

## RESEARCH ARTICLE

# AI Models for Life-Cycle Assessment of Bio-Energy Technologies and Pollution Quantification

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## ARTICLE INFO

Received: 12 December 2025  
Accepted: 6 January 2026  
Available online: 20 January 2026

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## ABSTRACT

Bio-energy systems are frequently promoted as low-carbon substitutes for fossil fuels and are closely related to SDG 7 (Affordable and Clean Energy) and SDG 13 (Climate Action). Actual environmental performance, however, is contingent on supply-chain design, choice of feedstock, set-up of the technology and local operating conditions. The life-cycle assessment (LCA) is currently the predominant scientific instrument for assessing these impacts in a comprehensive approach linked to SDG 12 Responsible Consumption and Production. Traditional LCA, however, has to deal with a variety of challenges including data scarcity, spatial and temporal variations, and the necessity to analyze several scenarios depending on changing circumstances. In recent years, some of these limitations can be mitigated by using artificial intelligence (AI) and machine learning (ML) techniques. This approach facilitates inventory data extrapolation, gap filling and estimation of the nonlinear function between process variables and environmental parameters, all leading to more dynamic and data rich assessment which reflects SDG 9 (Industry, Innovation and Infrastructure). This review consolidates a summary of up-to-date studies on AI-enabled LCA approaches for bio-energy systems and pollution assessment methods that interface directly with sustainability evaluation. The paper describes a general description of key aspects related to bio-energy supply chains in LCAs

regarding impact categories, including greenhouse gas (GHG), air pollutants, land use and water use with relevance to SDG 6-Clean Water and Sanitation and SDG 15-Life on Land. It subsequently provides an overview of AI and ML applications covering the full bio-energy life cycle, including aspects related to biomass resource assessment and feedstock production as well conversion, upgrading, refining, distribution to end use. Particular focus is given to works that integrate ML with LCA metrics for the prediction of environmental performance or for the optimization of process conditions through sustainability-based indicators. The review also presents AI-facilitated pollution monitoring applications, such as deep learning techniques for emissions detection using remote sensing data, carbon emissions prediction, and air quality monitoring through ML for betterment of SDG 11 (Sustainable Development Goals: Sustainable cities and communities). Major challenges including model interpretability, system boundary consistency, uncertainty propagation and hybrid modelling requirements have been identified. Next, AI focusing on digital twin, scenario analysis supported by AI and interactive LCA tool for informed decision making.

**Keywords:** bio-energy; life-cycle assessment; artificial intelligence; machine learning; pollution quantification; emissions monitoring; remote sensing

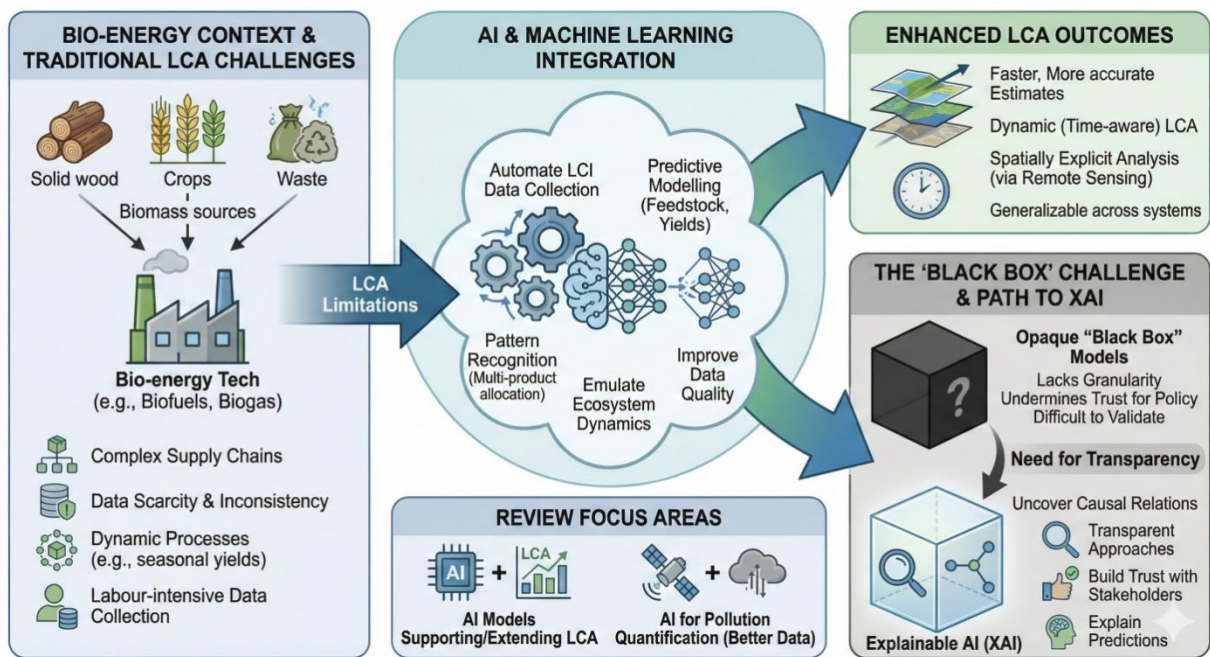
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## 1. Introduction

