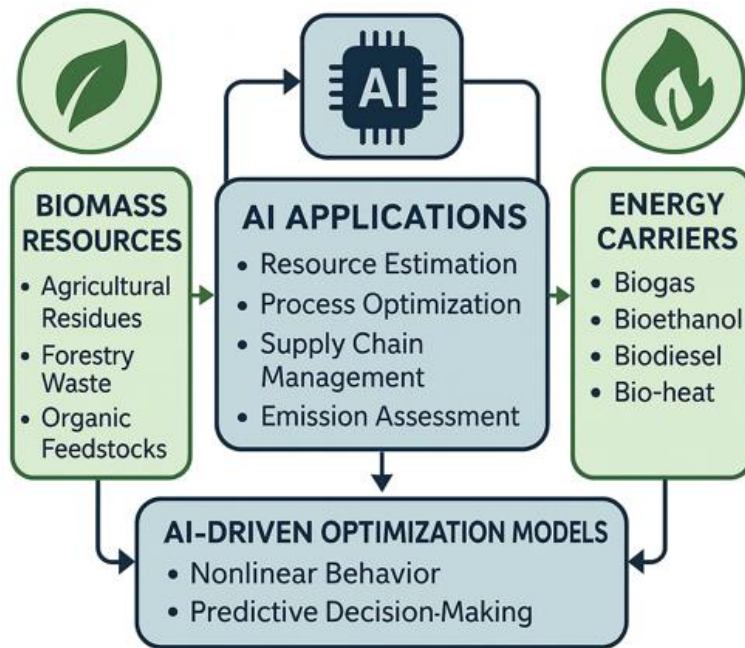


Figure 1. AI-Integrated Framework for Bio-Energy Systems

Figure 1 illustrates how AI methods interact across resource assessment, conversion, logistics, and emission management, showing the flow of information that links these stages. The figure highlights that predictive models function as decision-support tools rather than isolated components.

Neural networks, random forest and support vector machines are applied in many studies since they can use online data learning to adapt current state [8]. This functionality is critical for anaerobic digestion, which exhibits rich and sensitive dynamics impacting renewable energy production [5, 9]. Digestion behavior under different circumstances can be estimated by machine learning, and real-time control power can enhance the stability and efficiency [8]. Hybrid ML– optimization techniques, e.g., GA and PSO to improve biogas and methane yield, minimize overfitting, and optimize prediction accuracy [10]. These models are faster than the mechanistic type and more appropriate for real use [10]. They can also rapid predict the main outputs in order to support online monitoring [10, 12]. AI methods continue to require extremely large and accurate training datasets, and may be unable to generalize without additional real-world constraints [8, 10]. They are not, however, arbitrary-function approximators and do not support parallel processing but are still effective in modelling bio-energy systems [11]. Biochemically detailed mechanistic models like ADM1 are hard to calibrate for use in real time [8]. Machine learning is not burdened with solving (heavy) differential equations and has smooth connections to heuristic optimization tools [10, 7]. Interpretable tools must also be incorporated to demonstrate why ML is successful, enhance yield prediction and lead to optimal operating points [10, 13]. Explainable AI can also enhance trust in industry [8]. The absence of benchmarking datasets and in-depth validation principles hinders scale-bridging as well as feedstock translation [14]. Interpretative models are necessary to go beyond black-box predictions and provide process understanding [13]. Hybrid mechanistic–ML models merging biochemical information with data-driven power bring great potential for the enhancement of anaerobic digestion and other bio-energy systems [15, 8]. Important challenges such as preprocessing, interpretability, scalability and model selection are open and data standards and benchmarking frameworks need to be improved before it can scale and be applied in bio-energy systems [13, 15].

Table 1. AI Applications and Research Directions in Bio-Energy Systems

Aspect	Description	AI Role	Common Algorithms	Strengths of AI Models	Limitations / Gaps	Future Directions
Bio-energy Resources	Biomass from agriculture, forestry, and waste converted into biogas, bioethanol, biodiesel, and bio-heat.	Predict biomass availability and properties.	ANN, RF, SVM	Handles nonlinear and uncertain data.	Needs large datasets; limited transferability.	Build standardized datasets.
Conversion Processes	Anaerobic digestion and other processes show nonlinear behaviour.	Forecast biogas/methane yields and optimize conditions.	ANN, GA-ANN, PSO-ANN	Rapid predictions; adaptive learning.	Black-box behaviour.	Develop explainable and hybrid models.
Process Control	Real-time control improves stability in digestion and conversion units.	Predict operating conditions for stable performance.	ANN, SVM	Fast response; adaptive updates.	Accuracy depends on training quality.	Use model-agnostic interpretability tools.
Supply Chain & Logistics	Biomass transport and storage depend on variability and demand.	Support planning and supply-chain optimization.	RF, GA, PSO	Addresses uncertainty in multi-stage systems.	Lack of unified validation protocols.	Establish evaluation metrics and model guidelines.
Environmental Assessment	Emission control and lifecycle impact prediction.	Predict emissions and environmental impacts.	Ensemble models	Captures complex interactions.	Lacks embedded physical laws.	Link mechanistic and AI-based models.
Model Integration	Mechanistic models give insight but are computationally intensive.	Combine data-driven and mechanistic models.	Hybrid mechanistic-ML	Reduces overfitting; improves reliability.	Integration complexity.	Strengthen hybrid modelling frameworks.
Research & Scalability Challenges	Data pre-processing, interpretability, and scalability issues.	Improve prediction quality and stability.	Explainable AI, hybrid models	Supports transparency and wider adoption.	Incomplete datasets; inconsistent metrics.	Create stronger validation frameworks.

The objective of this study is to conduct a systematic review on use of artificial intelligence techniques along the bio-energy value chain i.e. biomass resource assessment, process optimization, supply-chain planning, and emission management in order to provide a knowledge base for researchers in this field. The research investigates how various AI models, datasets and unified hybrid optimization approaches cope with system nonlinearity, operation uncertainties and environmental constraints of the bio-energy system. By analyzing the recent trends, and finding shortcomings of present methodologies, this review aims to elucidate research gaps and provide future directions that can facilitate developing more effective, scalable and low-emissions bio-energy systems. **Table 1** explains AI Applications and Research Directions in Bio-Energy Systems.

