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AI-Based Pollution Monitoring in Bio-Energy Production Chains: Methods, Applications, and Gaps

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ABSTRACT

The rapid growth of bio-energy production is closely aligned with global sustainability agendas, particularly the Sustainable Development Goals (SDGs) related to **Affordable and Clean Energy (SDG 7)**, **Industry, Innovation and Infrastructure (SDG 9)**, and **Climate Action (SDG 13)**. Effective pollution monitoring across the bio-energy production chain is essential to ensure that renewable energy expansion does not lead to unintended environmental burdens. Current research largely treats artificial intelligence (AI) applications in environmental monitoring and bio-energy systems as separate domains, creating a research gap in integrated, process-wide frameworks that connect emission sources, sensor networks, data pipelines, and AI models across all production stages. The objective of this study is to critically review AI-based pollution monitoring approaches for bio-energy systems and to assess their capability to support sustainable and responsible energy production in line with SDG targets. The methodology involves a structured synthesis of recent literature on sensing technologies, data acquisition and preprocessing, machine learning and deep learning models, and hybrid physics-informed approaches applied from biomass handling to biofuel refining. The key findings show that AI-enabled

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monitoring improves real-time emission estimation, early detection of abnormal events, and short-term forecasting, supporting cleaner production pathways. At the same time, challenges related to sensor drift, data scarcity, model transferability, and interpretability limit large-scale adoption. The implications of this review highlight the need for open benchmark datasets, robust calibration strategies, and explainable AI models to strengthen regulatory trust, promote sustainable industrial practices, and contribute directly to achieving SDG-linked environmental and energy objectives.

Keywords: AI Monitoring, Bio-Energy, Emissions, Hybrid Modelling, Sensor Networks, Affordable and Clean Energy; Climate Action

1. Introduction

Bioenergy production involves several stages, including biomass collection and pre-treatment, anaerobic digestion, thermochemical conversion (combustion and gasification), and liquid biofuel processing. Pollution may arise at each stage. Typical examples include fugitive methane emissions and odor release from digesters, particulate matter (PM) and nitrogen oxides (NO_x) from combustion units, and volatile organic compounds (VOCs) and liquid effluents during refining operations. Monitoring these emissions is essential for regulatory compliance, effective process control, and protection of public health. Recent advances in low-cost sensors, IoT-based data transmission, and artificial intelligence provide new opportunities for improved, continuous monitoring and early mitigation of environmental impacts. Existing reviews on AI applications in environmental monitoring and bioenergy systems indicate rapid growth in sensor–AI integration and predictive control modelling. Environmental monitoring of bioenergy systems has attracted significant interest due to the temporal variability and complex behavior of pollutants ^[1]. AI-based approaches can offer faster response and higher reliability than manual sampling, which is often constrained by cost, scalability, and time, particularly in resource-limited regions ^[2,3]. AI systems support automated data acquisition, processing, and interpretation, shifting monitoring practices from static measurements toward predictive and real-time assessment of environmental impacts associated with bioenergy production ^[1,3,4]. Methods such as inductive learning, computer vision, and advanced sensor networks enable high-level data analysis and improve the accuracy, efficiency, and spatial coverage of environmental monitoring activities ^[4,5]. This integration strengthens risk prediction and environmental control across bioenergy supply chains ^[2]. AI-based models also support the analysis of complex natural and ecological phenomena that are difficult to capture using classical analytical tools, including habitat assessment, wildlife monitoring, and deforestation detection ^[4,6]. In the bioenergy context, AI is applied to multiple operational aspects, including feedstock management, optimization of conversion efficiency, and continuous environmental monitoring at both bio refineries and distributed bioenergy plants. Neural network models linked with air and water sensor networks are increasingly used for pollution estimation, waste treatment monitoring, and sustainability assessment ^[7,8]. Recent review studies summaries a wide range of AI techniques applied specifically to bioenergy process monitoring and environmental management ^[9]. Deep learning plays a central role by extracting complex patterns from large-scale environmental datasets, which is critical for climate modelling, pollution detection, and dynamic monitoring of bioenergy systems ^[10,11]. It improves classification accuracy for high-resolution satellite, drone, and ground-based sensor imagery used in land-use analysis and ecosystem surveillance within bioenergy landscapes ^[10,12]. These capabilities support assessments of land suitability for biofuel production and evaluation of associated environmental impacts ^[13]. Machine learning methods also assist in waste sorting and routing for bioenergy applications ^[14] and support planning and optimization of bioconversion processes through data-driven, adaptive decision-making in refinery environments ^[15,16].

Although there have been several state-of-the-art reviews on the use of artificial intelligence for environmental monitoring or bioenergy system optimization alone, this review is unique in providing a process-integrated, chain-wide context for pollution monitoring throughout the entire production pathway of

bio-energy. More specifically, it connects the sources of emission, sensing devices and data transformation into AI models at every stage -from biomass handling to anaerobic digestion as well as from thermochemical conversion and biofuel processing-into a single analytic framework. The review goes beyond prior works by critically deciphering the hybrid and physics-informed AI models to improve adaptability under varying operating conditions, as well as consolidating deployment-level issues including sensor drift, calibration consistency, domain shift, and regulatory acceptances. By identifying targeted research priorities in the form of open benchmark datasets, transferable calibration pipelines, explainable models, and closed-loop field validation, this work makes a focused contribution to the translation from AI-based pollution monitoring in experimental studies to reliable industrial practice.

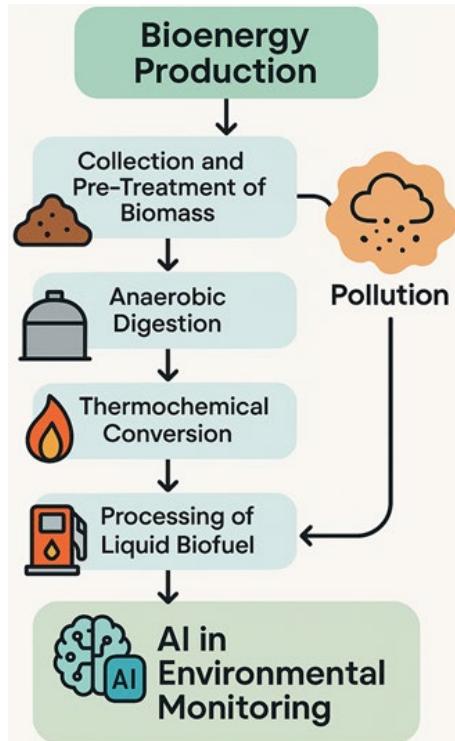


Figure 1. Overview of Bioenergy Production Stages and Points of Pollution with AI-Based Environmental Monitoring Integration