Bio-energy technologies (solid biomass, biogas, bioethanol, biodiesel, advanced bio-oils) are an essential component for many decarbonization pathways – especially in hard-to-electrify sectors such as heavy industry; aviation and shipping. But the climate and environmental benefits of bio-energy are not a no-brainer. They rely on LUC, fertilizer, feedstock logistics, conversion efficiency, by-product use and a point of use emission control. This weight is imposed by bringing LCA from the cradle to grave and comparing these impacts between Bio-energy options, fossil and other renewable systems. Although useful, classical LCA methods face great difficulty in addressing the complexities, data rich nature and dynamicity of bioenergy systems: such shortcomings can potentially be addressed by artificial intelligence (AI) and machine learning <sup>[1]</sup>. For example, machine learning can help improve data quality and facilitate more realistic LCA modelling by analyzing large-scale environmental datasets and emulating ecosystem dynamics <sup>[2,3]</sup>. This combination of machine learning and LCA allows one to deal with uncertainties in the data and employ less efforts than traditional inventory gathering <sup>[4]</sup>. ML facilitates the automatic calculation of CFs, increases precision of impact estimations, and closes typical data gaps in classical LCA background datasets <sup>[5–6]</sup>. In bioenergy, ML allows fast prediction of environmental impacts. Configuration when multiple-products make allocation difficult <sup>[1–2, 7]</sup>. It also assists in the evaluation of biomass properties, conversion efficiency and fuel characterizations that are generally challenging to be measured directly and hence more comprehensive evaluations <sup>[8]</sup>. These attributes potentiate assessments along the complete bio-energy chain; from feedstock growth to end use <sup>[2]</sup>.

**Figure 1** illustrates how implementing AI technology can benefit these existing challenges and strengthen the traditional practice of bio-energy LCA. In particular, it facilitates analysis interpretation from data scarcity and chaotic system complexity that arise when conducting such disclosure, since this structured learning improves our understanding of complex interrelationships. It's also a wake-up call to move away from black-box opaque algorithms and toward Explainable AI (XAI), because transparency and causal transparent is critically important for sensible environmental policy.

LCA of bio-energy remains difficult due to spatially dispersed feedstock chains, strong dependence on local and seasonal conditions, and inconsistent system boundaries across studies. AI and ML support feedstock prediction, process optimization, and direct estimation of inventory flows and impact indicators, reducing data gaps and computational effort <sup>[1]</sup>. Many existing black-box models lack transparency and process-level detail, which limits traceability and robust attributional or consequential LCA <sup>[7,9]</sup>. This highlights the need for explainable AI to improve interpretability, trust, policy relevance, and model generalization under data scarcity and uncertainty <sup>[10–15]</sup>.



**Figure 1.** Framework for Integrating Artificial Intelligence into Bio-energy Life Cycle Assessment (LCA)

In addition, advances in deep learning and remote sensing analyses are revolutionizing how emissions and air pollutants are tracked across space and time, allowing for LCAs of bio-energy projects that can be both dynamic (in time) and spatially explicit.

This review focuses on these two intersecting themes:

- AI models that support or extend LCA of bio-energy technologies.
- AI models for pollution quantification that can supply better emission data to LCAs.

Differences in depth by life-cycle stage reflect the distribution of extant work, not scope imbalance. Conversion technologies and pollution monitoring are emphasized more as there is a relatively greater volume of literature in the field with richer data and more diverse methodologies, especially for AI/machine learning. These perturbations also facilitate a direct connection between operational conditions and environmental effects. Other life-cycle phases are presented more summary-like due to still scarce data and evidence on dedicated AI studies. Such view considers the whole life-cycle, though it is consistent with level of maturity of current literature.