While there is no shortage of studies that show the promise of AI for resource mapping, process optimization and emission reduction in this field, a unified overview considering all classes of models over the full range of processes along the bio-energy chain as well as their relevance with respect to data availability, the complexity of processes and operational constraints has been lacking. The majority of these reviews concentrate on single processes such as anaerobic digestion or specific algorithms, without

consideration to addressing realistic decision-making requirements at a system level. This results in a disjointedness between the performance of different AI methods, where they fail to perform, and how they can be coordinated with mechanistic knowledge and new tools such as digital twins and federated learning. Filling this gap is a crucial step toward implementing AI-based workflows that enhance the reliability, transparency and scalability of real bio-energy applications.

2. AI applications in biomass resource assessment

AI methods have broadened the scope of bio-energy research by providing means to capture relative nonlinear dynamics, to respond to varying operational and environmental contexts, and learn from different data sources. These models contribute to more accurate predictions for biomass availability, biogas yield and emission patterns that are problematic to estimate using only traditional methods. Their increasing popularity through laboratory studies, pilot plants and, industrial-scale plants demonstrate the trend towards a data-driven process monitoring approach for both tactical planning and daily operation decisions. This shift also underscores the requirement for thorough evaluation of data quality, model interpretability and scalability to enable practical and reproducible results at the scale required for a range of bio-energy systems.

2.1. Biomass quantity estimation using remote sensing and ML

Determining the biomass resource is crucial for planning of any bio-energy project. It serves to screen plant sites, forecast annual material spectrally and minimize supply risks. Remote sensing has attracted attention in recent years, since it offers regular and extensive measuring opportunities. From satellite imagery, drone surveys and airborne LiDAR, we can acquire very fine details on land cover, condition of vegetation dynamics as well as surface structure. This data is then consumed by machine learning models which predict biomass more accurately compared to traditional field surveys. Methods such as RF, SVR and CNNs examine the correlation between spectral signatures, vegetation indices (VIs), soil moisture, and land surface temperature (LST). By incorporating these inputs with field measurements from reference sites, the models generate spatial maps of agricultural residue availability, forest biomass density and municipal waste output. These maps are useful for long-term planning and offer better use of biomass estimates.

In addition, AI application in remote sensing also supports the ability to monitor biomass growth and yield over different landscapes, enabling a more responsive resource-management approach. This facilitates the dynamic realignment of feedstock supply chains, mitigating logistical inefficiency and securing a continued supply of biomass for bio-energy plants^[16]. AI-based strategies are also vital to facilitate genetic selection and engineering of energy crops while enhancing biofuels production yield and total system efficacy^[17]^[18]. The applicability of these models is highly dependent on the availability of high-quality, application-specific data, which are often expensive and time-consuming to collect^[4]. More powerful data augmentation and transfer learning strategies across different geospatial datasets should be designed to solve this shortcoming and enhance model generalizability. Despite these improvements, reliable biomass mapping in complex forest structure areas is still challenging and the selection of appropriate algorithms and approaches for resource estimation at different scales is needed^[19]^[20].

2.2. Predicting feedstock quality

The quality of the biomass feedstock is a key factor in the conversion of biomass (including combustion, gasification, pyrolysis and anaerobic digestion). Characteristics such as the moisture, ash, carbon/nitrogen ratio and volatile matter contents are directly related to energy production and process efficiency. Machine learning models built on the basis of proximate and ultimate analysis data could provide a more accurate prediction as opposed to general empirical correlations. Modelling methods, including gradient boosting and ANNs, are trained with vast laboratory datasets to recognize patterns and predict critical parameters such as HHV, biodegradability, and methane potential. These predictions enable operators

to estimate the applicability of agricultural and forest residues, the choice of blending options and proper pre-treatment routes prior to conversion. The ability to predict saves expensive and time-consuming experiments, leading to improved process optimization and root performance in bio-energy systems.

AI will also be able to predict the impact of storage conditions and season on feedstock quality, enabling proactive actions to keep these at suitable properties for conversion processes [21]. For the case of biomass pyrolysis, machine learning is also utilized to predict bio-oil yield and quality, which have been shown to achieve higher predictive accuracy than conventional empirical models [22]. During the biofuel life cycle, machine learning has been used for applications, especially in aspects relevant to Industry 4.0 to enhance feedstock screening and supply-chain management [23]. These tasks range from logistics optimization, rheological property analysis and impact on biofuel quality, serving the purpose of a more efficient conversion [23]. The combination of machine learning with advanced analytical methods provides an excellent route for the online feedstock characterization and adaptive control of process settings and permits a basis to optimize bio-energy production [17].

Table 2. AI Applications in Biomass Resource Assessment and Feedstock Quality Prediction

Topic	Focus Area	AI / Data Sources	Key Contributions	Current Challenges
Biomass Quantity Estimation	Assessment of agricultural residues, forest biomass, and municipal waste	Remote sensing (satellite, drones, LiDAR); RF, SVR, CNNs	Spatial biomass maps; supports site selection, forecasting, and supply-risk reduction	Limited datasets; difficult mapping in complex forest regions
Remote Sensing Integration	Continuous monitoring of vegetation and land-use patterns	Spectral indices, soil moisture, LST with ML	Dynamic resource management; improves feedstock supply stability	Costly data collection; limited transfer learning ability
Energy Crop Improvement	Selection and improvement of biomass crop varieties	ML with remote sensing and genomic data	Improves crop breeding and yield prediction	Need better data augmentation and generalization strategies
Feedstock Quality Prediction	Estimation of moisture, ash, C/N ratio, volatile matter, HHV, biodegradability	Gradient boosting, ANN, large lab datasets	Predicts conversion suitability; guides blending and pre-treatment	Seasonal and storage-related variations need stronger models
Biofuel Process Support	Quality prediction in pyrolysis, gasification, and Industry 4.0 supply chains	ML with analytical and process data	Forecasts bio-oil properties; supports logistics and rheological assessment	Needs stronger real-time datasets and integration frameworks

Table 2 outlines how AI combined with remote sensing improves biomass resource assessment by generating accurate spatial maps, supporting long-term supply planning. It also highlights predictive tools used to evaluate feedstock quality, which help refine conversion processes and enhance overall bio-energy system performance. Insights from biomass availability and feedstock quality assessment. It is these materials discussed in "Process understanding in bio refining application of AI to bioenergy processing" that help underpin the performance of the materials under downstream conversion pathways and hence naturally lead to consideration of AI-backed optimization within bio-energy conversion processes.

