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ORIGINAL RESEARCH ARTICLE

Smart Biorefineries: Machine Learning for Process Control, Resource Utilization, and Emission Monitoring

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ABSTRACT

Bio-refineries are central to achieving a sustainable bioeconomy by converting renewable biomass into fuels, chemicals, and energy, directly supporting global climate and resource-efficiency targets. Their operation remains challenging due to nonlinear process behavior, feedstock variability, and the need to simultaneously address productivity and environmental compliance. While machine learning (ML) has been increasingly applied to individual bio-refinery operations, existing studies lack an integrated perspective that links process control, resource use optimization, and emission monitoring with sustainability objectives defined under the Sustainable Development Goals (SDGs). The objective of this review is to analyze and synthesize recent advances in ML applications for smart bio-refineries, with a focus on improving process efficiency (SDG 9: Industry, Innovation and Infrastructure), reducing energy and water consumption (SDG 7: Affordable and Clean Energy; SDG 6: Clean Water and Sanitation), and minimizing environmental emissions (SDG 12: Responsible Consumption and Production; SDG 13: Climate Action). A structured review methodology was adopted, covering peer-reviewed studies on supervised, unsupervised, and reinforcement learning methods applied to fermentation, thermochemical conversion, heat integration, and emission monitoring. The review shows that ML models, including artificial neural networks, ensemble methods, and hybrid ML–physics frameworks, enhance predictive accuracy, stabilize process operation, and enable proactive emission control. Reported case studies demonstrate measurable reductions in energy demand, improved resource utilization, and better compliance with emission limits. These findings underline the role of ML as a practical enabler of sustainable, low-emission bio-refineries. By linking operational performance with SDG-oriented outcomes, this review provides a clear framework for deploying ML technologies to support environmentally responsible and economically viable bio-refinery systems.

Keywords: Bio-refinery; emission monitoring; machine learning; process control; resource optimization; sustainability

1. Introduction

Bio-refineries are sophisticated processes that convert biomass feedstock to value added products (e.g., biofuels, bioplastics and high-value chemicals). Regulation of these processes is difficult because of their nonlinear patterns, diversity in feedstocks, and multi-stage relationships. Machine learning (ML) provides data driven methods for predictive modelling, process optimization and monitoring of environmental discharges. This review presents a critical overview of recent research on the application of ML for process control, resource consumption and emissions estimation in bio-refineries. In this context, ML algorithms have a great potential to revolutionize the bio-refinery design and operation due to their ability of increasing system performances (to obtain better multi-objective performance graphs) through more accurate models of different biomass valorization pathways using Multi - response models [1]. These high levels of computation allow the estimation of stability as well as conversion yields in thermochemical processes based on feedstock characteristics and blend mixtures, frequently without the need for mathematical formulations [2]. Combining machine learning with digital twins would enhance this possibility because different pretreatment scenarios could be simulated from which strategies can then be optimized without physical experiments [3,4]. This integrated manner allows not only the accurate tuning of operational conditions but also the flexible operations in feedstock variations for product yields maximization and waste minimization [5]. In addition to process optimization, machine learning is used in the identification and genetic manipulation of microorganisms and plants that lead to increased biofuel yields as well as making accurate predictions about technology economics and life cycle assessment results for biomass-to-biofuels [4]. This broad scope throughout the microbial strain optimization, scale-up from laboratory to industrial process scale process design, highlights the potential disruptive power of ML for expediting a sustainable bioeconomy. Moreover, machine learning is used to build surrogate models and predict the cost, mass/energy balances that improve techno-economic analysis and life-cycle assessment approaches in a variety of bio-refinery configurations [4,6]. The incorporation of such systems integration provides a complete picture of the intricate connection throughout biorefinery processes, which would lead to better design for energy efficient and sustainable technologies [3]. Challenges for conventional modelling methods are the complexity of many biorefinery systems, which feature interdependencies between a variety of feedstock options, process parameters and product streams [1], makes the identification or development of detailed input-output models unfeasible as is done in previous work on other CMPs.