The review progresses with a systematic approach in the selection of studies for comprehensiveness and reproducibility of this review, meeting study scope criteria on artificial intelligence applications to LCA and pollution quantification from bio-energy systems. Peer-reviewed articles were searched through extensive searches on main scientific databases (Scopus, Web of Science and ScienceDirect). The timescale of the literature reviewed mainly includes publications from 2010 to 2025, as these data-driven and AI-assisted LCA methods have been increasingly researched in this period.

The following criteria were used to select studies: (i) explicit use of artificial intelligence or machine learning, (ii) specific connection with life-cycle assessment, life-cycle inventory construction or procurement procedure method impact assessment pollution analysis for bio-energy systems; and (iii) detailed methodological information provided so that the model structure and context can be interpreted. Review or extended abstracts, methodological concepts and some selected high-impact cases were incorporated to ensure a balance between the theoretical progress and applied enhancements. Conference abstracts, non-peer-reviewed reports, and studies without clear method descriptions were excluded.

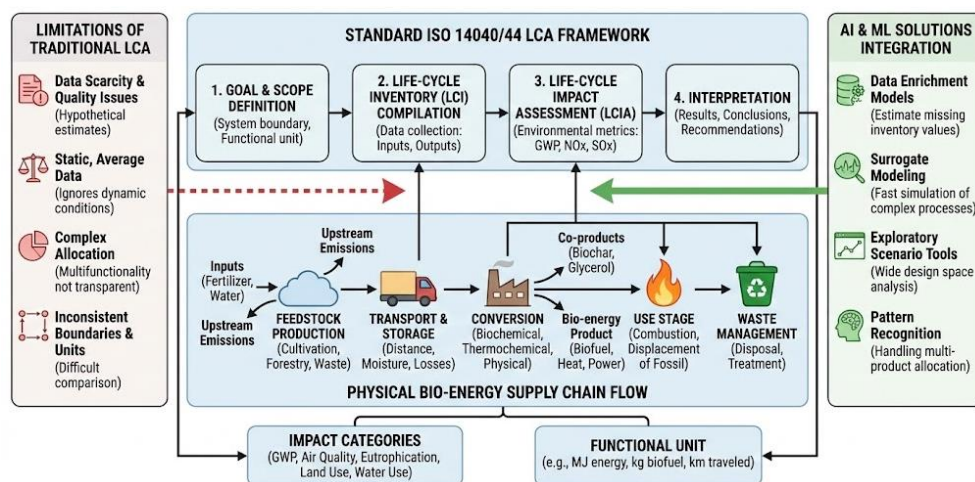
The references were classified based on the main contribution they have to bio-energy life-cycle: feedstock production, logistics, conversion processes and end-use emissions calculation, direct LCA indicator prediction. Another categorization was made in terms of type of AI model (i.e., regression and tree-based methods), artificial neural networks, deep learning, probabilistic models, explainable AI). This two-dimensional classification allows for a methodical comparison of methodologies' trends, domains of applications and identified research gaps in the reviewed source literature.

## 2. Life-Cycle Assessment of Bio-Energy systems

### 2.1. Standard LCA framework

The ISO-based LCA framework provides a structured approach to evaluate environmental impacts of bio-energy systems from resource extraction to final energy use. It consists of four stages: goal and scope definition, life-cycle inventory (LCI), life-cycle impact assessment (LCIA), and interpretation. In bio-energy studies, system boundaries generally include all stages that influence the overall environmental burden of the fuel or product. The biofuel life cycle begins with feedstock production, including crop cultivation, forestry, residue recovery, and waste handling. These steps determine land use, input requirements such as fertilizers and water, and upstream emissions. This is followed by transport and storage, where distance, moisture content, and handling conditions affect energy demand and losses. Biomass then undergoes pre-treatment and conversion through biochemical, thermochemical, or physical routes, each with distinct material flows and energy efficiencies. Final use involves combustion or application of the bio-energy product, leading to direct emissions and potential displacement of fossil fuels [16].