Figure 1 sets the scene for pollution monitoring as a chain-level rather than unit-level problem. Here, the figure shows the mapped emission sources across biomass handling, digestion, thermochemical conversion and refining to demonstrate why single approach monitoring is not enough. It further illustrates the visual concept of continuous, AI-driven sensing and data integration along stages where emissions are intermittent, diffuse, and operationally coupled. Application of AI driven analytics to Earth observation data is enhancing monitoring by providing rich spatiotemporal insights into land-use change, biomass growth and pollution associated with bio-energy production ^[17]. These approaches can be used to enhance resource management and conservation planning and also inform ecosystem health assessment determination as well as the prediction of ecological response to bio-energy practices ^[6,18]. One of the typical examples is the application of AI models for detecting deforestation through satellite images in order to identify illegal logging which impacts carbon balance and biodiversity ^[4]. Remote sensing techniques, for instance satellite imagery, LiDAR and hyperspectral, have permitted the AI in forest composition studies at a large scale and have an impact on biomass resource surveillance ^[19]. AI plays a significant role in predicting the properties of biomass, optimizing conversion processes and facilitating biofuel characterization, which aids in the improved efficiency and environmental profile of bioenergy systems ^[20]. Integrating AI and EO data also aids in early detection of environmental anomalies and understanding temporal trends, which are necessary for decision-making processes and sustainable development ^[17]. This integrated approach allows surveillance

from broad land-use trends to specific pollutant signals, favoring risk-based and adaptive management across bio-energy chains. Among them, there are multi-criterion decision making tools where AI is able to evaluate the environmental, economic and social aspects of bio-energy projects [21]. AI Over the Horizon AI predictive spatial data can assist farmers and planners in adaptive management at bioenergy landscapes by accounting for carbon sequestration, species distribution and ecosystem conditions [22]. Responsible application of such systems is essential to ensure that they are used for beneficial purposes in sustainability rather than exacerbating inequality and new environmental stresses [17]. That would require strong frameworks around data governance, model transparency and ethical protection. Clear description of recent advances, the present status and barriers of AI based pollution monitoring for bio-energy systems is required to foster environmental sustainability and technological advancement. This review provides an in-depth description of the state-of-the-art along the bio-energy production chain, including AI supported pollution monitoring as well as applications for air, water and soil and future research directions. **Table 1** describes the way in which AI can be applied to environmental monitoring through the bioenergy chain, connecting each step of processes to a set of received pollution problems and responses according with appropriate AI methods and applications. It also outlines the main research deficiencies, particularly demand for adaptive models and multi-source data integration, along with transparent governance structures.

Table 1. AI-Based Environmental Monitoring in Bioenergy Production

Aspect	Bioenergy Processes	Pollution Sources	Role of AI	Applications & Examples	Key Insights / Research Gaps
Process Chain & Context	Biomass collection, pre-treatment, anaerobic digestion, combustion, gasification, liquid biofuel refining	Fugitive methane, odour emissions, PM, NOx, VOCs, wastewater	AI improves tracking of dynamic, complex pollution patterns	Use of sensor networks, IoT telemetry, inductive learning, computer vision	Need for systematic AI-based monitoring across each production stage
Monitoring Challenges	Manual sampling, laboratory testing, low temporal resolution	Limited scalability in developing regions	AI handles large, heterogeneous, real-time datasets	Automated data gathering, adaptive algorithms	Research gap in affordable, high-resolution environmental monitoring
AI Techniques	Applied throughout bioenergy operations	Identifying hidden pollution trends	Deep learning for pattern detection, classification, forecasting	Satellite imagery, drones, ground sensors, LiDAR, hyperspectral imaging	Integration of multi-source data remains limited in many chains
Environmental Applications	Feedstock logistics, land use assessment	Pollution during conversion, transport, waste handling	Predictive analytics for early warnings	Land cover classification, deforestation tracking, biomass estimation	Lack of unified models linking land-use change and real-time pollution
Operational Benefits	Improved conversion yield, optimized bioconversion	Reduction of emissions and resource loss	Data-driven decision support for sustainable processes	Waste sorting, routing, resource allocation, process optimization	Need for adaptive models that react to rapid system fluctuations
Ethical & Governance Needs	Sustainable production planning	Potential bias in environmental decision systems	Fair, explainable and transparent AI frameworks	Multi-criteria decision analysis for socio-environmental balance	Research gap in ethical guidelines and governance for AI deployment

2. Measurement hardware and data pipelines

Bio-energy plants require a variety of sensors and different measurement principles, drift behaviors and cross-sensitivities need to be dealt with in one way. These discrepancies underscore the importance for combined pipelines which unify all readings from optical, electrochemical (EC), oxidised metals and reference-grade instruments into a common approach. Here, in conjunction with hybrid networks and AI-based calibration, this joint work further enhances the accuracy of pollutant measurement results, making monitoring more continuous across combustion, digestion and fuel-processing units.

2.1. Sensor types and characteristics

Bio-energy applications use a number of sensor types to monitor gas emissions, particulate activity and component status along components including the economizer, exhaust line and ash-handling units. NDIR sensors are typically used for CO and CH₄ because they are sufficiently stable in humid condition and readily suitable for continuous field measurement. These sensors are also popular for methane because they offer the rapid detection required in applications such as leak detection. Industrial and commercial applications catalytic bead sensors are used for industrial and commercial only not residential. For NO_x, SO₂ and O₃, electrochemical sensors are commonly recommended because of selectivity [and power requirements plus they are suitable for deployment in networks]23.

Particulate concentrations (PM_{2.5}, PM₁₀) are determined by optical counters providing real-time and gravimetric samplers (reference methods). Sensors that measure VOCs are usually metal-oxide, but their readings may change depending on temperature or humidity. In these cases, laboratory methods for chemical speciation (e.g., gas chromatograph or FTIR) are still necessary to determine more detailed components of the reaction mixture that low-cost sensors are not able to distinguish [23]. The AI-enhanced sensor networks are designed for compensating the individual sensors biases, through aggregating data from different sources to form more complete pollution and source estimations. The infrared gas sensors are crucial for the carbon-based gases due to their ability to detect a specific absorption wavelength, and presents with sensitive and accurate readouts and low interference towards other species [24]. Flow monitoring, despite its importance in interpreting energy use measurement and verification is still expensive and technically demanding, which justify the demand for models based on hybrid measurement-modelling methods [25]. Other alternative techniques including infrared absorption spectroscopy and optical interferometry also provide choices, and have their working range and limitation [26]. Low-cost sensor networks are now being deployed in proximity of combustion and digestion units to map pollutant concentrations at high spatial resolution. Low price allows dense monitoring, but problems like drift and cross-sensitivity limit its reliability. "Master special of many families-Master special for all-more or less obsolete now Reference standards are still needed for calibration and long-term validation. A number of investigations propose hybrid networks, where low-cost sensors share the coverage function with a few well-located reference monitors, can provide an effective trade-off between network extension and accuracy for bio-energy applications. Real-time online detection can compensate for the deficiencies of the casualty-based instrument and offline laboratory devices which are expensive to use and work in stops and starts [27]. To make such hybrid systems more reliable, AI solutions that can compensate sensor drift and cross-sensitivities, as well as fusion multimodal datasets into a single monitoring structure, must be developed [24,28].