3. AI for process optimization in bio-energy conversion

The optimization of process performance is a key concern for enhanced stability, efficiency and environmental impact of bio-energy system operation because the conversion pathways are frequently characterized by complex reaction pathways and narrow operating potentials. AI approaches provide a systematic technique to examine such nonlinear behaviors by estimating the input-output relationships of processes, identifying early symptoms of instability and offer appropriate control actions. These methods supplement the traditional kinetic and mechanistic models to minimize computational expense with

acceptable predictive performance. Their increasing deployment in bio-gas production, thermo-chemical conversion and integrated bio-refinery processes are indicative of the possibilities for enhancing on-line control, resource utilization and emission footprints.

3.1. Anaerobic digestion and biogas systems

The anaerobic digestion process is sensitive to temperature, pH, organic loading rate (OLR) and the composition of feedstock. AI methods are currently applied to predict biogas yield, monitor the first indications of the process instability and propose appropriate feed ratios. Models including ANNs, LSTMs and ensembles have all been used to predict methane production with high accuracy. Hybrid ML–kinetic models Hybrid ML–kinetic models add machine learning (ML) to the kinetic M–CMBD model so as to achieve better generalization scenarios. For instance, ANNs have been successfully combined with particle swarm optimization to predict and maximize biogas production from palm oil mill effluent in solar bioreactors [17]. This kind of integration allows for real-time optimization of operating parameters and better energy conversion efficiency, particularly under changing environmental conditions [22]. Reinforcement learning (RL) has begun to be used in the context of real-time control of digesters. RL agents are capable of adjusting the operating factors, OLR or mixing strength, for example, according to observed digester behavior and may be applied on-the-fly. This approach also optimizes the biogas yield and process stability, so that the accumulation of toxic matter can be avoided for a stable bio-energy production [15]. The improvement of dynamic optimization is even more pronounced by integrating it into operation with online sensor information or forecasting data in order to predict transitions between feedstock quality or environmental states [15]. Machine learning also enables more general decision-making. The inclusion of ML in the life cycle assessment and techno-economic analysis allows for a rapid identification of viable equipment configurations and cost estimates as opposed to using conventional process simulations [17]. Applications of machine learning in ad have expanded to monitoring, modelling and optimizing the bioprocesses key parameters, and have led to considerable improvement in biogas production efficiency [15].

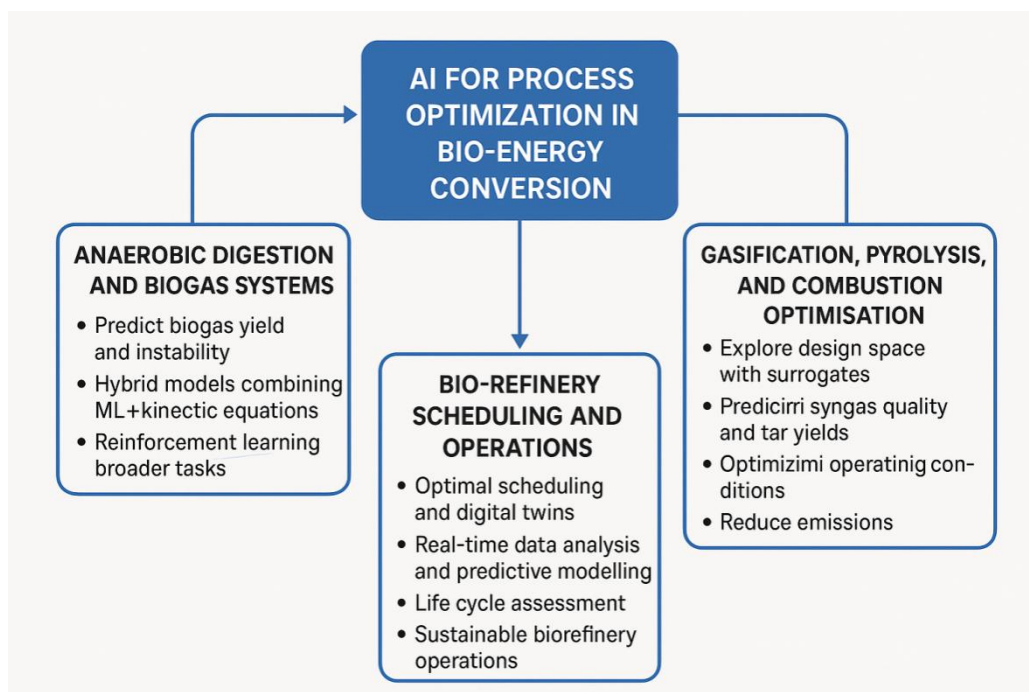


Figure 2. AI-Driven process optimization framework for bio-energy conversion systems

Figure 2 outlines how AI supports monitoring and control in major conversion pathways, showing the shift from static modelling toward adaptive, data-driven operation. The layout makes clear that process optimization relies on iterative feedback between reactor conditions and model predictions.

3.2. Gasification, pyrolysis, and combustion optimisation

Gasification or pyrolysis are (high temperature) processes, particle size-dependent and sensitive to temperature, residence time and equivalence ratio. Artificial neural network models enable fast screening of the design space and help in finding conditions in which syngas can be enhanced or tar formation suppressed. ML techniques have also been successfully applied to the air–fuel ratio control for combustion systems, and a feedstock blending strategy based on ML for reducing the pollutant emissions.

Sophisticated machine learning-based methods are used to forecast outputs (methane, hydrogen, carbon monoxide, carbon dioxide and higher heating value) from the downdraft biomass gasification process with R^2 values greater than 0.9, demonstrating better predictive ability compared to conventional modelling techniques [22]. Combining machine learning methods, such as artificial neural networks with genetic algorithms, has been proven to be quite effective in optimizing the biomass pyrolysis and gasification, resulting in better performance in terms of energy recovery [24]. These techniques well extend to predict the combustion efficiency and very appropriate for the determination of optimal operating conditions in regard to emission reduction with data sets covering various operational modes [17]. In addition to the prediction, ML algorithms are also used for the optimization of bio-oil products and experiment-based studies have demonstrated their high yield and good energy recovery [22]. To this aim, it is necessary to develop accurate, fast and robust models for complex thermos-chemical processes. Machine learning offers robust alternatives to time consuming conventional methods, and provides dependable performance over a range of scenarios [25]. High predictive accuracy ($R^2 > 0.90$) of syngas composition and product distribution in gasification was obtained using models like support vector machines, random forests or artificial neural networks and in certain cases, these models performed better to conventional mechanistic models [26] [24]. A combination of machine learning with computational fluid dynamics (CFD) aids in the improvement of predictive performance. These models will be more useful to predict the yield of tar and the content of hydrocarbon in gas, which provides the possibility towards pyrolysis and gasification processes optimization [27] [28]. ETR has proven to be especially effective in the prediction of syngas properties in biomass chemical looping gasification when few data samples are available [29], outperforming artificial neural networks and random forests in terms of accuracy. These AI-assisted optimizations lead to smaller emission footprints and higher sustainability in bio-energy systems by optimizing process parameters [30]. They tend to use resources more efficiently and produce cleaner energy, enabling the bio-economy to become more environmentally sustainable [31].