Conversion pathways such as combustion, gasification, pyrolysis, anaerobic digestion, fermentation, and transesterification differ in efficiency, emissions, and co-product generation, making this stage central to LCA comparisons. Waste recovery includes management or beneficial use of residues, which may add or offset environmental burdens [16]. Functional units, commonly expressed as MJ, kWh, or mass of fuel, enable consistent comparison across systems [17,18]. For example, bioethanol comparisons with gasoline often rely on energy content or vehicle distance rather than volume to reflect performance differences [19]. Co-products such as biochar, digestate, and glycerol influence burden allocation and system credits. The ISO 14040/44 standards of the International Organization for Standardization provide guidance for impact assessment and result interpretation [20]. Impact categories typically include global warming, air pollution, eutrophication, acidification, land use, biodiversity, water use, and ecotoxicity. Despite this, selecting an appropriate functional unit remains challenging due to the multifunctional nature of biorefineries, which limits direct comparison across studies without harmonization [21–25].



**Figure 2.** Standard Bio-Energy Life Cycle Assessment (LCA) Framework and Supply Chain



The **figure 2** illustrates the ISO-standardized LCA stages—Goal, Inventory, Impact, and Interpretation—applied across the full bio-energy lifecycle, mapping the physical flow from feedstock cultivation to final energy use. It underscores the relationship between life cycle operational stages and environmental impact categories while pointing out key methodological constraints such as complexity of allocation, or data paucity that influence assessment reliability.

## 2.2. Limitations in traditional Bio-Energy LCAs

Numerous studies have identified common shortfalls in the use of classical LCA methodology for bio-energy systems. One of the main limitations is the lack of standard units, which do not allow comparison between trials. Multipurpose-application is usually only partially taken into account, even if more than one co-product such as heat, biochar or glycerol is involved. Decisions concerning allocation or system extension heavily influence outcomes, but are not always well documented. Moreover, the accuracy of LCA results is critically dependent on data quality and availability, and due to lack of access to primary industrial information (in most studies) could be based on hypothetical assumptions or laboratory-scale calculations <sup>[16]</sup>. Consequently, LCAs of the same bio-energy pathways can vary to a large extent and cast doubts about their utility in informing policy or investment <sup>[26]</sup>. Many biorefinery LCAs also present limited value-chain data, generic datasets not including uncertainty analysis or overlooking important impact categories, reducing the confidence in the results <sup>[27]</sup>. Standard LCAs concentrate on a subset of indicators (primarily greenhouse gas emissions) with little attentiveness to land-use change, biodiversity and water-related effects. They also assume average spatial and temporal characteristics, whilst there is strong regional and seasonal variability in yields, emissions and land impacts. The inability to explore multiple scenarios is largely due to static databases and computational intensity, even though bio-energy systems are dynamic and transforming rapidly. The flexibility of determining system boundaries, co-product treatment and allocation under ISO standards makes the comparison between studies even more troublesome and inconsistent results appear even for similar pathways <sup>[11,28]</sup>. These methodological variances diminish the reliance on LCA for policy-relevant findings, as noted in previous reviews <sup>[16,29]</sup>. These gaps can be addressed through practical applications of artificial intelligence, such as enriching absent inventory data, model surrogate for complicated processes or facilitating fast exploration design space. Such methods bring versatility and rigor into consideration, which is not normally the case in classic LCA methodologies.

**Table 1.** Summary of the Standard LCA Framework and Key Limitations in Bio-Energy Assessments

Key Point	Description	Key Processes / Factors	Environmental Indicators Affected	LCA Challenges Identified	Notes / Examples
Goal & Scope Definition	Defines purpose, system boundary, and functional unit for bio-energy assessment.	Feedstock production, conversion stages, use phase, and waste handling.	All impact categories depending on boundary decisions.	Inconsistent functional units; incomplete boundary definitions.	Functional unit often MJ, kWh, or kg biofuel.
Life-Cycle Inventory (LCI)	Compilation of input–output data across the bio-energy chain.	Crop cultivation, fertilisers, water use, residues, transport, storage.	GHG emissions, nutrient runoff, land occupation, water consumption.	Data gaps, use of generic datasets, limited industrial data.	Many studies rely on secondary lab-scale data.
Life-Cycle Impact Assessment (LCIA)	Translates inventory flows into environmental indicators.	Combustion, gasification, pyrolysis, digestion, fermentation, transesterification.	GWP, eutrophication, acidification, NO <sub>x</sub> , SO <sub>x</sub> , CO, PM, biodiversity, ecotoxicity.	Narrow focus on GHGs; limited land-use change and spatial–temporal detail.	Water use, biodiversity often omitted.