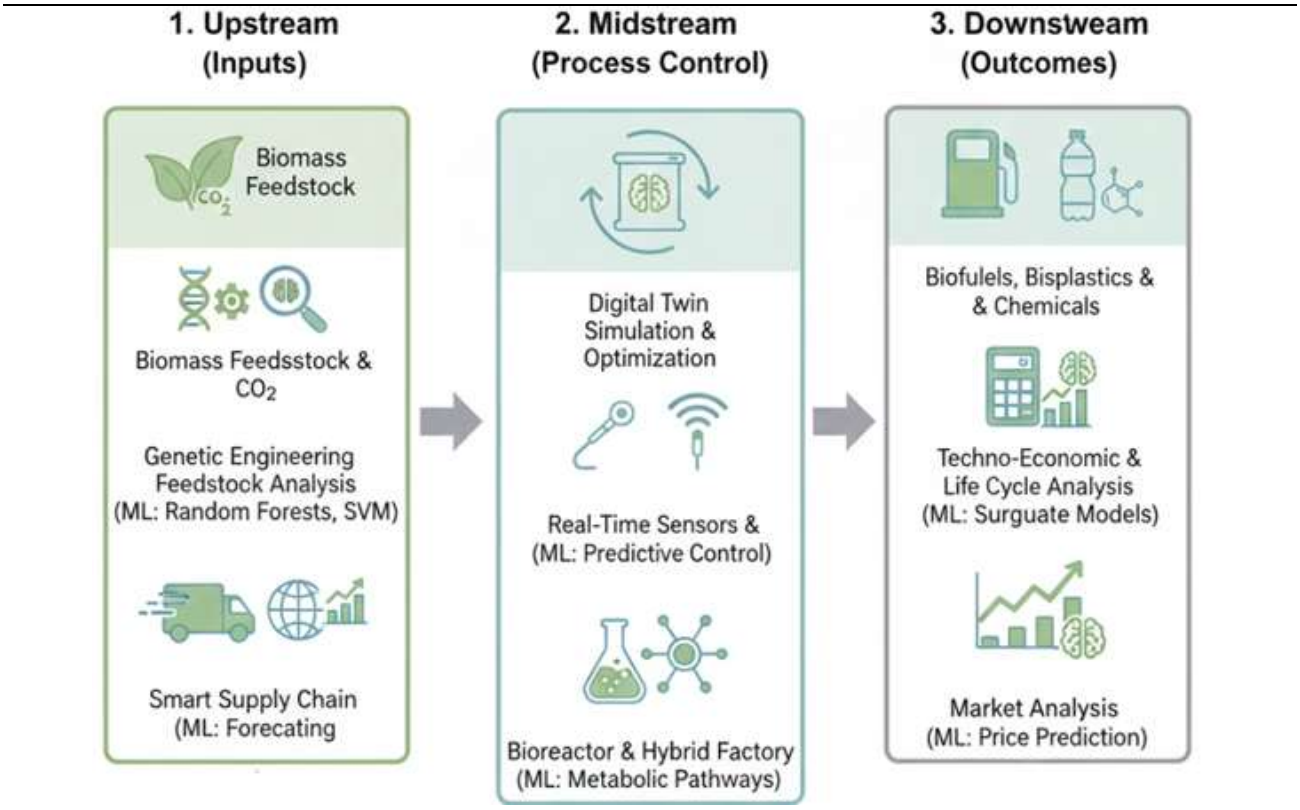

Figure 1. Machine Learning-Integrated Framework for Smart Biorefinery Optimization

Figure 1 illustrates the integration of machine learning across the biorefinery value chain, from Upstream feedstock engineering and supply chain forecasting to Midstream real-time process control using Digital Twins. It highlights how ML-driven predictive modelling enables adaptive management of complex biomass dynamics, ensuring stable conversion rates. Finally, the Downstream phase utilizes surrogate models to optimize product yields and provide accurate techno-economic and life cycle sustainability assessments.

Machine learning is a promising tool to overcome these challenges by unearthing unknown patterns in massive datasets that can enable model building for optimizing biofuel systems, and for compliance with environmental, social, and governance (ESG) criteria [4]. These data-based findings are critical for predicting biomass properties and conversion efficiencies in connection with the choice of optimal pretreatment and bioconversion paths [4,7]. This predictability is an essential tool for optimizing use of resources and reducing cost-of-operations throughout the entire bio-refinery value chain. Moreover, machine learning has been essential to the development of decentralized and sustainable supply chain networks for bioethanol production with efficient resource allocation and demand prediction [8]. This also involves using algorithms to predict demand for products, and the availability of feedstock (and inventory management), which minimizes supply chain disruption. These functionalities are complemented by machine learning-based estimation of optimum parameters for microalgae cultivation to achieve maximum biomass production and nutrient removal efficiencies [9]. The intricacy of biorefinery operation requires sophisticated computational tools to appropriately model and optimize them, particularly with variability in biomass composition and rates of reaction. Accordingly, ML approaches are increasingly utilized to create reliable predictive models capable of handling these variabilities and thus improving the process stability and yield [4,10]. Notably, machine learning contributes to metabolic pathway prediction and system regulation of potential importance for the realization of hybrid bio factories combining microalgae and engineered microbial consortia [11]. They are then used to optimize cultivation parameters and control bioreactor conditions on-line, for the purpose of maximizing biofuel productivity [11]. Furthermore, such algorithms can learn from market trends, oil costs, and policy decisions to develop reliable forecasts of biofuels demand, pricing and competitiveness upon which producers and investors can make strategic decisions [12]. Apart from economic prediction, the ML models Furthermore, outside to cost forecasting have been increasingly used for online monitoring and controlling of important process conditions (i.e., pH, temperature, nutrients in the corn) laterization through fermentation that immediately influences the conversion rate alongside quality of product [13]. Such real-time control and predictive analysis can be used to predict the upsets and adjust the process in advance so as to keep good operation conditions, which helps avoid an upset on a process or system level and improve system reliability [14]. This is particularly crucial as conventional mathematical programming finds it difficult to cope with the growing complexity of the variables, objectives and constraints in biomass supply chain operations whereby solving problems in real-time or at a large scale becomes very difficult [15]. This limitation underscores the demand for sophisticated machine learning techniques which can manage these complexities, providing solutions to optimize different components of smart bio-refinery process from feedstock to product [16]. In addition, machine learning is used to automate process control and in-situ long-term monitoring with the aim of revolutionizing algae culturing through substantial labor cost reduction as well as enhancing general enterprise efficiency and economy [17]. The integration with artificial intelligence and machine learning algorithms, also permitted the prediction of the optimal growth conditions, as well lipid accumulation in different microalgae species by using techniques such as Support Vector Machines, Random Forests or Deep Neural Networks [11,18]. These developments can enable accurate perturbation of environmental and genetic variables to optimize biomass production and synthesis of specific bioproducts [19,20]. These complex models provide adaptive learning and pattern generalization, which are essential for enabling the continuous changes in biological systems and complicated datasets observed in biorefineries [21].