3.3. Bio-refinery scheduling and operations

Bio-refineries handle several products and processes depending on each other, where optimized feedstock input, reactor operation, and energy flows become a key point. Machine learning-enabled optimization integrates machine learning predictions with mathematical programming models to reduce energy and emission levels. With Twins, advanced operating results tracking in real time is made possible by the digital twins underpinned by machine learning. Such digital twins enable predictive maintenance, anomaly detection and proactive adjustments to operating conditions, with the potential that they lead to enhanced refinery efficiency and profitability [32]. Even in the smart integrated bio refinery case, machine learning is used to analyses data and make predictive models in real-time monitoring for better utilization of resources, decrease waste [32]. The use of machine learning in combination with LCA tools enables assessment of the environmental and economic impact across various pre-treatment strategies, to promote sustainability considerations in bio refinery design and operations [17]. The support by AI and ML shines a light on the commercial developments of innovative bio refineries by giving assistance and improvements to critical aspects, toward future biofuels and biochemicals. These technologies favor the integration of data) processing, and system-level decision making in catalyst design, synthesis and characterization critical to the effective conversion of ligno-cellulosic biomass [33]. This integrated analytical and predictive framework

offers a better understanding and control of complex bio-refining operations, advancing ourselves toward a sustainable bio-based economy [17] [34]. Smart models can further support lignocellulosic biomass bioconversion thanks to the possibility of do a preliminary screening and identifying compatible windows on operating the needed pre-treatments as well as also for optimizations [17]. **Table 3** shows how AI techniques promote important bio-energy conversion processes for prediction, monitoring and operational control. It emphasizes the use of machine learning and hybrid models for the enhancement of anaerobic digestion, thermos-chemical reactions, and bio-refinery operations towards improved efficiency and stability.

Table 3. AI for Process Optimization in Bio-Energy Conversion

Area	Process Focus	AI Methods Used	Key Contributions	Challenges / Needs
Anaerobic Digestion & Biogas Systems	Stability control, methane prediction, feed ratio management	ANN, LSTM, ensemble models, PSO-ANN hybrids, RL	Forecasts methane yield, detects instability, supports real-time adjustments, improves system efficiency	Needs high-quality sensor data; limited generalisation across feedstocks
Hybrid ML-Kinetic Modelling	Mechanistic-data fusion for digesters	ML combined with kinetic equations	Better prediction across varied conditions; supports adaptive optimisation	Integration complexity; varied performance across reactor scales
Thermo-Chemical Conversion	Gasification, pyrolysis, combustion	ANN, GA-ANN, SVM, RF, Extra Trees	Predicts syngas composition, reduces tar, improves bio-oil yield and emission control	Requires robust datasets; complex reaction pathways still difficult to capture
ML-Enhanced CFD & Surrogate Modelling	High-temperature reactor optimisation	Hybrid ML-CFD models, surrogate models	Faster design exploration; better prediction of tar and hydrogen output	Accuracy depends on calibration; limited transferability
Bio-Refinery Scheduling & Operations	Feedstock scheduling, pretreatment, energy flow control	ML with optimisation, digital twins	Real-time monitoring, predictive maintenance, improved scheduling and resource use	Needs strong data integration and coordination of complex workflows

Based on the set of studies reviewed, several points of consensus and contestation emerge. A large number of studies consistently claim that black-box models (e.g., ANN and ensemble methods) provide good predictive accuracy for nonlinear biomass and conversion processes, in line with observations across anaerobic digestion, pyrolysis and gasification literature. There is, however some imprecision from studies which describe the model's generalization differently, with conclusions regarding strong model transferability across feedstocks as well as claims for lack of transfer since data is scarce and operating conditions vary are published. A smaller number of studies present hybrid or physics-driven models, which present better reliability and interpretability, providing insights beyond pure prediction. Such differences illustrate that, although the literature concurs generally with regards to AI benefits in bio-energy improvement operations, various modelling approaches address distinct concerns and overcome them only given an appropriate level of data quality, reactor scale and process variability. These comparisons serve to make clear why the guidance on model selection is so varied across the field. As the process-level optimization ensures more stable and efficient individual conversion units, attention is shifted to the supply-chain rationale that supports continuous operation, including the usage of AI to make transport-, storage- and planning-decisions safer.

4. AI-enhanced supply-chain optimization

AI increasingly assists in the efficiency and stability of bio-energy supply chains, which tend to be subject to seasonal, spatially dispersed, and high transport costs influencing factors. The use of data-driven models to improve the accuracy of the decision-making process by associating the physical information with real-time operational data. **Figure 3** depicts how AI algorithms coordinate routing, scheduling, and multi-objective planning across dispersed biomass networks. The structure underscores that supply-chain stability emerges from combining real-time data with optimization routines.



Figure 3. AI-Enhanced supply-chain optimization framework

4.1. Transport and logistics planning

Bio-energy supply chains represent multi-stage networks of systems, involving harvesting, collection, baling, storage and transportation. At every stage, uncertainties due to weather, biomass quality, labor availability and equipment performance are added. AI tools can help to mitigate these uncertainties through route optimization, vehicle schedules, and cost predictions. Machine learning models analyse historical and real-time data to predict travel delays, fuel consumption and loading efficiency. These methods can also help to determine suitable transportation modes and storage accordingly (including aspects as, moisture content, crop variability and degradation risk due to handling and storage). All these help logistics to be more reliable, timely and economical.