Key Point	Description	Key Processes / Factors	Environmental Indicators Affected	LCA Challenges Identified	Notes / Examples
Interpretation	Analyses results, checks consistency, identifies uncertainties.	Scenario comparison, sensitivity checks, uncertainty evaluation.	All indicators included.	High variability of results; low transparency in assumptions.	ISO flexibility reduces comparability.
Multifunctionality & Co-Products	Handling of multiple outputs such as biochar, digestive, glycerol, heat.	Allocation, system expansion, fossil fuel substitution.	GHG balance, energy credits, land-use offsets.	Inconsistent allocation rules; weak justification.	Co-product method strongly influences results.
Structural Limits & AI Needs	Conventional LCA is static, data-heavy, and slow.	AI-based data enrichment, surrogate models, scenario exploration.	Potential to improve all indicators.	Missing data, static modelling, high computational cost.	ML surrogates mimic complex models efficiently.

**Table 1.** (Continued)

The main steps of the ISO-compliant LCA framework used for bio-energy systems and the related environmental indicators and methodological issues are summarized in **Table 1**. It delivers an abridged comparative snapshot to illustrate where conventional LCAs are limited and which analysis gaps still exist.

### 3. AI and machine learning techniques relevant to LCA

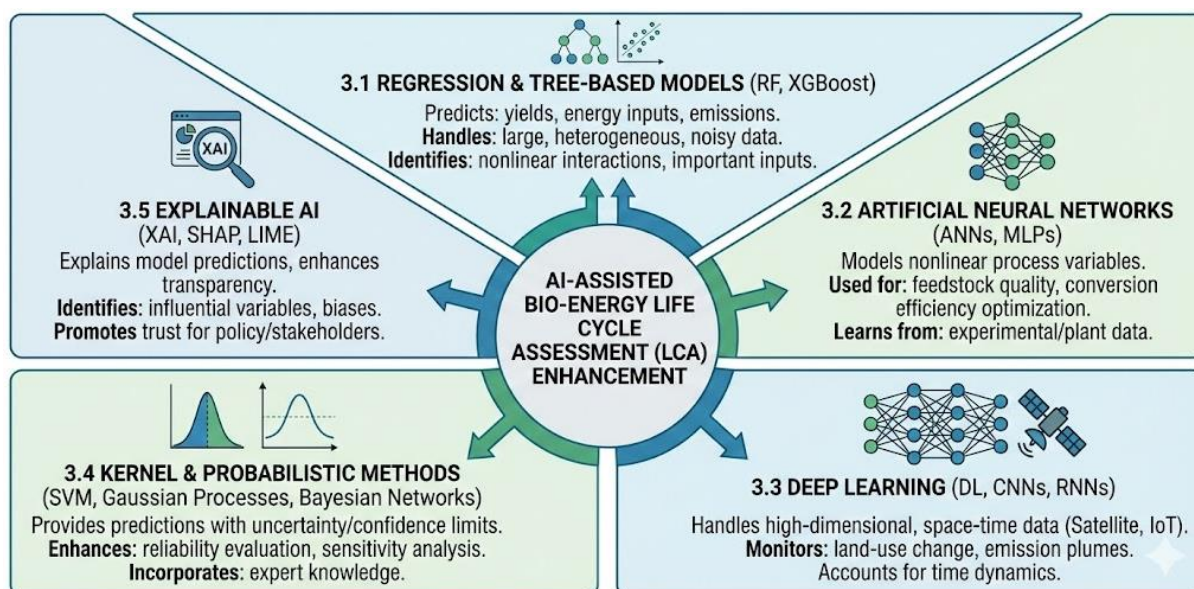
The **figure 3** groups the main AI methodologies—from regression and tree-based models, for instance used to predict yield, to deep learning applied in spatial analysis—by a generic class of function they play in life cycle assessment. It also shows how various algorithms accommodate distinct needs, e.g., employing neural networks for tracking complex process optimization as opposed to probabilistic methods in estimating uncertainty and risk. Lastly, it emphasizes the importance of Explainable AI (XAI) in establishing the validity of these models and bringing transparency to those making real life decisions.