2. Bio-Refinery systems: Overview

Biomass processing plants contain numerous unit operations, e.g., pretreatment, fermentation, enzymatic conversion, and separation/purification. The primary performance goals are to achieve highest possible product yield, minimize energy consumption and ensure compliance with all environmental laws. The complication is characterized by feedstock variability, inter-unit processes interaction and multiple but frequently contradictory objectives. To tackle these challenges, consistent with the sophisticated demands of industrial processes, intelligent biorefineries incorporate advanced machine learning methodologies for process control on-the-fly, resource management and emission monitoring enabling more robustness in handling complexities of varying feedstocks and multidimensional process dynamics [22]. They could provide predictive modelling and adaptive control strategies to maximize the performance on a wide range of spatial and temporal scales in the bio-refinery [23]. In detail, artificial intelligence and machine learning algorithms play an important role in breaking these technological bottlenecks associated to production and characterization of algal bioactive ingredients, allowing real-time control/monitoring of intelligent bioreactors as well as predicting cultivation yields and market needs with extreme precision [24]. This is particularly crucial given the forecasted expansion of industrial biotechnology (to USD 546.8 billion) and global biorefinery (USD 1.1 trillion) markets by 2027, highlighting an immediate requirement for optimization design approaches to address future requirements [25]. Successful application of machine learning methods including artificial neural networks, support vector machines and random forest algorithms for predicting non-linear interaction and handling multivariate data in biohydrogen production from microalgae implies that these are more promising [26]. These models are essential to automatically improve the performance of bioprocesses like complex biochemical pathways submitting multiple operational variables and go beyond usual “trial and error” approaches, which often fail in catching the interdependence among factors [27]. Moreover, the utilization of reinforcement learning provides high potential to deal with the uncertainties and complications that are found in biorefining processes (especially followed by various waste feedstocks situation) since it can provide model-free decision making [22]. This allows the systems to optimize their control policies through trial and error, and do so far more efficiently in response to changes in feedstock composition and operational disturbances than traditional controllers [22]. Furthermore, there is a growing emphasis on implementing AI-driven machine learning methods in the biotech sector to automate various processes and to monitor as well as control them, based on their ability to efficiently capture challenging relationships between process parameters and performance [28]. These features include high-level application frameworks such as active learning that are capable of selecting experimental samples efficiently, thereby minimizing the number of experiments benchmarked on microalgae studies [29]. These approaches are especially useful for the fine tuning of microalgal growth conditions and product characteristics, as they can quantitatively determine the effects of input values on cultivation and increase our comprehension of microalgal biology [21]. For example, advanced genetic algorithms and particle swarm optimization have been successfully employed in an ethanol yield increase of 18% combined with life cycle assessment models to adequately deal with greenhouse gas emissions [4]. These AI-based methods are also very useful in improving the resource use efficiency and reducing environmental degradation for a variety of biofuel production schemes such as corn ethanol, sugarcane feedstock, cellulosic, waste-to-fuel product pathways [9]. Keeping the above-mentioned comments in perspective, it can be concluded that all aspects of these related methodologies help achieve the goal of smarter biorefineries to not only increase economic gains but also meet strict environmental sustainability requirements by increasing process efficiency and minimizing environmental footprints [9,28].

Table 1. Machine Learning Applications in Smart Biorefineries

Unit Operation / Stage	Key Objectives	Major Challenges	ML / AI Techniques Applied	Control & Optimization Role	Environmental / Sustainability Focus	Representative Outcomes
Pretreatment	Improve biomass accessibility and conversion efficiency	Feedstock heterogeneity and variable composition	ANN, SVM, Random Forest	Predictive modelling of pretreatment severity and yield	Reduced energy use and waste generation	Improved conversion rates with stable operation
Fermentation / Bioreaction	Maximize product yield and productivity	Nonlinear kinetics and process disturbances	ANN, Deep Learning, Reinforcement Learning	Adaptive real-time control of operating conditions	Lower emissions and efficient resource use	Enhanced yield and robust process stability
Enzymatic Conversion	Improve reaction efficiency and selectivity	Complex biochemical pathways	ML regression, Genetic Algorithms	Multi-variable parameter optimization	Reduced enzyme consumption and by-products	Higher conversion efficiency
Separation & Purification	Achieve high purity with low energy input	Energy-intensive multistage interactions	Tree-based models, ML–LCA integration	Energy and process optimization	Reduced greenhouse gas emissions	Cleaner outputs with lower energy demand
Microalgal Bioprocessing	Optimize growth and bioactive compound production	Sensitivity to cultivation conditions	ANN, Active Learning, PSO	Intelligent bioreactor monitoring and control	Sustainable biomass production	Accurate yield prediction and quality control
Integrated Smart Biorefinery	Balance yield, cost, and sustainability	System-level complexity and conflicting objectives	Reinforcement Learning, GA–PSO hybrids	System-wide multi-objective optimization	Regulatory compliance and reduced footprint	Up to 18% yield improvement

Table 1 summarizes the major unit operations in smart biorefineries and links them with key objectives, operational challenges, and suitable machine learning techniques. It shows how AI-based predictive modelling and adaptive control support yield enhancement, energy efficiency, and robust process operation under

feedstock variability. The table also highlights the role of these tools in reducing environmental impacts while enabling system-level optimization across integrated biorefinery stages.

3. Machine learning for process control

3.1. Predictive modelling

Predictive modelling is the cornerstone of data- driven process controlling since it bridges process condition to target-predicting yield parameters. In biorefineries as well as in process industries, product yield, biomass conversion efficiency, selectivity or stability are determined by a complex combination of strong non-linear and interacting variables like temperature, pH, residence time, substrate composition and catalyst characteristics. Supervised learning methods are suitable to capture such behavior given the availability of enough historical or experimental data. For example, ANNs were successfully applied in modelling of the complicated fermentation process such as for predicting biomass and product concentrations with excellent prediction accuracy derived from various input parameters [30]. Other predictive models, including support vector machines and Gaussian process regression can also provide strong predictive capabilities, especially with small or high-dimensional data sets, in which they are able to efficiently capture non-linear relationships between input-output pairs [31]. These models allow for a proactive fine-tuning of process settings to avoid the drift from optimal operating conditions, improving global system robustness. Machine learning–based models better handle the strong nonlinearities and complex interactions in biorefineries by learning directly from process data, unlike conventional mechanistic models that rely on simplifying assumptions. ML models adapt to variability, manage high-dimensional data, and can be updated in real time, enabling more accurate prediction, improved control, and efficient optimization of biorefinery operations.