Real-time supply chain data-supported digital twin technology that allows for dynamic optimization, for example, facilitates antifragility supply-chain development through autonomous adaptation or corrective action in unplanned events ^[16]. Other reinforcement learning algorithms could further aid to resilience by determining reliable suppliers and forecasting how adaptable they are towards uncertainty, such as price fluctuations and delivery delays, using previous information ^[35]. In such a configuration, the inclusion of AI not only maximizes current operational efficiency but also renders the whole bio-energy supply chain resistant to uncertainties, aiding in efficient and reliable energy systems. ^[36]. Artificial intelligence in clean energy - Market potential. The worldwide AI market for clean energy is estimated to grow over USD 75.82

billion by 2030, registering a strong annual growth as the strategic role of AI in the optimization of renewable energy supply chains and power generation continues to expand [37].

4.2. Multi-objective optimization

It is a problem of the trade-off between the factors associated to economic, environmental and social. Multi-objective optimization methodologies integrate NSGA-II, particle swarm optimization and machine learning models to search for very large numbers of potential supply-chain configurations. Such hybrid methods balance considerations of transport distance, carbon footprint, energy loss and total cost. By visualizing the resulting Pareto-optimal solutions, decision-makers can select strategies that minimize emissions while enhancing resource utilization and ensuring an economical supply. This is conducive to long-term planning and enhances bio-energy systems' resilience. AI also assists in drawing up more cognitively nimble and resilient supply chains, which help support decarbonization efforts as well as wider sustainability targets [37, 38]. Furthermore, AI can help to detect potential health and safety hazards in bio-energy supply chains, for ensuring ethical behavior, fair labor standards and human rights are respected [39]. AI-based apps also help in transparency by recording the flow of biomass and ascertaining compliance with sustainability certificates or ethical sourcing norms [37]. Use of explainable AI The use of explainable AI would aid in decision-making by providing the transparency and clarity into how complicated models work, and this can help decrease mistakes, highlighting any possible flaws in strategies to optimize the supply chain [35]. These analyses also make it possible to conduct a trade-off review based on the reduction of GHG emissions, contributing to decision-making that balances economic productivity and environmental conservation [39]. Recent developments also apply to predictive analytics, with machine-learning logic predicting demand and the generation of energy. It helps in the better utilization of the grid and reduces reliance on fossil fuels [40] [41].

5. AI for emission prediction and reduction

AI techniques are increasingly integrated into bio-energy systems to measure, predict, and manage emissions with greater accuracy. These tools address both real-time operational needs and long-term planning by analyzing large datasets and identifying patterns that are difficult to capture through conventional models.

5.1. Real-time emission monitoring

AI models are being utilized to predict emissions in combustion, fermentation or gasification units through training with process conditions including temperature, pressure, feed rate and moisture content. These analytical tools predict major pollutants, such as CO₂, CH₄, NO_x, SO_x and particulate matters, allowing operators to correct the emissions before things get worse. Machine-learning-based an early warning system is utilized for early detection of methane slip in anaerobic digestion systems when patterns are detected in sensor data. If deviations are identified, the system can suggest changes to load rate, mixing intensity, or digester temperature to minimize losses and keep the reactor running efficiently. The Bayesian Networks and Extreme Gradient Boosting similarly improve the prediction accuracy for biogas production by properly addressing uncertainties and aggregating weak learners into strong ensembles. Such models convert qualitative and vague information into quantitative knowledge in order to assist in process decisions and optimizations [15]. Such proactive control of emissions becomes relevant, considering the stringent environmental legislations and in the direction of achieving net-zero emissions [40]. Big data analytics platforms for e.g. Hadoop, Spark, are employed to filter large datasets and discover emission patterns or trends that in turn facilitate a better understanding on how emissions react to operational changes [42]. These considerations assist in dynamic calibration of emission abatement measures and provide guidance in selecting the value range of operational parameters under which to minimize the environmental impact but

still produce a relatively high level of energy [43]. AI techniques also increase biogas production monitoring accuracy, which leads to higher productivity and lower operating cost [44]. More sophisticated machine learning and deep learning models can also enhance computational efficiency and predictive accuracy in real-time modelling of carbon emissions involving various sectors [45] [46].

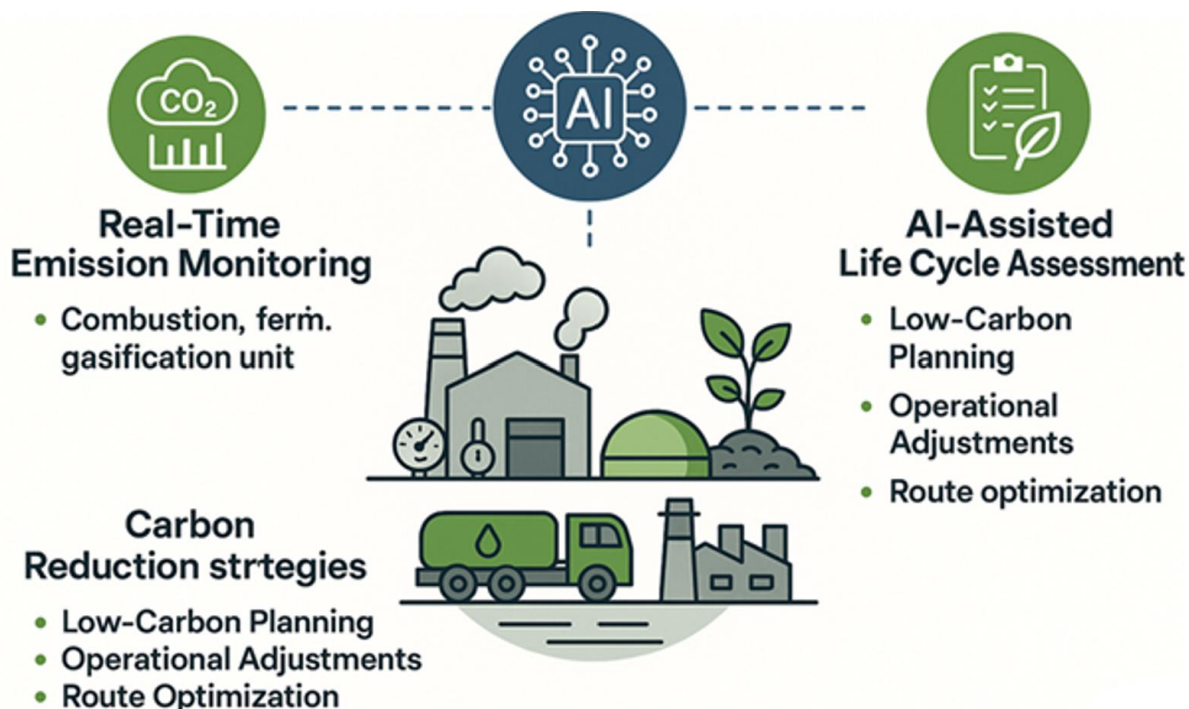


Figure 4. AI for Emission Prediction and Reduction

Figure 4 presents the role of AI in detecting emission patterns and linking them to operational parameters. It shows that real-time analytics combined with predictive models enable more proactive emission control.