#### 3.1. Regression and tree-based models

Regression and tree-based techniques are commonly used to predict crop yield, energy input, emissions and bio-oil outputs in bio-energy systems. Ensemble models including the random forest, gradient boosting and XGBoost are able to address heterogeneous, large-scale data sets with non-linear couplings between feedstock, climate and operations variables. Regularized and stacked ensembles decrease noise and enhance robustness while recovering critical influences on environmental effects <sup>[30]</sup>. Support vector machines help implement classification and predication with small samples, which contribute to inventory estimation and LCIA if only little empirical information is available <sup>[1,4,9,31]</sup>.

#### 3.2. Artificial Neural Networks (ANNs)

ANN are used when strong non-linear relationships between process variables and environmental responses occur. MLP have been applied in biodiesel and bioethanol studies to correlate quality of the feedstock, process conditions, type of catalyst used, to conversion efficiency and emissions for optimization or life-cycle inventory purposes. Recurrent and convolutional networks solve time-series and image data, both of which are now emergent in operational data and remote sensing as the field of LCA matures <sup>[1]</sup>. ANNs have also been employed to predict the biomass pyrolysis activation energy, enhancing comprehension of thermal decomposition and making it possible to estimate better efficiency and pollutant generation w.r.t. different conditions <sup>[32]</sup>. The capacity to learn complex patterns from data by avoiding prior assumptions in form of equations favor ANNs to predict conversion and stability in biodiesel and numerous thermal processes involving many concomitant parameters <sup>[33–35]</sup>.



**Figure 3.** Classification of AI and Machine Learning Architectures for Bio-Energy LCA

### 3.3. Deep Learning (DL)

High-dimensional and space-time data are particularly suitable for methods based on deep learning. Deep learning applied to pixels from satellite images can be used to estimate the supply of biomass, observe land use change and track emission plumes stemming from bio-energy plants. Models based on sequences (like recurrent networks) encapsulate the time-varying nature of emissions, power generation, and plant efficiency, which conventional LCAs tend to simplify <sup>[36]</sup>. This enhances the resolution in time of the estimates of environmental impact, which is crucial for bio-energy systems characterized by variable feedstock quality and operating conditions. The fusion of classical and deep neural architectures with Ios and mobile inferencing provides real time data driven LCA analysis, continuous environmental monitoring <sup>[37]</sup>.

### 3.4. Kernel and probabilistic methods

Predictions are made with quantified uncertainty based on kernel-based methods (e.g. support vector machines) and probabilistic models (e.g. Gaussian process regression). Such methods yield confidence intervals to the environmental indicators, which is useful in LCA since inventory data frequently are uncertain because of regional variation, measurement constraints and small sample sizes. Sensitivity analysis is used to investigate inputs that dominate overall uncertainty and guides focused data collection for improved robustness. Probabilistic graphical models, and in particular Bayesian networks represent dependencies over life-cycle stages, allow for uncertainty propagation and scenario analysis, including incorporation of expert knowledge on drivers of the scale of land use change <sup>[38]</sup>. In general, probabilistic ML techniques can tackle both epistemic and aleatory uncertainty issues by providing distributions of possible values other than point estimations in enabling more risk-informed decisions in bio-energy LCA <sup>[1]</sup>.

### 3.5. Explainable AI (XAI)

Explainable AI techniques reveal why models achieve certain predictions, which is crucial for AI-supported LCA. Techniques such as SHAP and LIME offer insight into how specific input features affect emissions, energy demand or land-use impacts that can be verified against well-known physical and process principles <sup>[39,40]</sup>. This transparency builds trust, assists in identifying biases, and facilitates communication with non-specialist stakeholders – particularly when the outputs of an AI model are informing bio-energy policy or industrial planning. New XAI methods such as Shapley values and Relevance propagation have

shown the potential in providing a richer understanding of complex environment processes, taking the analysis further from mere correlation to that of causal investigation <sup>[41–45]</sup>.