2.2. Data acquisition and pre-processing

Contemporary bio-energy facilities store high-frequency data sampled by on-board loggers using IoT telemetry into time-series databases for later analysis. For most pipelines calibration is performed by field co-location of sensors and reference instruments applying simple linear correction factors or more advanced

drift correction techniques. For smaller ($< 1\text{mW}$) plants and farms, which may be reliant on uncalibrated sensors, hierarchical validation: synthetic-benchmark-trained-and-real-microdata-refined improves model accuracy [29]. This method enables strong AI modelling even if sensor data is heterogeneous or noisy [30]. Calibration Technically, AI models also refine calibration by training on co-located reference monitors and employing additional parameters such as temperature and humidity to correct for drift [31]. After calibration, data cleaning removes missing values and noise via statistical or machine learning based methods for preparing the dataset for analysis [32]. Outlier removal compensates for electrical noise, warm-up behavior and abrupt system changes; interpolation retains temporal coherence. Features like rolling averages, variance, gradients and frequency-based features are frequently taken out of these studies and combined with plant-level information as feedstock composition, the feed rate of the digester, and temperature in the digester, combustion load and flow rates were used together with meteorology. These manual inputs are designed to assist in the interpretability of global emission estimates and to refine high emission activity periods. Clean, high-quality data is of crucial importance as poor quality data can impact on model accuracy in a dynamic plant environment [33]. Those virtual sensors, based on machine learning models, also correct distorted readings and ensure that the data is continuous [34]. Robust pre-processing is still crucial; even sophisticated models don't work well when trained with uncalibrated or noisy input. **Table 2** lists the principal hardware and data-pipeline components with a focus on sensor roles, typical limitations, and the necessity of hybrid systems together with AI methods to achieve an accurate and reliable monitoring throughout different parts of plants.

Table 2. Hardware, Sensors, and Data Pipeline Structure in Bioenergy Monitoring

Component	Purpose	Sensor / Tools	Key Issues	Role of AI / Hybrid Systems
Measurement Hardware	Track gases, PM, and operating conditions	NDIR, catalytic bead, EC, metal-oxide, optical PM, gravimetric, GC/FTIR	Drift, cross-sensitivity, humidity effects, high cost	Unifies signals, compensates drift, improves continuity
Sensor Characteristics	Provide pollutant-specific measurements	NDIR (CO/CH ₄), EC (NO _x /SO ₂ /O ₃), metal-oxide (VOCs), PM counters, FTIR/GC	Humidity effects, limited speciation	Multisensor fusion and calibration improve accuracy
Low-Cost Sensor Networks	Enable dense spatial monitoring	Low-cost multi-pollutant nodes	Strong drift, low stability	Combine with reference stations for balanced accuracy
Data Acquisition	Collect and store high-frequency readings	IoT loggers, cloud databases	Noise, missing data, communication gaps	Supports hierarchical validation pipelines
Calibration & Pre-Processing	Prepare clean and reliable datasets	Drift correction, imputation, outlier removal	Heterogeneous and noisy industrial data	AI correction, virtual sensors, feature extraction
Overall Outcome	Achieve stable and continuous monitoring	—	Mixed pollutants and dynamic conditions	Reliable long-term monitoring across units

3. AI methods: tasks and algorithms

This section outlines the main AI tasks and algorithmic families used for pollution monitoring in bio-energy systems. It focuses on how prediction, forecasting, and anomaly detection are matched with process data and sensor characteristics. Emphasis is placed on selecting methods that remain reliable under dynamic operating conditions.

3.1. Tasks

AI approaches for bio-energy involve prediction and diagnostic tasks to provide real-time monitoring & operational planning. A central task is regression, in which models learn the connection between multimodal

sensor inputs (process settings), and measured pollutant values. It enables low-cost sensor arrays together with process data to emulate reference-quality measurements. Many works focus on predicting trends, by short-term (minutes to days) forecasting of time series. These predictions provide an early alarm that emissions may be increasing, and allow the operator to take action on air–fuel ratios, feedstock input or on digester conditions. Anomaly detection is also quite crucial, as it detects abnormal trends or noise present in sensor readings that could help to identify equipment failures or process upsets which can lead to high emissions^[29, 35].

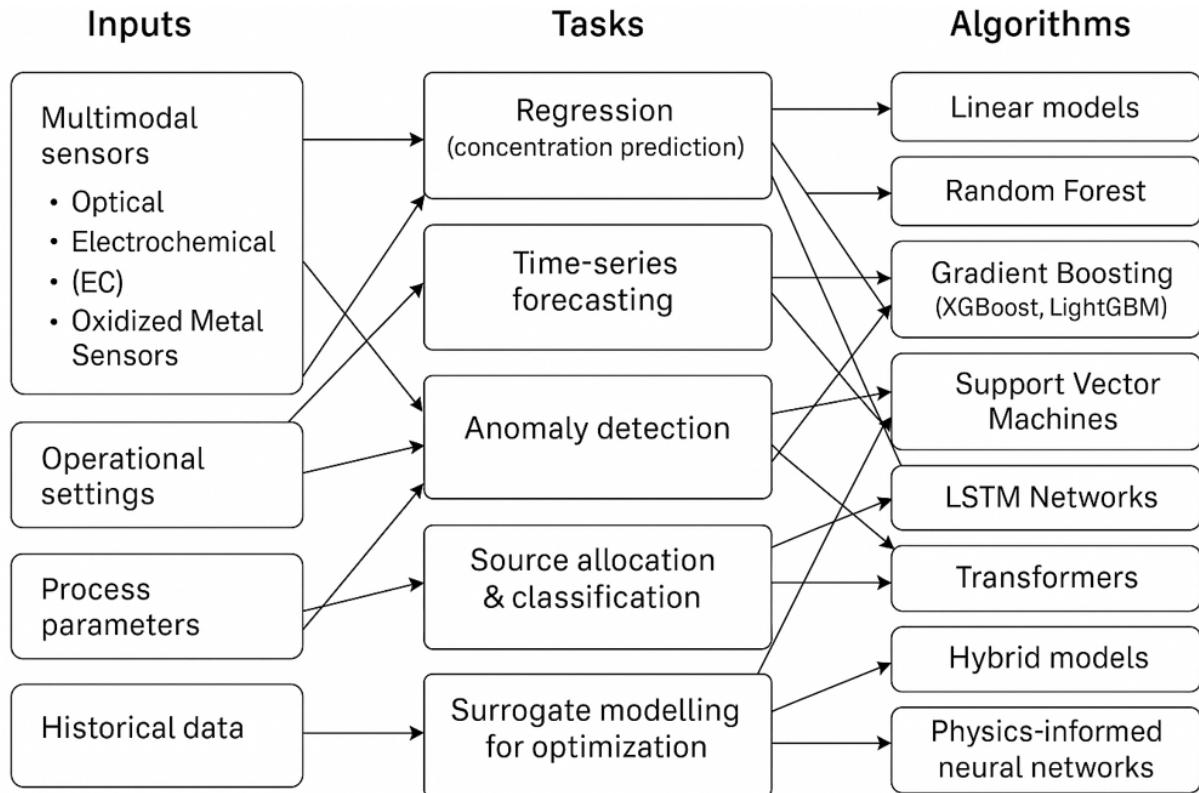


Figure 2. Input–Task–Algorithm Framework for AI Applications in Bio-Energy Systems