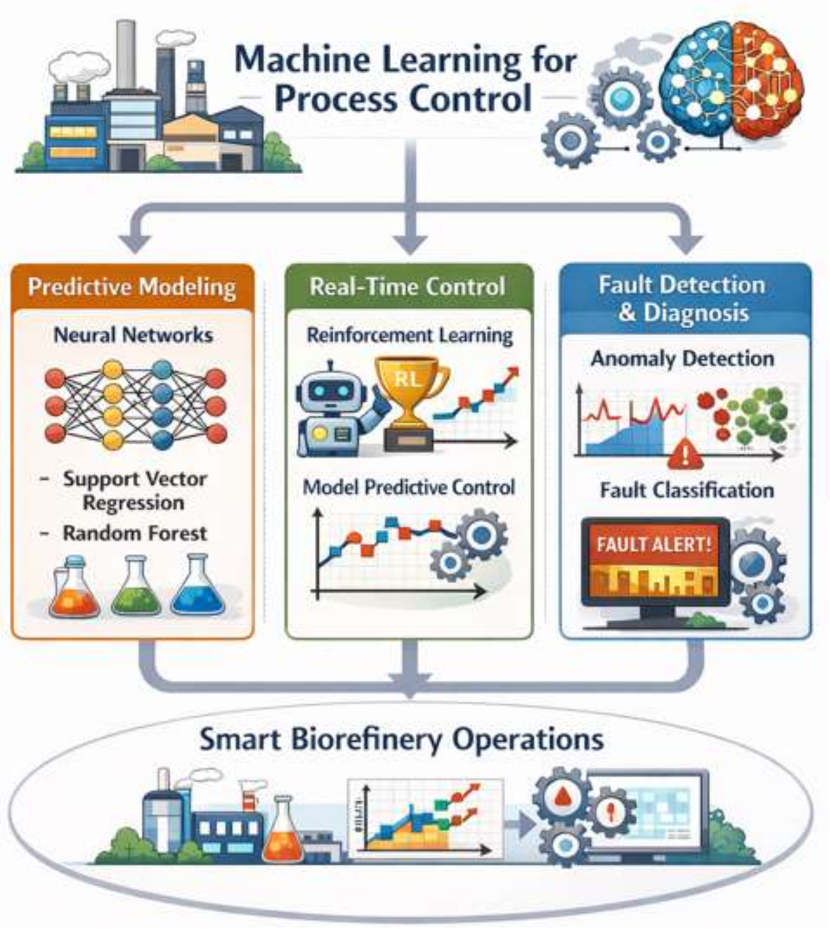

Figure 2. Machine Learning Framework for Process Control in Smart Biorefineries

Figure 2 presents a simplified conceptual diagram illustrating how machine learning (ML) techniques are integrated into process control systems for smart biorefinery operations. Artificial neural networks, support vector regression, and random forest models are widely reported due to their ability to represent nonlinear trends without explicit mechanistic assumptions. Among these, neural network models show particular strength in lignocellulosic fermentation and biochemical conversion processes, where microbial kinetics and inhibition effects introduce complex dynamics. These models work with better accuracy of prediction and greater ease in operating range, as opposed to linear regression or any simple empirical correlations. Therefore, predictive models can serve as virtual process maps to aid offline optimal solution and online decision actions. In addition, machine learning is utilized for online process monitoring and control thereby allowing systems to adjust themselves in face of unexpected disturbances and to continuously enhance performance [31]. For instance, artificial neural networks were reported to show high predictive accuracy and flexibility in simulating several steps of bioethanol biorefineries process such as pretreatment and fermentation considering input variables like yeast cell count and pH associated with the outputs (bioethanol concentration and yield) [4].

3.2. Real-time control

Machine learning to control biorefineries in real-time, adapting to variations between operations and feedstocks. Reinforcement learning (RL) learns optimal control policies for maximizing rewards such as yield or energy efficiency, making it well-suited to systems where explicit control laws are hard to obtain, for example on nutrient feeding strategies without detailed mechanistic models [32]. ML-enhanced model predictive control (ML–MPC), on the other hand, can also predict process behavior in the future over a receding horizon while it takes account of operational constraints to actively adjust for unstable process or better economic performance [32]. Spectroscopic data-aided ML models can be employed for real-time correction of important parameters during cultivation with almost zero control delay [33], and such hybrid data-driven–mechanistic approach also improves supervisory control in complicated fermentation systems [34]. The use of ML-enhanced MPC is specifically powerful in multivariable and constraint-ridden bioprocesses (such as fed-batch cell culture) where it allows to optimize the feeding strategy on-line without loss of product quality or process safety [35–37].

These approaches, RL and ML-aided model predictive control (ML–MPC), widely vary in their philosophy of control where they are relied for real-time bio-refinery operation. RL is a model-free method which learns the optimal control policy by interacting with the process, and it is highly flexible for non-linear, uncertain and time-varying problems such as biorefinery systems. However, RL often needs a large amount of training data, and it also brings difficulties in safety and satisfaction of constraints. ML–MPC, by contrast, retains the structure and model knowledge integration of classical MPC in combination with the ability to use ML models for representing complex nonlinear dynamics such that operational limits and regulatory constraints can be explicitly accounted for. Therefore, RL is more flexible and adaptable while ML–MPC gives a more predictable, interpretable and industrially robust control. Both are complementary and hybrid RL–MPC approaches have increased as a promising avenue for intelligent biorefineries.