5.2. AI-assisted life cycle assessment (LCA)

Life cycle assessment (LCA) demands comprehensive data on energy consumption, water use, air emissions, transportation, and land-use effects. Some of these datasets are noisy or incomplete. Serving as a complement to LCA, AI can predict missing parameters, create artificial datasets, and facilitate the quick study of scenarios. Machine-learning surrogate models can mimic the computational requirements of detailed LCA calculations, but on a much coarser timescale, which is enough to rapidly compare feedstocks and conversion technologies. This gives a more accurate picture of environmental burdens and improves decision-making along the bio-energy value chain. AI is also used to evaluate building carbon emissions through the analysis of real-time energy consumption data, providing effective plans for reaching carbon reduction targets, and helping other sustainability objectives [45]. In a similar field, infrared spectroscopy combined with machine learning helps measure carbon content in biological or fossil samples to determine the impact of solid refuse burning on emissions reduction and resource efficiency [47]. Advanced AI calculations have been growing in popularity for comparative studies such as comparing emissions from 2G ethanol production chains to fossil-based processes, used to guide the transition towards biofuel transport systems [48]. Machine learning also has helped in the LCA process, for instance, by using it to predict biogas production curves from different compositions of lignocellulosic feedstock blends and optimization of anaerobic digestion as well as predicting ethanol yield and NaOH requirement in bio-ethanol refineries [17]. These findings improve the accuracy of the estimation process using advanced techniques and big data, which leads to precise predictions with negligible errors [45]. Indeed, this integration facilitates a new

perspective of how LCA can be included in design, which overcomes long-standing limitations stemming from the limited data availability and static system boundaries [49]. By using AI-powered methods to derive proxy values for missing information, they can also narrow down data gaps and enhance the completeness and accuracy of estimated environmental impacts [50].

5.3. Carbon reduction strategies

AI enables low-carbon planning that could identify feasible ways of reducing emissions at various stages within the bio-energy system. Typical approaches include using feedstock blends on a predicted emission factor basis, identifying high-emission conversion or transport process steps, suggesting process adjustments to decrease pollutant generation and assessing land-use-change impacts using spatial AI as well as geospatial data. These methods enable planners to compare the performance of alternate system designs, evaluate mitigation potential and implement measures that reduce overall carbon intensity while continuing to serve system load. AI-enabled platforms can automate data collection from a wide variety of sources, analyse emissions information and churn sustainability reports, which are in line with regulatory bodies; hence empowering more accountability in organizations [51]. AI can optimize transportation routes over traffic, road condition and even weather information to reduce travel time, save fuel and alleviate pollution [46]. This type of AI-leverage optimization of transport systems (also, incorporating the renewable energy and biomass technologies) are significant in terms of carbon reduction in the mobility sector [52]. AI is also employed to analyse the traffic data, estimate congestion and propose real-time re-routing with minimum fuel consumption and emissions [46]. The AI-aided advanced LCA models have been adopted by urban mobility for its journey toward zero emissions. This approach allows the modelling, assessment and optimization of transport systems based on data-driven policy-inducing measures [53]. AI can process intricate models of mobility and measure impact towards the environment, thus enabling valuable inputs into policies for decreasing carbon emissions and favoring sustainable urban transport [53]. This comprehensive approach enables cities to be in harmony with international environmental targets, such as the Paris Agreement, while also supporting tailored carbon-emission analyses for mobility-hub location selection and operations planning [54]. **Table 4** contributes to gaining and reducing emissions, including its ability of real-time monitoring, life cycle assessments and low-carbon strategies. It also discusses the most relevant tools employed, the primary contributions of each approach and the main challenges to be addressed for broader deployments.

Table 4. AI for Emission Prediction and Reduction

Area	AI Methods / Tools	Key Contributions	Challenges / Needs
Real-time Emission Monitoring	ANN, XGBoost, Bayesian Networks, Hadoop, Spark, Deep Learning models	Predicts CO ₂ , CH ₄ , NO _x , SO _x , PM; detects methane slip; enables proactive control; improves accuracy	Needs high-quality sensor data; uncertainty in real-time datasets; integration across diverse systems
AI-assisted LCA	Surrogate ML models, data imputation, infrared spectroscopy + ML	Fills missing LCA inputs, generates synthetic data, speeds scenario analysis, supports environmental comparisons	Incomplete datasets; static system boundaries; difficulty capturing spatial and temporal variations
Carbon Reduction Strategies	Spatial AI, route optimisation models, transport analytics, automated reporting systems	Identifies high-emission steps, improves feedstock selection, optimizes transport routes, supports emission-focused policies	Requires large geospatial datasets; coordination across mobility networks; regulatory compliance needs

In bio-energy, AI-supported reviews are increasingly important for policy and decision-making. Biomass availability and conversion efficiency estimates will be improved, leading to more reliable emission profiles that help the design of well-founded sustainability criteria and benchmarks for bio-energy plants. In combination with AI-supported LCA tools and real-time emission monitoring systems can form the basis for

dynamically adjustable compliance thresholds instead of having only static compliance limits. Such capacities also help policymakers in better estimating the impact of land-use, carbon intensity ratings and technology-specific incentives. Through increased transparency and predictive consistency as AI technologies advance, the latter can be reinforced even more through certification schemes, subsidy allocation and in the development of risk-responsive regulatory regimes consistent with national and international climate goals.

6. Key research trends

Current research highlights several directions that are shaping the use of AI in bio-energy systems.