**Table 2.** AI and Machine Learning Techniques Used in Life-Cycle Assessment

Technique	Purpose in LCA	Common Models	Key Strengths	Typical Applications in Bio-Energy LCA	Handling of Uncertainty / Nonlinearity
Regression & Tree-Based Models	Predict inventory parameters such as emissions and yields	Random Forest, Gradient Boosting, XGBoost, Laplacian Regression	Manage large heterogeneous datasets; capture nonlinear interactions; identify important variables	EV energy-use prediction, bio-oil yield estimation, feedstock quality classification	Ensemble modelling reduces noise; strong sensitivity analysis capability
Artificial Neural Networks (ANNs)	Map nonlinear relations between process variables and outputs	MLP, RNN, CNN	Learn from plant/experimental data; strong nonlinear prediction ability	Biodiesel/bioethanol conversion efficiency, pyrolysis activation energy, emission prediction	Captures complex patterns without predefined equations
Deep Learning (DL)	Analyse high-dimensional spatial and temporal data	CNNs, RNNs, hybrid ANN–DL models	Extract features from images/time series; model time-varying emissions	Biomass availability mapping, LUC monitoring, time-variant emission modelling	Models dynamic changes often ignored in traditional LCA
Kernel & Probabilistic Methods	Predict indicators with quantified uncertainty	SVM, Gaussian Process Regression, Bayesian Networks	Provide confidence intervals; represent complex dependencies	Sensitivity analysis, land-use change modelling, scenario evaluation	Handles epistemic and aleatory uncertainties; probabilistic outputs
Explainable AI (XAI)	Improve transparency of ML predictions for LCA practitioners	SHAP, LIME, LRP, feature-importance scores	Reveals variable influence; supports verification with physical processes	Identifying emission drivers, policy-oriented LCA, model diagnostics	Explains model decisions; supports ethical and robust decision making

The **table 2** gives a comparative view of major AI and machine learning techniques used in life-cycle assessment, highlighting how each method supports prediction, interpretation, and uncertainty handling. It shows the strengths of models such as regression, neural networks, deep learning, probabilistic tools, and explainable AI for analyzing bio-energy systems. The summary helps readers understand which techniques are suitable for tasks like emission estimation, land-use assessment, scenario analysis, and transparent decision making.

## 4. AI Models across the bio-energy life cycle

### 4.1. The Production of feedstock, land-use and the biomass availability

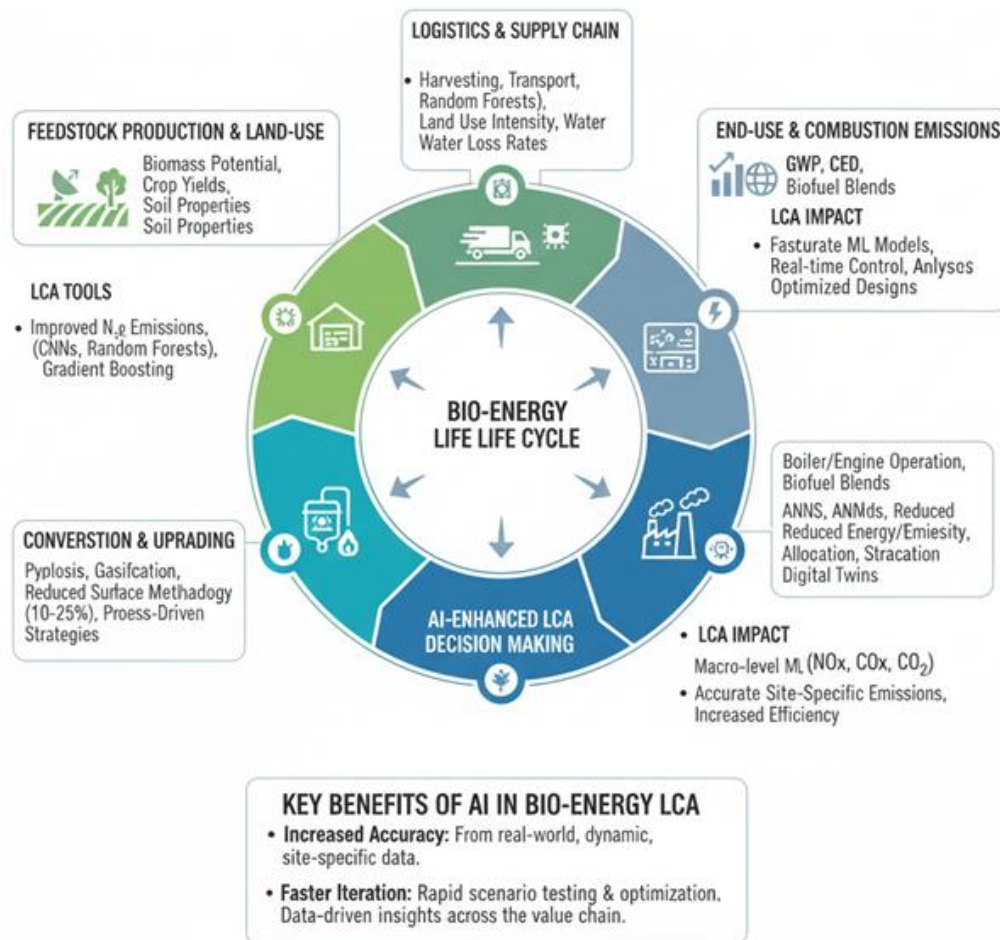
Bio-energy LCAs depend strongly on accurate estimates of biomass potential and upstream impacts. Remote sensing-based machine-learned products provide very stylized spatially and temporally resolved information on crop yields, forest biomass and residue availability. The use of deep convolutional networks and random forests with multi-spectral satellite data (e.g., Landsat or Sentinel) can map biomass patterns and land management. Gradient boosting machines are also applied to estimate soil properties, fertilization requirement and irrigation needs from field measurements and climatic information. The methods contribute to the development of better life cycle inventories for cultivation by improving estimates on soil emissions, particularly N<sub>2</sub>O as result of fertilizer application, and providing more accurate indicators for land use intensity and water consumption. Moreover, farm management can be further optimized as machine learning