The logical relationship between AI tasks, algorithm selection and heterogeneous sensor inputs are described in **Figure 2**. It demonstrates that model selection is a function of task demand—either prediction, novelty detection or source identification—and not simply an algorithmic whim. The approach corresponds to the notion of aligning data semantics with an appropriate learning target and is supportive of the widely accepted view that good pollution monitoring entails that data-specific will effectively mediate between mission goals and collected input. Anomalies make it possible to detect abnormal emission spikes, equipment failures or sensor malfunctions. These models are trained on normal patterns of behavior and produce notifications when sensor behavior deviates from the learned pattern. In plants that must be monitored constantly is the operator to ensure safe operating limits are not exceeded, this is useful. Advanced AI approaches take this further by identifying and correcting drifts to increase the quality of sensor data, thus enhancing for example prediction tasks and control actions downstream^[36]. Several approaches employ unsupervised learning for the anomaly detection based on the deviation from operational baselines, enabling effective real-time monitoring and more accurate predictive maintenance^[35]. ALE source allocation and classification techniques can identify which unit (combustion, digestion or storage) is responsible for an emission event - a particularly valuable function for facilities with several combustion, digestion or storage units. Classification algorithms tie sensor signatures to likely sources, simplifying targeted abatement and supporting regulators in understanding the contribution of each process. And in the

field of transformers, instead of stacking different layers, self-attention is applied to extract fine features from industrial data for refining pollution source identification and prediction [37]. Predictive emissions monitoring systems can be substituted for traditional continuum monitoring by employing AI to predict pollutant concentrations from process variables, e.g. by using machine-learning techniques such as gradient boosting machines [38]. AI models are also stand-ins for process enhancements. They predict emissions given different operating conditions, and facilitate multi-objective optimization between power generation, operational stability and the environment. Such surrogate models are especially useful when the physical simulations are slow or computationally expensive.

3.2. Algorithms and hybrid approaches

In bio-energy research, a variety of ML techniques are implemented. Older methods like linear regression, random forests, gradient boosting (XGBoost, LightGBM) and SVMs are ubiquitous because they work well and are interpretable. Tree ensembles are particularly attractive in this regard, because they model nonlinear dependencies, and cope well with noisy input data while these models offer transparent variable-importance assessments. Random forests have found promising results in biomass-to-biochar prediction [39], whereas gradient-boosting techniques and XGBoost have provided precise NO_x predictions for combustion and boiler systems [38,40]. Deep learning-based models are more appropriate for temporal patterns when system behavior is predominantly sampled in interval timing. LSTMs are able to capture long-term time-series dependencies, while transformers work well with irregular or multivariate data. They can be employed for short-term prediction in AD (Anaerobic Digestion), biomass combustion and upgrading of biogas. Hyper parameter tuning is also widely realized with the Bayesian optimization, by which more accurate prediction programs for gasification outputs / engine emissions can be obtained as a result. Hybrid models are gaining popularity. Some methods marry mechanistic process models with a data-driven component to compensate for the remaining errors, and full physics-informed learning which encapsulates process constraints into neural networks. Human-in-the-loop AI can benefit from expert judgment in the course of model refinement, which is useful especially for complex bio-energy processes where laws of physics and domain knowledge enhance reliability and interpretability [42]. AutoML solutions automate feature processing and model choice. Additionally, ensemble stacking improves prediction stability. Research on anaerobic digestion demonstrates that tree-based AutoML models, when joined with neural networks, yields higher accuracy. Hybrid systems combining ML and metaheuristic optimization also underpin optimal operating conditions and pollutant mitigation for enhanced system efficiency and environmental acceptability. These models allow for improved accuracy, robustness, and generalization in the context of renewable-energy and biofuel applications [43]. Deep-learning-mechanistic hybrids model nonlinear behavior while enforcing physical consistency by reducing reliance on large dataset [44].

This section shows the technical depth of HPC through an extensive discussion of hybrid and physics-informed AI models. The paper describes how data-driven approaches are integrated with scales in mass balance, thermodynamic relationships and process kinetics. Moreover, it demonstrates how in human-in-the-loop techniques expert knowledge is also leveraged to enhance robustness, interpretability, and reliability under changing bio-energy operating conditions.

4. Applications across the bio-energy chain

This section examines how AI-based monitoring is applied at different stages of the bio-energy production chain. Applications are reviewed from biomass handling to biofuel refining, with attention to pollution sources and process variability. The discussion highlights differences in maturity across stages.

4.1. Biomass collection and pre-processing

Operations for biomass—chipping, drying, conveying and transport—are a source of suspended dust/particulates. AI models connect equipment variables (e.g., conveyor speed, moisture content and mechanical load) with meteorological conditions in order to predict particulate release for varying operating conditions. Research has shown that integrated models can predict for periods of high dust generation. Drones or fixed camera sensors allow the online remote sensing and visual examination of biomass piles, where image features such as color changes, surface cracking and local heating are useful for detecting degradation (or early self-heating). High VOC and CO events occur under similar meteorological conditions and therefore early notification may be useful for preventive action. AI methods such as ML and neural networks further enhance the prediction of feedstock quality for optimum anaerobic digestion conditions with the production of biofuels at higher efficiency with a better sustainability [45]. The tools contribute to limit the environmental pollution, optimize the logistics of biomass, and that waste is reduced simultaneously with the increase in material quality. Above and beyond these, AI can also facilitate biodiesel production prediction, engine-emission model estimation and biofuel quality forecasting [40]. Furthermore, AI based approaches help in microbial or crop selection, and conducting genetic engineering for maximizing biofuel yields, and allow early stage techno-economic & life-cycle studies of a biomass-to-biofuel process [46].

4.2. Anaerobic digestion and biogas facilities

Artificial intelligence (AI) methods have been employed for explanation and control analysis. AI methods are employed to investigate emissions from the AD process by developing a methane yield model as a function of feedstock characteristics, OLR, digester temperature and indicators about microbial activity. They also allow for the estimation of methane slip, i.e., the unintentional release of methane before combustion or upgrading. Such sensor-based classifiers can focus on pH, redox potential or temperature as well as gas composition to detect the occurrence of unstable states such as acidification or overloading. Regression models are developed up to the prediction of methane, CO₂ and total gas production first to design an early intervention strategy. Predictions of these emissions in real time can be interfaced with modern control systems for controlling processes to minimize GHG emissions automatically. Machine learning exhibits better predictive accuracy for methane yield from AKR than linear regression, however it is less reliable [47], demonstrating the potential application in WWTP models. ANN and SVM methods are also employed to optimize running states and predict biogas production for sustained, efficient AD operation [29,35]. AI-driven models also aid in optimization of that processes and reduction in pyrolysis, gasification, and combustion toward better system performance through the improvement in BE aspect [35]. Deep learning integrating with neural networks is a further method to enhance methane prediction by overcoming the disadvantages of classical models (dealing with complicated inputs and having slow characteristics in responding biogas systems) [48]. **Figure 3** summarizes how AI tools are applied in various links of the bio-energy chain, and highlights that pollution benefit is achieved through holistic application rather than isolated optimization. It shows disparities in research maturity: among available biomass-based technologies, anaerobic digestion and combustion have attracted much more interest than upstream (e.g., biomass pre-treatment) or downstream (e.g., bio-oil upgrading) processes showing the future studies gaps.