Although ANN-based controllers can model nonlinear fermentation dynamics, it difficult to use these models on a large scale. These include lack of sufficient high-quality training data, biological variation and drift in processes that reduce model generalization, and also the black-box nature of ANNs which constrain interpretability and operator confidence. There are also considerations like safety and robustness (extrapolation outside the training domain can lead to unstable or unsafe behavior). Integration with other control systems, reliability of sensors and low-latency calculation as well as hybrid architectures (e.g. ANN models inside frameworks like MPC) are also necessary to manage industrial scale reliability and compliance.

3.3. Fault detection and diagnosis

Another emerging application of machine learning in process control is on-line fault detection and diagnosis. Multivariate sensor data are generated in massive quantities by industrial processes, which tends to make manual monitoring unfeasible. Unsupervised and semi-supervised learning algorithms are often used to identify anomalies in behavior. Methods like principal component analysis, clustering and autoencoder models detect deviations on temperature, pressure, flow rate or composition patterns. These approaches are particularly attractive for detecting subtle perturbations that may herald an equipment failure or process upset prior to a major operational failure [38]. Learning algorithms can then classify the nature of a fault and infer actions that should be taken, e.g. for maintenance or process adaptation [39]. For example, deep learning (DL) model such as RNN and CNN have demonstrated outstanding performance on time-series data compression from biorefineries to a prediction of the equipment failures and construction of the specific fault condition with high accuracy [30]. This predictive ability enables operators to proactively plan for preventative maintenance, minimizing the likelihood of unexpected downtime and improving total system reliability [40].

Table 2. Machine Learning for Process Control

Application Area	ML Technique	Control Objective	Typical Input Variables	Predicted / Controlled Outputs	Key Advantages	Representative Applications
Predictive Modelling	Artificial Neural Networks (ANN)	Model nonlinear process behavior	Temperature, pH, residence time, substrate composition	Yield, biomass concentration, conversion efficiency	High accuracy, strong nonlinear mapping	Fermentation and biochemical conversion
Predictive Modelling	SVM, Gaussian Process Regression	Robust prediction with limited data	Operating conditions, catalyst properties	Yield, selectivity, stability	Effective for small, high-dimensional datasets	Biorefinery process modelling
Real-Time Control	Reinforcement Learning	Adaptive policy optimization	Process states, sensor data	Feeding rate, nutrient supply	Model-free, disturbance tolerant	Nutrient feeding in bioprocesses
Real-Time Control	ML-Enhanced Model Predictive Control	Setpoint tracking under constraints	Spectroscopic and kinetic data	Cell growth, metabolite concentration	Handles nonlinear multivariate systems	Fed-batch and biopharmaceutical processes
Fault Detection & Diagnosis	PCA, Autoencoders, Deep Learning	Detect and classify process faults	Multivariate time-series sensor data	Fault indicators, failure prediction	Early warning and predictive maintenance	Equipment monitoring in biorefineries

Table 2 summarizes key machine learning applications in process control, highlighting how different algorithms are used for prediction, real-time control, and fault management. It links ML techniques with their objectives, inputs, advantages, and practical applications in biorefineries and related process industries.

Early identification of faults in reactors, heat exchangers, separators, or auxiliary units allows operators to intervene before failures escalate. This reduces unplanned downtime, improves safety, and limits material losses. Beyond detection, diagnostic models can also assist in isolating the likely source of a fault, supporting maintenance planning and continuous process improvement.

4. Resource use optimization

4.1. Energy efficiency

Energy is of the highest operation cost and environmental concern in bio refineries and other like industries. ML models help fostering energy efficiency through learning relationship between historical operating data and end energy demand over process units, including reactors, distillation columns, heat exchangers or utilities. Mathematical models are up till now used to estimate energy consumption at different working conditions. For instance, a random forest model was reported to achieve a R2 of 0.98 in predicting the bio-oil yield from pyrolysis data, highlighting the advantage of using it over other ML methods for energy related predictions [13]. Moreover, these models are able to reveal potentials for process intensification or for waste heat recovery by detecting inefficiencies in energy use and thus allowing measures at specific points to reduce overall consumption [41]. For hydrothermal liquefaction of lignocellulosic biomass, machine learning can be used to optimize the reaction time [42], temperature, and pressure towards maximizing biofuel production at lowest energy input. Such optimization is likely to result in substantial reduction on the total energy demand of a biorefinery and thus facilitate the economic and environmental viability of such complexes. In addition to process optimization, ML contributes to preventive maintenance strategies with substantial savings in energy consumption through avoiding process interruptions and optimizing plant operational scheduling [43].

They enable recognition of the operating windows with minimum specific energy consumption, while maintaining throughput and product quality. In heat integration systems, the optimization based on data helps in choosing temperatures well as a method for recovering heat and distributing the load of utilities. Combine with online monitoring and ML-based tools can allow real-time monitoring of the plant energy performance, continuous tracking for feedback control so that actions can be taken when needed, helping toward a more stable and efficient plant operation.