6.1. Hybrid models combining mechanistic principles with ML

These models combine physical laws with data-based learning, resulting in increased accuracy of prediction without compromising on process behavior. They are especially useful when sensor information is scarce or the system has a nonlinear behavior. For instance, fitting neural networks to thermodynamic equations can yield more accurate predictions of biofuel yields for a range of operating conditions ^[3]. This makes the prediction more robust and generalizable, especially for predictions outside of the range of observed data ^[2]. Insight ability - Hybrid models provide stronger interpretability, allowing to gain an insight into the mechanisms that influence how systems respond, instead of merely observing their outputs. This interpretability is crucial for the input design of process and risk assessment in bio-energy systems. Another popular theme is the construction of multi-fidelity models that incorporate information from multiple resolutions and data sources in order to achieve a more accurate overall representation of the system while minimizing computational costs.

6.2. Remote sensing with AI for regional biomass mapping

Satellite and drone information analyzed through machine learning techniques provides valuable information on biomass to then move towards crop conditions and spatial variability. This enables even better anticipation on feedstock supply and making plans for harvesting and transport. This ability is especially significant for regional evaluations, due to the inclusion of finer information relative to that obtained with traditional ground-truthed surveys, and helps in more detailed resource estimation for bioenergy production ^[55]. The integration of remote sensing data with AI enables the real-time monitoring of biomass growth and health, providing early signals for disruptions in supply from climate events, disease etc ^[3]. They also assist in developing predictive models for yield optimization and sustainable land-management practices ^[4] ^[17]. Such developments are needed if bioenergy systems are to be improved through enabling for a stable and well-managed feedstock supply that influences the economics and environmental sustainability ^[36]. Lastly, AI-based interpretation of remote sensing data can be applied to assist with land use planning by pinpointing appropriate locations for energy crop cultivation, dedicated areas that minimize competition with food production and promote biodiversity conservation ^[1].

6.3. Digital twins for real-time plant monitoring and optimization

Digital twins link data on actual operations to a virtual model of the plant, enabling detection of operational anomalies, experimentation with operational concepts, and prediction of system behavior without risk to real-time operation. This coupling facilitates predictive maintenance, enhanced operational efficiency and smarter decisions for complex bio-energy plants ^[36]. Digital twins also offer immediate feedback on simulations and optimization, and they can be combined with techno-economic performance analysis for directing system enhancements ^[56]. With AI technology embedded, these digital twins inform predictive maintenance, real-time of energy optimization and grid resourcing for better process efficiency and resilience ^[57]. Through coupling state-of-the-art simulation and real-time data analysis, digital-twin architectures enable

multi-criteria decision-making concerning environmental, economic and social issues in bio-based sectors [58]. The advancement of automated experiments with artificial intelligence, coupled with AI research systems, advances the optimization in bio-energy processes for optimal operating conditions and materials [59].

6.4. Reinforcement learning for adaptive control of digesters and gasifiers

Reinforcement learning agents acquire control strategies through interacting with the system and getting feedback from distributed performance scores. This has to be considered in terms of stability, disturbance rejection, and permanent process efficiency. It allows optimization of the law degree, temperatures, and feeds ratios and thus leads to higher biogas yields and lower operational costs in AD (anaerobic digestion) as well as gasification plants [17]. In fact, given that RL can deal with changing environments and learn from historical data, it is well suited for the complex and nonlinear dynamics exhibited by bio-energy production systems, and can be used to support incremental improvements in both efficiency and system stability [60]. Recent trends involve using transformer-based models to predict failures in biogas generators, as well as utilizing generative adversarial networks in digital twin environments towards dynamic optimization. Those approaches replicate several operating conditions and suggest appropriate operation strategies for online process control [15].

6.5. Automated feature extraction through deep learning for feedstock classification

Deep learning models process images, spectra and sensor signals to determine the type of biomass, its quality and contamination. This results in less hand on testing time and enables better process planning for the pre-processing and combustion facilities. Automation is crucial to maintain consistent feedstock quality, which in turn significantly impacts the efficiency and stability of the bioenergy conversion process [17]. These methods also permit fast, non-destructive feedstock characterization so that reactor operating conditions can be optimized and process upsets avoided [15]. In this context, machine learning (and in particular artificial neural networks) is applied to optimize the operations of bio refineries and to enhance the bioethanol extraction process by determining suitable operating conditions [17] [25]. Artificial neural networks have also been used in highly efficient biomass gasification combined power generation systems to predict key process variables, and provide according good prediction of parameters such as gasification temperature and air-to-fuel ratios [61-75].

6.6. AI-LCA integration for rapid sustainability assessments

AI methods allow life cycle assessments to be performed faster through interpolation of missing data, creating alternative scenarios, and tracking uncertainty. This permits quick comparison of technologies and feedstock pathways. The application of AI in LCA systems can shorten the time to assess environmental impacts and resource consumption, and provide a more adaptable and comprehensive assessment on sustainability issues related to bioenergy systems. Such a quicker review is crucial for decision-making and investment because it allows for the quick selection of environmentally and economically viable bioenergy routes. It also allows for flexible analysis of a broad array of potential bioenergy technologies, from a sighting perspective to full implementation, while including all appropriate environmental footprints [76-86]. The capacity to compare different designs and anticipate environmental results enables stakeholders to make choices that foster sustainable bioenergy development while minimizing negative impacts.

6.7. Federated learning for multi-plant model training without sharing raw data

Federated learning, where trained parameters but not sensitive operation data are exchanged to build joint models, allows for cooperation among facilities without releasing plant-level details. This was made possible by the decentralized approach, hence going on to encourage the development of anti-fragile and more generalizable AI models for bio-energy optimization that can leverage different data sources without violating privacy or security information issues [87-98]. Federated learning promotes collective intelligence in

the bioenergy sector by accelerating the convergence of predictive models and optimizers. Experience from a diversified operational environment can be integrated, and thus more resilient and effective bioenergy systems will be established. Federated learning also enables continuous learning, such that models can cope with new data flows as well as operational changes across a distributed network of bioenergy plants and remain relevant over-time [99-105]. This strategy can alleviate the drawbacks of single-plant databases, which might lack sufficient samples for achieving highly accurate and generalizable AI models [106-115]. Such a decentralized learning scheme is of great advantage for future bioenergy technologies, where the lack in data from single sites may compress model building and application [116-122]

Overall, these developments are indicative of a move towards higher levels of automation, real-time decision-making support, and enhanced model transparency throughout the bio-energy sector.