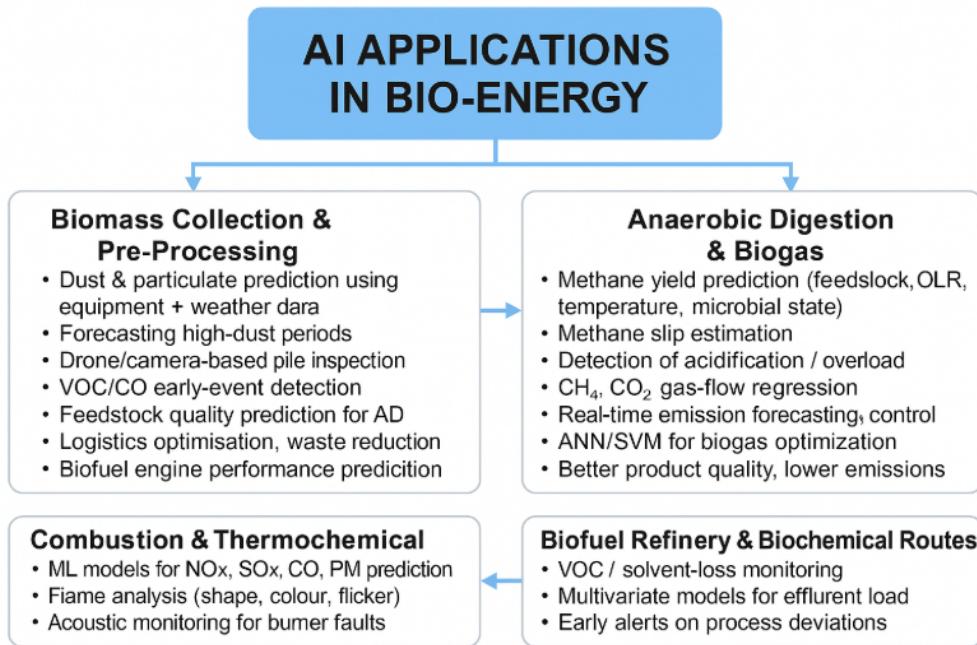


Figure 3. AI Applications across the Bio-Energy Chain

4.3. Combustion and thermochemical conversion

Regulated pollutants NO_x, SO_x, CO and PM are emitted when biomass is combusted in bio-energy plants. These emissions are estimated by the machine learning models, which considers the fuel type, moisture content, air-fuel ratio, furnace temperature and load variations as inputs. Such models are used to determine operating windows for emissions compliance at a cost of low energy generation. Computer vision has been applied to the analysis of flame shape, color and flicker (which relate to combustion quality) while acoustic signals help identify noise patterns related to/mismatch in combustion or burner damages. Early diagnosis of the abnormalities is possible by both these techniques. AI methods, e.g. ANN and machine learning models predict stability and conversion rates of thermochemistry reactions for bio-oil and syngas production with lower experimental requirements ^[47]. These instruments also provide a better understanding of waste-to-energy processes, such as incineration by determining optimum erosion conditions for high energy recovery with minimal emissions ^[35]. Moreover, AI enables the comprehension of intricate biochemical paths to biofuel production and assists shifting to advanced- or next-generation nonfood biofuels ^[40]. These strategies enhance the biofuel value chain from feedstock generation to ultimate conversion ^[40]. Above and beyond process optimization, AI enables adaptive and predictive maintenance for emissions-control systems. It is also possible to combine it with GIS in order to identify and monitor polluted areas suitable for bioremediation, boosting environmental management ^[49].

4.4. Biofuel refinery and biochemical conversion

Processing biofuels (e.g., production of ethanol from fermentation, of biodiesel from transesterification, and biochemical upgrading) create three waste products including compounds in gaseous form, waste water and off-gases. Solvent loss and VOCs emissions are monitored by the AI platforms via sensors in the vent lines and process units. Multivariable models are constructed, taking into account temperature, pressure, flow rate, solvent composition and reaction indicators to predict pollutant loads online. These predictions assist operators to detect abnormalities in time, making them respond before having an impact on emissions or effluent quality. Through early prediction, AI enhances the environmental performance and improves process stability in biofuel refining. Similarly, machine learning methods are also used to measure and tune the associated chemical parameters for conversion of waste oils to biodiesel whose output yield and quality is increased ^[49]. These optimization approaches also help with removing impurities from feedstocks and

compost, leading to reduced environmental load and higher economic returns [48]. These prediction tools aid in regulatory compliance and development of an environmentally and economically sustainable bio economy [35]. Machine learning with predictive modelling facilitates automatic and real time monitoring in the biomass conversion process and thus reduces labor cost as well as improves its efficiency [50]. AI also scales to the broader strategic control of systems in bio refineries, where digital twins represent and optimize processes systems to optimize resource consumption and waste minimization [51-60]. The role in which AI can play at different stages of the bioenergy chain for improved efficiency, process stability and emissions management is summarized in **Table 3**.

Table 3. Role of AI in Biomass, Biogas, Combustion, and Biofuel Refinery Processes

Stage / Process	Key Activities	AI / ML Applications	Benefits	Examples / Outcomes
Biomass Collection & Pre-Processing	Chipping, drying, conveying, transport, storage pile monitoring	Dust forecasting; drone/camera inspections; feedstock quality prediction; biodiesel & engine performance modelling; microbial/plant selection	Early detection of dust/VOC events; improved quality; optimized logistics; reduced wastage	Predicting dust peaks; detecting pile degradation; ANN for digestion feed quality; AI for biodiesel and emissions
Anaerobic Digestion & Biogas Facilities	Biogas yield monitoring; stability assessment; methane slip detection	Regression, ANN/SVM for methane yield & CO ₂ ; classifiers for overload/acidification; deep learning for digestion dynamics	Stable operation; reduced methane slip; early fault detection; real-time emission prediction	ML-based methane yield estimation; AI control to reduce GHG; optimization of pyrolysis/gasification
Combustion & Thermochemical Conversion	Combustion control; flame analysis; emission monitoring	ML for NO _x /SO _x /CO/PM; computer vision for flame patterns; acoustic burner fault detection; ANN for thermochemical reactions	Controlled emissions; early abnormality detection; improved bio-oil/syngas production	AI optimization of waste-to-energy units; predictive maintenance; GIS-AI for remediation
Biofuel Refinery & Biochemical Conversion	Fermentation; transesterification; biochemical upgrading	Multivariate VOC/solvent models; ML for process optimization; impurity removal; digital twins for control	Lower emissions; early upset warnings; improved yields; reduced cost	AI for biodiesel yield; automated monitoring; refinery digital twins