4.2. Feedstock allocation and scheduling

Bio-refinery processes often use varied feedstocks including agricultural residues, energy crops or organic wastes with different physical and chemical characteristics. Differences in moisture, composition and heating value make feedstock choice and delivery scheduling difficult. This AI can handle this problem by predicting conversion behavior, yield and the processing limitations for various feedstock types and blends. Such learning algorithms can help predict the best ingredient mixing ratio to keep high-quality product and processing efficiency under control in a production line [5]. Such mechanism provides with intelligent control of feedstock supply lines, which result in lowering of logistic costs and optimize processing resource [12]. For instance, support vector machines and artificial neural networks can predict optimum feedstock blends for maximum biofuel generation with minimum environmental cost [13]. This allows biorefineries to adapt their operation in real-time to changes in feedstock availability and market demands so as to maximize financial profitability and operational flexibility [2]. This predictive performance is advantageous for management control of raw material feeding in a biorefinery where process energy input should be optimized and waste minimized very consistently, on top of the fact that variability of feedstock composition may occur [12].

Ensemble learning methods, such as random forests, and tree boosting algorithms are well suited for dealing with heterogeneous data and nonlinear combinations of feedstock parameters. These tools help decision makers choose the best feedstock blend, order and inventory. Play the Podcast as a result, feedstock allocation becomes more robust with respect to supply fluctuations but also performance stability is achieved and operational risk is reduced.

Figure 3. Machine Learning–Based Resource Use Optimization in Smart Biorefineries

Figure 3 illustrates how machine learning supports efficient utilization of energy, feedstock, and water/nutrients in biorefinery operations. Predictive and optimization models enable optimal load distribution, feedstock scheduling, and precise input control based on process data. Together, these strategies reduce waste and resource consumption while improving productivity and sustainability.

4.3. Water and nutrient use

Water and nutrient supplements are essential in the fermentative and cultivation processes which is involved in determining those biomass growth and product formation. Its overuse is not only increasing the operating expenditure, but also magnified ecological cost. Water demand and nutrient uptake as a function of operating conditions, microbial activity, and substrate features are predicted by means of supervised learning models. For example, ANN models were successful in predicting the optimal operating conditions for glucose and reducing sugar yields during enzymatic hydrolysis, demonstrating their versatility to optimize resource utilization without detailed information on feedstock [2]. These systems also provide excellent control over nutrient delivery, so that there is very little waste of either the growth medium or the microbes/enzymes, and they find applications in maintaining optimum physiological conditions for microorganism/enzyme processes [2,14]. In this case, water use and nutrient release will be less, fitting in with the sustainable principles of biorefinery operation [44]. In addition, predictor models can already predict the demand for water recycling or adding nutrients along-side with on-line process monitoring to close material loops and optimize overall resource efficiency [3].

When combined with optimization frameworks, such predictions enable accurate tuning of input flows to meet process specific needs. This precise control minimizes waste and prevents the inhibitory effects of overfeeding. Through time, these data-centric approaches can assist in the sustainability of operation through reduction of freshwater utilization and enhanced nutrient usage efficiency throughout bio-refinery platforms. In addition, there are also the possibilities that ML-based methodologies can simulate complex nutrient availability of microbial consortia in (waste)water to bioreactors favoring resource allocation for higher production and minimal waste [45].

5. Emission monitoring and environmental compliance

5.1. Predictive emission models

Environmental compliance monitoring is an essential part of sustainable bio-refinery operation including greenhouse gas (GHG), VOC, and particulate emissions originated by conversion and auxiliary processes. Access to all emission streams by means of direct continuous measurement may be practically restricted because of sensor availability and the costs and efforts due to maintenance. To fill this gap, ML-based predictive models are developed that predict the emission levels from readily accessible process and environmental data. For instance, ANN can estimate pollution levels using operational parameters that facilitates real-time control to abide by environmental laws [46-54]. These smart models can further predict future experiments from current data, which provide powerful means for preliminary screening and optimization of biorefining processes [55-58]. This foresight also applies to the ability of anticipating potential roots of contaminant spread via sensing data in a water distribution system and expediting responses if any [59-62]. Moreover, ML algorithms can detect if deviations in the process are correlated with increased emission, by having timely intervention which will target and prevent environmental pollution effects. Such models likewise apply to the prediction of wastewater treatment efficiency and methane emissions from fermentation, these being important to minimize the global environmental footprints [63-72]. Reinforcement learners can learn from energy consumption, raw material usage and emissions data to determine process conditions which lead to a reduction in the environmental impact without losing productivity [73-80]. Predictive emissions models overcome the shortcomings of CEMs by predicting emissions based on existing process data. Soft sensors, which supply continuous and reliable emission estimate when physical ones are expensive, unavailable or corrupted by noise and drift. These models facilitate early detection of deviations from normal emissions trends and facilitate anticipatory, process-based control that relies to a lesser extent on end-of-pipe measurements. Thus, they enhance the level of monitoring of emissions as well as regulatory compliance and plant operations within smart biorefineries.

Supervised ML models, with reference outputs from historical sensor data, laboratory analyses or operational logs can describe the relationship between operating conditions and emission formation. These models help identify the significant influences, such as temperature spikes, feedstock variation or incomplete conversion. Purely predictive emission modelling also provides alerts regarding abnormal emission trends at an early stage so that the operators can modify their process control before a limit value prescribed by law is nearly reached.