6.8. Key Limitations of Current AI Approaches in Bio-Energy Systems

Though the AI technologies are advancing bio-energy research, there are some common challenges that have been limiting the accuracy and applicability. The reliance on large, high-quality datasets is also a key issue as these are often unstable across feedstocks, climates and plant designs. Small data sets for training models are suboptimal, leading to reduced generalization and possible overfitting. Furthermore, a major issue is the low interpretability of most black-box models, whose obstacle course decision space makes it difficult to deploy in practice and discourages their use within regulated industrial sectors. Combining AI and mechanistic knowledge is challenging, particularly at the level of biochemical/thermo-chemical reactions that are poorly understood. The scale-up is also a limitation because, generally, processes worked out in lab and pilot plants are not directly operable at an industrial scale. Inconsistent performance in studies is also aggravated by variation in the quality of sensors, data pre-processing and evaluation metrics. Moreover, AI implementation relies on steady data pipelines and computational resources that are hard to maintain in distributed bio-energy plants. Taken together, these constraints highlight the necessity for standardized datasets, transparent model architecture and closer integration of data-driven and physics-based frameworks to promote more accurate and affordable bio-energy optimization.

7. Future Directions

Future research in AI-driven optimization of bio-energy systems is moving toward more integrated, reliable, and scalable solutions.

7.1. Building large, standardised, and open datasets for biomass and process variables

creating shared datasets that cover diverse feedstocks, climates, and operational conditions will improve model robustness and enable fair benchmarking across studies. Standardization of data formats and metadata will also support reproducible research.

7.2. Designing physics-guided ML models for more reliable performance

Embedding physical constraints and mechanistic principles into ML architectures can reduce prediction errors, improve extrapolation, and strengthen trust in model outputs. Such approaches are especially important for safety-critical and regulatory applications.

7.3. Developing plant-wide digital twins that link sensors, ML, and control loops

Digital twins spanning pre-processing, conversion, and emission-control units can serve as real-time decision-support tools. These virtual systems can test operational changes, forecast failures, and help maintain optimal performance without interrupting plant operations.

7.4. Integrating AI into LCA tools to support policy and planning

AI-enabled LCA frameworks will allow rapid evaluation of emerging technologies, supply-chain designs, and regional scenarios. This integration can assist policymakers in comparing pathways and selecting options with lower environmental burdens.

7.5. Using reinforcement learning for multi-objective optimization under uncertainty

Reinforcement learning can help manage trade-offs among efficiency, cost, and emissions when system conditions fluctuate. It offers adaptive strategies that update continuously as new data becomes available.

7.6. Adopting edge-AI hardware for faster on-site computation

Deploying lightweight AI models on edge devices reduces dependence on cloud platforms and supports real-time monitoring in remote or distributed facilities. This leads to quicker responses to faults, process variations, and emission spikes.

Together, these directions will contribute to stable plant operations, lower emissions, and improved sustainability across the bio-energy sector.

8. Conclusion

The data-driven method of AI from an ADDC has changed its role from an additional support tool for analysis to the cornerstone tool for optimization in bio-energy systems. Throughout the value chain — from resource assessment and conversion to supply-chain planning and emission management — AI approaches offer speedier predictions, better pattern recognition, and more stable operations. It is demonstrated that machine learning, hybrid physics-guided methods, deep learning and reinforcement learning consistently improve the prediction accuracy of biomass availability, biogas yield as well as emission behavior, such models and decrease computational time for intensive simulations. These improvements help in designing, operating and predicting more secure and efficient operation of both biological as well thermo-chemical routes. The manuscript also addresses ongoing issues in relation to the quality of data, scalability or interpretability and generalization capabilities of models. Advancing in these areas will be facilitated by standardized datasets, tighter integration of mechanistic knowledge and accelerated adoption of digital-twin platforms. Novel tools like federated learning, edge-AI deployment, and AI-embedded LCA are promising in revolutionizing real-time decision-making and sustainability assessment for future bio-energy systems. Further, an effective partnership between data scientists and researchers in energy processes will be indispensable to transition these innovations into scalable, low-emission, industry-ready solutions. In this work, such a unifying contribution is provided by converging model-level with process-level and system-level analysis of the entire bio-energy chain into one integrated analytical framework. It not only compares capabilities and weaknesses of black-box, hybrid, physics-guided and explainable models but also relates these differences with the operational requirements for resource assessment, conversion processes, supply-chain planning and emission management. An integrated perspective as such is not often covered in prior reviews, which usually discuss individual stages or zoom in on particular algorithms. By specifying model appropriateness, highlighting cross-cutting challenges and profiling emerging trends such as digital twins, federated learning and AI-assisted LCA the manuscript offers a structured basis for researchers and practitioners seeking to enable verifiably scalable low-emission bio-energy systems.

Glossary of Abbreviations

AD – Anaerobic Digestion

AI – Artificial Intelligence

ANN – Artificial Neural Network

CFD – Computational Fluid Dynamics

CNN – Convolutional Neural Network

C/N Ratio – Carbon-to-Nitrogen Ratio

DT – Digital Twin

ETR – Extra Trees Regression

GA – Genetic Algorithm

GA-ANN – Genetic Algorithm–Optimized Artificial Neural Network

HHV – Higher Heating Value

LCA – Life Cycle Assessment

LST – Land Surface Temperature

LSTM – Long Short-Term Memory Network

ML – Machine Learning

NSGA-II – Non-dominated Sorting Genetic Algorithm II

OLR – Organic Loading Rate

PM – Particulate Matter

PSO – Particle Swarm Optimization

PSO-ANN – Particle Swarm Optimization–Optimized Artificial Neural Network

RF – Random Forest

RL – Reinforcement Learning

SVM – Support Vector Machine

SVR – Support Vector Regression

VI – Vegetation Index

Author Contributions

Sajal Suhane and **Anant Sidhappa Kurhade** conceptualized the study and defined its scope. **Smita Suhane**, **Rushali Rajaram Katkar**, and **S. Sugumaran** contributed to the literature survey, data collection, and synthesis of review content. **S. Sugumaran**, **Santosh Bhauso Takale** and **Surekha Dehu Khetree** supported the methodological framework and thematic organization of the manuscript. **Shyamsing Thakur** and **Shital Yashwant Waware** assisted in the critical analysis and interpretation of results. **Anant Sidhappa Kurhade** supervised the overall work and provided technical guidance. All authors contributed to writing the original draft, reviewing, editing, and approving the final manuscript.

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Conflict of interest

The authors declare no conflict of interest

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