5. Evaluation metrics and benchmarking

The assessment of AI models in the application of bio-energy emission studies employs commonly used metrics for model evaluation that assess prediction accuracy, classification reliability and forecasting skill. For regression purposes, RMSE, MAE and R² are the three measures used to express respectively total error, average deviation and goodness of fit. For classification tasks, precision, recall and F1 score are commonly used, particularly to find rare events like faults, emission spikes or sensor anomalies. Or similarly, in time series forecasting comparison of fit to simple baseline methods is usually done using skill values or relative errors. Biomass' higher heating value, for instance, can be accurately estimated by advanced machine learning techniques contributing to the determination of complicated biomass arrangements [61-75]. Cross-validation and external validation will help to improve the robustness of models, which is necessary as bio-energy feedstocks and operations are in general diverse (and often heterogeneous) [76-83]. The feedback from a variety of sensors in real time must also be combined correctly in order to maintain coherence when predicting with AI in systems featuring movement. Strong validation procedures are going to ensure that AI-engine based monitoring tools have a solid base for their use and will effectively contribute to wider

adoption in bio-energy industries. In work that focuses on temporal patterns, time-order-based validation is due for a requirement furthermore, techniques like temporal blocking and rolling-window splits are necessary. The former prevent leakage of information from the future while providing an estimate how a model would behave in practice. In imbalanced data classification, the model performance is commonly monitored by sensitivity, specificity, accuracy, precision, F1 score and Matthews's correlation coefficient [84-88]. Recent evaluation measures involve spatiotemporal out-of-distribution scores, sensitivity scores related to aleatory uncertainty and outlier scores for biased subgroups [89-90]. One considerate limitation is the absence of standardize data sets and most of the works use sensor logs from each plant, making them difficult to compare. Some recent work has made codes, sample data or synthetic benchmarks available to ease transparency. The lack of open source data is still crucial, and the usage of standard benchmarks would help making comparison more consistent. It is important to generate available and standardized data set with reference implementations, which can make a widely researched while AI-based bioprocess engineering in designing reliable [91-101]. To establish robust models, such data should cover a wide spectrum of operating conditions and pollutant characteristics [102-104]. Comprehensive benchmarks for accuracy, robustness and fairness of AI models are also critical as with other ML subfields [105-107], e.g., as initiated by NREL for biogas algorithms. These benchmarks should provide the community with public datasets and standard classification, regression and prediction challenges, applicable across bio-processing studies [108-116]. Shared data sets and evaluation methodologies enhance reproducibility and promote the development of powerful, generalizing predictive models [117-120]. Developing benchmark data sets containing documented sources of uncertainty is also critical to advance uncertainty quantification in the context of bio-energy [121-123]. Even though diverse AI models have been reported for pollution prediction in bio-energy systems, the validation techniques applied in each study vary. Cross-validation is the most frequently used method that provides robust internal performance estimates and is preferable when there is limited data, although such a method tends to assume stationarity and can lead to an overestimate of generalization in highly dynamical bio-energy processes. External testing, based on data from other independent plants or operating periods, provides more evidence of transferability, but this is infrequently applied because requisite data are rarely available and limitations on confidentiality. Temporal validation techniques, such as rolling-window or blocked time-series splits, are of special interest to emission forecasting and anomaly detection; since they maintain the causal nature of process data and prevent information leakage from future states. A systematic comparison reveals that none of these strategies is universally effective on its own; however, a combination of cross-validation for model selection with temporal and external testing for deployment-level assessment can provide a more accurate profile of model robustness and generalization.

6. Case studies (selected)

This section presents selected case studies that demonstrate practical implementations of AI-based monitoring in bio-energy systems. The examples illustrate how different modelling approaches perform under real operational conditions. Attention is given to both achieved benefits and observed limitations during deployment.

6.1. Auto ML by tree for the prediction of biogas

In the last few years, a number of studies have utilized automatic machine learning algorithms in biogas producing systems with emphasis on lignocellulosic substrates. AutoML frameworks for tree-based models can explore an enormous search space of ensemble learners and hyperparameters, relying on a simple operational protocol to discover the best model without a significant amount of human intervention. These models have performed well in predicting methane yield for a range of feedstock characteristics, loading rates and digester conditions. Besides reliable predictions, in this case they also yield ranked feature importance estimates which are useful to understand the relative impact of variables like fiber content,

volatile solids, and temperature and retention time. The resulting balance of accuracy and interpretability makes tree-based AutoML a valuable method for plant operators who want to change feedstock mixes while keeping gas stability.

6.2. IoT and deep learning for industrial air detection

Another strand of research involves combining inexpensive sensor networks with deep learning on air emissions detection in industrial bio-energy environments. Dense distributions of gas, particulate and meteorological sensors are these deployed interconnected to IoT platforms for real time data streaming. Highly accurate sequence models, typically LSTM- or transformer based, can predict in the short-term range, that is to say forecast emission levels ahead of time such that operators still have a reaction time until threshold values are crossed. There are works that have claimed advancements in the early detection of spikes in emissions [5, 4]. However, there is a need for periodic calibration and model retraining as degraded environmental conditions can cause the sensors to drift. Such practical experiences the difficulties and opportunities of operating large AI-enabled monitoring systems in production.

6.3. AI for optimization of organic waste treatment

Studies in bio-waste treatment show how AI is applicable to a broader range of bioenergy processes. Composting, aerobic digestion, and other treatment systems were shown to exhibit instabilities when the temperature, moisture, aeration rate, and gas composition trends were analyzed using data-driven models. Predictive models can be used to optimize the operating parameters, ensuring desired microbial activity will not be lost or odor formation/ emitted. From the case studies, enhanced stability results in more efficient processing with corresponding reduction in environmental burden. These results indicate the scalability of AI-based monitoring and control concepts for use cases also outside the specific scenario of the biogas plant, helping to achieve a further sustainable tech-supported transformation.

7. Challenges and gaps

This section identifies key technical and operational barriers that limit the deployment of AI-based monitoring systems. It focuses on sensor reliability, data quality, model transferability, and interpretability. These issues are discussed in relation to long-term industrial use. **Figure 4** illustrates the systemic barriers hindering the deployment of AI in bio-energy monitoring, starting with sensor inaccuracies and data scarcity that compromise model reliability.