5.2. Sensor integration and data fusion

The modern bio-refinery network use layers of distributed sensors for temperature, pressure, gas composition, flow rates and energy consumption in multiunit. Individual measurements are noisy or may be drifted. Data fusion methodologies connect these different data streams to gain robust, comprehensive estimates for emissions. For instance, Kalman filters or Bayesian networks can use information from multiple sensors and historic data for rendering accurate estimates of pollutant concentrations even in the case when some sensor's reading is missing or noisy. This holistic strategy improves the accuracy and precision of the emission monitoring for a complete picture of biorefinery foot printing on environment [81-85]. Advanced deep learning-based models, exploiting satellite imagery, IoT sensor data and climate models can further help improve such assessments by incorporating information over a large scale of environmental impact [96-90]. Moreover, these unit systems support in-line detection of anomalies and predict elevation that may be predictive of future environmental exceedances to act and adjust processing conditions on a real-time basis to improve process performances with a reduced ecological footprint [91-92]. Sensor data fusion enhances real-time environmental compliance by integrating information from a variety of sensors to form coherent pictures of emissions and operational conditions. It cross-validates and filters measurements to alleviate noise, drift, sensor failure and paucity of coverage. The fused data had improved emission estimates which were more stable and were able to identify unusual trends at an earlier stage, as well as differentiate between real changes in emissions and sensor errors. This works for building a more reliable compliance confidence, monitoring, and decision making in the industrial systems.

Techniques like Kalman filtering, ensemble learning and deep learning-based architectures integrate sequential as well as spatial information from multiple sensors. This combination enhances reliability in the face of incomplete or uncertain data and provides better real-time emission estimation. Data fusion also facilitates consistent monitoring of emission profiles across process units, enhancing the connection between operational control and environmental performance monitoring.

5.3. Regulatory reporting

Emission levels, operating situation and compliance status for a given reporting period have to be accurately recorded in order to comply with environmental regulations. Manual generation of such reports is time-consuming and error prone, particularly in large data-intensive sites. Machine learning enable the automation of data aggregation, validation and trend analysis in regulatory reporting. For example, ML models can be designed to analyze historical emissions and recognize trends and risks of non-compliance in future by biorefineries avoiding or warning potential polluters [93-105]. These systems can also correlate sensor data with established regulatory ranges and create alerts in anticipation of potential excursions, as well as reports that align with specific regulatory paradigms. It is this level of automation that simplifies reporting, guarantees correctness and minimizes the administrative work for bio-refinery operators. In addition, machine learning supports the development of real-time inferential sensors for monitoring renewable carbon content, a requirement for co-processing bio-feedstocks to meet regulations – The online approach renders obsolete costly and slow offline measurements [106-112]. The network will provide national scale, near real-time assessment of environmental and regulation related performance well beyond the capability of existing manual reporting-based methods [113]. AI systems can adjust the collection and reporting of data to new emissions standards or reporting guidelines to maintain compliance with changing regulations [114-117]. Use of machine learning for regulatory reporting also applies to predictive modelling on permit renewals and environmental impacts assessment, enabling a justification to show evidence-based maintenance of the environment. ML-driven regulatory reporting systems facilitate proactive compliance as they provide real-time assessment and early detection of non-compliance risks. These systems are used to monitor trends and deviations based on real-time and historical data, stopping further dispersion before the regulatory limits will be exceeded in time to perform some corrective operation. They also enhance data validation, consistency and auditability in regulatory submissions. Hence, this post-event documentation based reporting becomes an ongoing compliance activity.

Determination and rule-based models can identify operating periods with potentially non-compliant values or high emitter-role risks. This enables immediate corrective action and facilitates open communication with the regulatory agencies. At longer time scales we can see that machine learning aided reporting enables companies to show consistent improvement in controlling emissions and facilitate an evidence-based approach to environmental auditing.

Table 3. Emission Monitoring and Environmental Compliance

Section	Focus Area	ML Techniques Used	Data Sources	Key Functions	Benefits
Emission Monitoring & Environmental Compliance	Overall emission control and sustainability	ML, AI, data-driven modelling	Process data, sensor data, logs	Emission estimation, optimization, compliance support	Reduced environmental impact, improved compliance
Predictive Emission Models	Prediction of air, water, and methane emissions	ANN, supervised learning, reinforcement learning	Historical sensor data, lab analysis, operating conditions	Emission forecasting, early warning, driver identification	Proactive control, minimized emissions, regulatory safety
Sensor Integration & Data Fusion	Accurate real-time emission estimation	Kalman filters, Bayesian networks, deep learning	IoT sensors, satellite data, climate models	Data fusion, anomaly detection, real-time monitoring	Improved accuracy, robustness, comprehensive footprint analysis

Table 3 summarizes how machine learning supports emission monitoring and environmental compliance in biorefineries by integrating predictive models, sensor data fusion, and automated regulatory reporting. It highlights the use of advanced ML techniques to improve emission estimation accuracy, enable proactive control, and ensure continuous compliance with environmental regulations.

6. Case studies

6.1. Fermentation control using ANN and MPC

Several experimental and pilot-scale studies report the successful integration of artificial neural network models with model predictive control for fermentation systems. ANN models are first trained to capture the nonlinear relationship between operating variables such as temperature, pH, substrate concentration, and biomass growth. These trained models are then embedded within an MPC framework to forecast future process behavior and compute optimal control actions.

Results indicate that ANN–MPC systems maintain fermentation variables closer to their target setpoints, with lower overshoot and faster stabilization compared to conventional PID-based control. Improved control precision directly translates into higher product yield and more consistent product quality. In addition, smoother control actions reduce excessive heating, cooling, and dosing, leading to measurable reductions in energy consumption while preserving overall process stability.

6.2. Emission prediction in biomass gasification

Biomass gasification processes are characterized by strong coupling between feedstock properties, operating conditions, and emission formation. Case studies show that ensemble learning models such as random forests and gradient boosting can predict carbon monoxide and nitrogen oxide emissions with good accuracy using inputs like moisture content, elemental composition, equivalence ratio, and reactor temperature.

These predictive models enable operators to anticipate emission spikes before they occur. By adjusting air–fuel ratios or operating temperatures in advance, emission levels can be kept within regulatory limits. Practical implementations report sustained operation below compliance thresholds, along with improved process transparency and reduced reliance on end-of-pipe emission control measures.