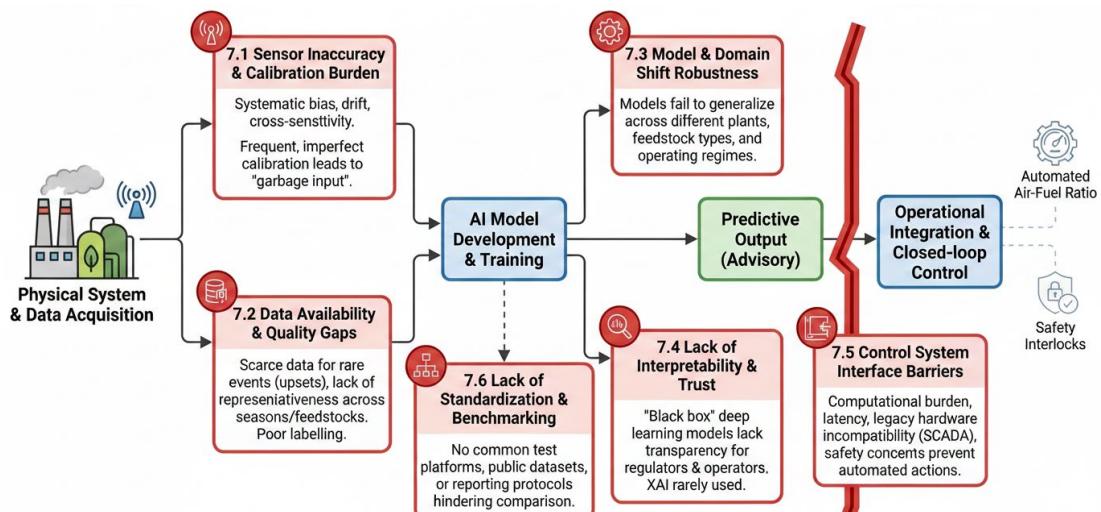


Figure 4. The "Pipeline of Barriers" in AI-Based Bio-Energy Monitoring

These upstream flaws, combined with poor cross-site generalization and a lack of interpretability ("black box" issues), create a trust gap for operators and regulators. Consequently, these technical and safety constraints prevent the integration of predictive AI into real-time, closed-loop control systems.

7.1. Accuracy of the sensors and burden of calibration

Affordable sensors are the preferred choice for high-density monitoring, but suffer from systematic bias, drift and cross-sensitivity. These problems result in non-robust datasets unless the calibration is accomplished frequently. Many studies continue to use ad hoc calibration procedures or do not consistently follow best practices (such as regular co-location with reference instrumentation or correction model based on transfer learning). If calibration is less than perfect, downstream ML models may be fed garbage input and will produce biased estimates or low confidence in predicted emissions or anomaly alerts. Inter-instrument calibration inconsistency further hampers inter-site comparison and long-term deployment reliability. The manuscript's power lies in its symptomatic dealing with calibration problems. This section covers all aspects of sensor drift, cross-sensitivity and long-term stability issues that could indirectly affect AI models due to inappropriate calibration. The emphasis on hybrid-sensor networks and AI assisted recalibration is indicative in pragmatic constraints for field deployment.

7.2. Availability, representativeness and labelling of data

Reliable datasets representing a wide spectrum of the feedstocks, seasonal variations, and process upsets are still scarce. The bulk of the works presented in the literature are based on data collected at one plant or equivalent short campaigns. For this reason models trained using a narrow scope generally does not generalize at other plants. In particular, the lack of labelled data for rare events such as digester upsets, combustion faults, or emission spikes is severe. This hampers the design of reliable classification and anomaly detection methods. Further systematic sampling, long-term observation and experiment are required to acquire representative data sets.

7.3. Robustness to model and domain shift

Design and operational characteristics of bio-energy systems differ widely in terms of style, size, and feedstock type, leading to a common source-shift issue. Models that work adequately with one feeding regime, feed energy types (mob and roughage balance), moisture/energy content may not behave as such when feed mix/feed energy types, load patterns, or environment conditions change. There is a growing body of knowledge in transfer learning, domain adaptation and physics-guided model designs, but very few such techniques are used in practice. Dealing with domain shift is necessary to construct models that are robust across plants and for extended operating periods. Here, the manuscript offers a transparent and rigorous examination of domain shift due to variations in feedstock, plant design, operation regimes or environmental conditions. The discussion reveals why models trained on site-specific data tend to generalize poorly and emphasizes that transfer learning and physics-informed methodologies are necessary for cross-site robustness.

7.4. Interpretability and regulatory acceptance

Regulations are focused on transparent and traceable decision processes. Interpretations via models like tree-based models result in partial interpretability via feature importance; however, many modern high-performing deep learning frameworks act as black boxes. Methods of XAI - For instance SHAP, counterfactual reasoning or structured surrogate models are scarcely used in emissions work. It's hard, though for operators and regulators to trust in AI-provided advisory without easy insight into why it made various predictions, especially if actions could impact a company's compliance with the law or safety.

7.5. Interface to control systems and decision process

Most of the reported work is predictive rather than closed-loop control. One subset are those that have some form of integration with AI predictions and automated actions, such as air-fuel ratio changes, digester feeding pattern changes, or the initiating safety procedures. Real decision-friendly workflows are built on trustworthy models, verified control strategies and intuitive operator interfaces. Fully integrated AI-control system demonstrations are limited, and there is still work left to be done in converting predictive outputs into operational guidance that can be acted upon.

Despite several studies with excellent predictions, few applications pass from a simple prediction to closed-loop operational control in the bio reporting area of air pollution assessments powered by bio-energy. A primary obstruction is computational burden; more sophisticated models, especially deep learning based and compositional sensitive-rigorous method could infeasible under the real-time control time frame or incompatible with the legacy plant hardware. Integration into existing systems is yet another challenge to overcome, as the AI model has to reliably communicate with supervisory control and data acquisition (SCADA) systems, programmable logic controllers and safety interlocks all of which require deterministic response time and high fault tolerance. Data latency, sensor fault and the necessity of periodical recalibration also bring great concerns to be in use under a dynamic plant environment. From an organizational point of view, mechatronic service operators and regulators may need explicit decision logic and reliable fail-safe mechanisms to authorize AI-exerted control actions. These are the reasons why most of the works reported in the literature never go beyond advisory or alarm-based systems, and motivate the pursuit than lightweight, interpretable models, edge-computable/adjustable computations, and incremental human-in-the-loop control strategies can be practical paths towards closed loop adoption.

7.6. Standardization and benchmarking

The lack of common test platforms hinders progress on the comparison of algorithms, validation of claims, and determination of best practices. Different types of sensors, pre-processing of data, evaluation of the models, and reporting hinder the ability to judge what methods carry over across contexts. Common tasks, public data sets, and clearer reporting instructions would improve replication and facilitate the generation of new methods. Creating such benchmarks is a necessary step in an effort to establish robust, comparable work in AI-based bio-energy monitoring.