6.3. Optimization of heat integration

Heat integration is a major opportunity for reducing energy demand in bio-refineries due to the presence of multiple hot and cold process streams. Machine learning-based optimization frameworks have been applied to analyze heat exchanger networks using historical operating data and process constraints. These tools identify alternative heat recovery pathways that may not be evident through traditional pinch analysis alone.

Case study results show that data-driven optimization can lower overall utility demand by improving heat recovery efficiency and balancing thermal loads across the plant. Such approaches support incremental retrofitting decisions and provide practical guidance for improving energy performance without major process redesign.

7. Challenges and limitations

Data availability and data quality remain the most significant constraints on the effective use of machine learning in bio-refinery process control and optimization. Many facilities operate with limited historical datasets, fragmented records, or data collected under narrow operating ranges. Such conditions restrict the ability of ML models to generalize across different feedstocks, loads, and transient states. In addition, missing values and inconsistent sampling rates further complicate model development.

Sensor reliability is another practical limitation. Industrial sensors are subject to fouling, aging, and calibration drift, which introduce noise and bias into measured variables. When these effects are not properly detected and corrected, ML models may learn misleading patterns, leading to reduced prediction accuracy and unreliable control actions. Continuous sensor validation and data preprocessing are therefore essential but often resource intensive.

Model interpretability also poses a challenge, particularly for complex architectures such as deep neural networks. Process engineers often require clear insight into cause–effect relationships to trust and act on model outputs. Limited transparency can slow adoption and reduce confidence in ML-based recommendations. Techniques for model explanation and sensitivity analysis are available, yet they add another layer of complexity to system implementation.

Solutions produced by purely data-driven resource optimalization can be statistically, but not physically (mass, energetics and thermodynamical conservation laws), optimal or unsafe. The models have also been found unable to generalize beyond historical data, thus being sensitive to fluctuations caused by different feedstocks, perturbations or scale up conditions often encountered in the biorefinery. Moreover, lack of interpretability decreases operators' trust so it is not easy to be used in practice. These considerations motivate the use of hybrid, data-driven and physics-based approaches for realistic and reliable resource optimization.

Finally, integration of ML models with existing control infrastructure demands careful validation and testing. Safety constraints, regulatory requirements, and fail-safe operation must be ensured before deployment. ML-driven control actions need to be evaluated under abnormal and extreme conditions to prevent unintended process upsets. These challenges highlight the need for gradual integration, strong validation protocols, and close collaboration between data scientists and process engineers.

8. Future directions

Future research on machine learning for bio-refinery systems is expected to move toward tighter integration between data-driven methods and established engineering knowledge. One important direction is the combination of machine learning with first-principles models. Hybrid frameworks that embed mass, energy, and reaction constraints within ML architectures can improve predictive accuracy while retaining physical meaning. Such approaches support better trust and acceptance among process engineers, as model outputs remain consistent with known process behavior. Another promising area is the development of transfer learning strategies. Bio-refineries differ widely in scale, feedstock type, and process layout, which limits direct reuse of models trained at a single site. Transfer learning allows models to be adapted using limited new data, reducing training effort and improving generalization across different configurations. This is particularly relevant for emerging facilities where long-term operational data are not yet available.

Advances in edge computing also open new opportunities for real-time application of machine learning. Deploying trained models closer to sensors and control hardware reduces data transmission delays and enables faster decision making. Low-latency inference is essential for safety-critical control loops and for handling rapid disturbances in dynamic processes. Finally, digital twin frameworks are expected to play a central role in future bio-refinery management. By coupling machine learning models with process simulations, digital twins allow systematic exploration of operating scenarios, fault conditions, and optimization strategies. These virtual representations support predictive analysis, operator training, and informed planning for process modifications under varying economic and environmental constraints.

9. Conclusion

Machine learning has become a crucial facilitator of smart biorefineries system by overcoming the difficulties of non-linear process dynamics, feedstock variability and multi-objective optimization. This paper demonstrates that ML-based predictive modeling, R-T control and fault detection systems provide significant process stability, product yield and energy efficiency beyond the capabilities of classical solutions. Evidence-based improvement in the use of energy, feedstock, water and nutrients also help to increase resource efficiency and improve economics. Machine learning is also important for emission monitoring and environmental compliance by predicting emission models, sensor data fusion, and automatic reporting systems. This functionality ensures proactive environmental management, and better understanding on how to align the media with sustainability and regulatory goals. Some challenges, ranging from data quality to interpretability and systems integration, however persist; but further development of hybrid ML–physics models and digital twin frameworks is likely to speed up industrial uptake. In general, machine learning offers a scalable pragmatic route to resource-efficient, low-emission biorefineries for a sustainable bioeconomy.

Authors' Contributions

Sonali Shrikant Patil led the conceptualization, literature review, and initial drafting of the manuscript. **Madhuri Karad** and **S. Manjula Gandhi** contributed to data curation, analysis of machine learning techniques, and preparation of technical tables and structured content. **Mahesh Ganpat Bhong** and **Kiran Dattatray Devade** supported the sections related to resource optimization, including energy efficiency and feedstock management. **Vishakha Avinash Mahajan** contributed to emission monitoring and sustainability analysis. **Ghanasham Chandrakant Sarode** and **Ganesh Patil** assisted in manuscript structuring, case study synthesis, and technical refinement. **Anant Sidhappa Kurhade** conceived the overall research framework, supervised the study, critically reviewed the manuscript for technical depth and clarity, and finalized it for submission as the corresponding author. All authors reviewed and approved the final version of the manuscript.

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Conflict of interest

The authors declare no conflict of interest

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