The lack of available data is partially compensated by a few new initiatives that contribute with partial benchmarks for AI-based monitoring on bio-energy and in environmental systems closely related to it. These span from plant-specific open data provided with particular studies, over synthetic / semi-synthetic benchmarks derived from process simulations, to domain-adjacent repositories established for air-quality prediction, biogas production, or industrial emissions monitoring. Although such resources are still fragmented and not standardized, they depict realistic avenues for reproducible evaluation. Prospective research could in practice help bridge this gap by publishing calibrated multi-sensor datasets with well-defined operating scenarios, embracing common evaluation criteria and providing to be used as reference selected baseline results for facilitating comparative analysis across the studies. Cooperative benchmarking using field-data from numerous bio-energy facilities, enabled by shared pre-processing and validation pipelines, would enhance model generalization to new sites, and greatly reduce the time from site-specific pilot demonstrations to deployable monitoring systems.

8. Research priorities and recommendations

This section proposes research directions aimed at improving the robustness and applicability of AI-based pollution monitoring. Priority areas include data availability, calibration practices, and hybrid modelling approaches. The recommendations are grounded in the gaps identified earlier.

8.1. Open benchmark datasets

Development in AI for emissions is hindered by the absence of openly available high-quality datasets. A priority is to develop multi-site, multi-sensor data collections with co-located reference measurements provided for e.g. CH₄, CO, NO_x, PM and VOCs. The operational meta information for these datasets should also be available, that is, feedstock properties, load pattern and biogas plant conditions as well as timestamps, of what was referred to in Sect. Such resources would facilitate benchmarking of algorithms, provide for replicability and assist in discovering methods that generalize to a range of bio-energy systems.

8.2. Calibration and transfer learning pipelines

Affordable sensors need to be calibrated regularly in order to stay consistent over time. Automatic algorithms with drift correction, cross-sensor transfer learning, and context-aware recalibration would alleviate the manual burden on operators and increase data reliability. Research in this field should then look into scalable methods to adapt calibration models on the sensor aging and, possibly, environmental changes. This would also help to standardize practices across different sites if these pipelines are made open and modular.

8.3. Physics-aware and hybrid modelling

Combining knowledge based on physical process and machine learning is a trend to enhance robustness under varying operating conditions. Hybrid approaches are able to incorporate mass-balance relationships, thermodynamic laws or reactor kinetics into the learning process, making the approach's performance less dependent on large sets of data and enhancing extrapolation capabilities as feedstock or load conditions vary. Further research is also needed to develop generally applicable frameworks that trade off physical limitations against data-driven flexibility.

8.4. Explainability for regulatory use

AI models need to be transparent, and predictions must have uncertainty estimates to be deployable in regulation/operation. Interpretability tools specific to emissions surveillance – e.g., structured surrogates, feature attribution methods, and uncertainty bands – should be automatically appended to model pipelines. This would explain to operators why a model had made a given prediction and give regulators the certainty needed for decisions on compliance.

8.5. Closed-loop field trials

However, in current deployments, a gap between modelled and active control is left out after the prediction step. Field tests are necessary to make links between AI predictions and actual control actions, for example, modulating air–fuel ratios, changing feedstock blends or actuating ventilation systems. These tests need to account for emissions reductions as well as operational both fuel consumption, stability and maintenance burden. There would be clear case studies as an example to stimulate it in industry.

9. Conclusion

This review presents a comprehensive and process-integrated analysis of AI-based pollution monitoring across the complete bio-energy production chain, spanning biomass handling, anaerobic digestion, thermochemical conversion, and biofuel refining. The discussion shows that artificial intelligence, when combined with modern sensing systems and data pipelines, can significantly improve real-time emission estimation, short-term forecasting, and anomaly detection under highly dynamic operating conditions. Such capabilities are essential for regulatory compliance, process stability, and the reduction of environmental impacts associated with bio-energy systems. The review also highlights that current progress is constrained by practical challenges, including sensor drift, inconsistent calibration practices, scarcity of representative

multi-site datasets, and limited robustness of models under domain shift. While advanced machine learning and deep learning models demonstrate strong predictive performance, their deployment remains limited by issues of interpretability, transferability, and weak integration with operational decision-making and control systems. Hybrid and physics-informed AI approaches emerge as a promising pathway to address these limitations by embedding process knowledge into data-driven models and improving reliability under variable conditions. Future research should prioritize the development of open benchmark datasets, standardized calibration and validation protocols, and explainable AI frameworks suitable for regulatory use. Equally important is the transition from prediction-focused studies to closed-loop, field-tested implementations that directly link AI outputs with operational control actions. Strengthening these areas will support the translation of AI-based pollution monitoring from experimental demonstrations to reliable industrial practice, contributing to cleaner bio-energy production and measurable progress toward sustainable energy and climate objectives.

Author Contributions

Madhuri Karad conceptualized the study, coordinated the review framework, and contributed to structuring the manuscript and synthesizing the literature across the bio-energy production chain. **Nidhi Sharma** contributed to the analysis of sensing technologies, data acquisition methods, and environmental monitoring practices, and assisted in drafting the corresponding sections. **Khaja Gulam Hussain** contributed to the review of AI algorithms, hybrid and physics-informed modelling approaches, and evaluation metrics used in pollution monitoring studies. **Vakiti Sreelatha Reddy** supported the discussion on instrumentation, sensor characteristics, calibration challenges, and regulatory aspects related to environmental monitoring. **Madhuri Ghuge** contributed to the sections on data preprocessing, machine learning pipelines, and benchmarking practices, with emphasis on practical deployment issues. **Sagar Arjun Dalvi** assisted in compiling application case studies across biomass processing, anaerobic digestion, combustion, and biofuel refining stages. **Rupesh Gangadhar Mahajan** contributed to the critical analysis of challenges, research gaps, and future research priorities, and reviewed the manuscript for technical consistency. **Shital Yashwant Waware** and **Anant Sidhappa Kurhade** supervised the overall study, provided methodological guidance, refined the technical content, and performed final review and editing of the manuscript. All authors read and approved the final version of the manuscript.

Abbreviations

Abbreviation	Full Form
AI	Artificial Intelligence
ML	Machine Learning
DL	Deep Learning
IoT	Internet of Things
SDGs	Sustainable Development Goals
GHG	Greenhouse Gas
PM	Particulate Matter
PM _{2.5}	Particulate Matter $\leq 2.5 \mu\text{m}$
PM ₁₀	Particulate Matter $\leq 10 \mu\text{m}$
NO _x	Nitrogen Oxides
SO ₂	Sulfur Dioxide
CO	Carbon Monoxide
CO ₂	Carbon Dioxide
CH ₄	Methane
VOCs	Volatile Organic Compounds
NDIR	Non-Dispersive Infrared

EC	Electrochemical
FTIR	Fourier Transform Infrared Spectroscopy
GC	Gas Chromatography
ANN	Artificial Neural Network
SVM	Support Vector Machine
LSTM	Long Short-Term Memory
XGBoost	Extreme Gradient Boosting
AutoML	Automated Machine Learning
RMSE	Root Mean Square Error
MAE	Mean Absolute Error
R ²	Coefficient of Determination
XAI	Explainable Artificial Intelligence
SCADA	Supervisory Control and Data Acquisition
GIS	Geographic Information System
UAV	Unmanned Aerial Vehicle
LCA	Life Cycle Assessment

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Conflict of interest

The authors declare no conflict of interest

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