algorithms are capable of processing vast amounts of agricultural data such as the weather, soil conditions and yield health to better predict crop growth and yield [3].

## 4.2. Logistics and supply-chain stages

The process of bio-energy chain consists from several subsequent tasks (cutting, gathering, baling or chipping) and interim tools such as storage and final disposable. Tools for AI have now been added to enhance these steps. Route optimization and fleet scheduling algorithms minimize fuel usage and overall transport effort. Stochastic models suggest that biomass moisture content, decay and loss rates during storage will all change. Sensor driven systems in real-time with ML (Machine Learning) algorithms are enabling better inventory tracking and supply predictability. These refinements have an impact on LCA stage results in reducing transportations emissions and updated loss fractions used in inventory calculations. The literature indicates that AI-informed routing has potential to decrease fuel consumption and CO<sub>2</sub> emissions by in the order of 10–25%, with observable reductions in life-cycle burdens per unit delivered bio-energy. For example, machine learning may enhance logistics of biomass supply chain by demand prediction and route optimization where decreasing transportation cost and better inventory management can be achieved [3]. Machine learning application in forest and biomass supply chain management have been proven to provide the powerful tool for sustainable forest management and biomass resources development, solving multifaceted logistics problem for building multi-feedstock – focused lines [46].



**Figure 4.** AI Applications across the Bio-Energy Life Cycle Stages

The **figure 4** maps specific AI interventions to each stage of the bio-energy value chain, from using satellite data for feedstock estimation to optimizing logistics and conversion processes. It highlights how

machine learning enables real-time emission monitoring during end-use and facilitates rapid "screening" assessments by directly predicting environmental indicators like GWP.

### 4.3. Conversion and upgrading processes

AI techniques are emerging for the optimization of conversion pathways such as pyrolysis, gasification, hydrothermal liquefaction (HTL), fermentation and transesterification in bio-energy production. Model-based machine learning couples process parameters (i.e., temperature, residence time, catalyst type and biomass composition) with product yield, energy use and emissions guiding LCA informed decisions in design. Biodiesel and bioethanol optimization by ANNs and response-surface methods, where the relationship between LCA down streaming chemicals separation process operating conditions required to outcome performance measures, such as efficiency, by-product formation and allocation choices in the product were presented. ML also facilitates the real-time control of fermentation variables and the development of microalgae-based systems. In general, the data-driven optimization makes technical goals consistent with life-cycle indicators (e.g. GHG emissions and cumulative energy demand <sup>[13]</sup>), whereas conventional models conceive most of the aspiration values exogenously or improperly in terms of constraints <sup>[34,47]</sup>.

### 4.4. End Use, combustion and operation emissions

In operation, the AI models predict emissions of boilers, engines and turbines when operating with bio-fuels or mixtures. NO<sub>x</sub>, SO<sub>x</sub>, CO, CO<sub>2</sub> and particulates generation models with fuel composition and operational input are calculated. In the biodiesel–diesel and ammonia–hydrogen systems, they also predict the combustion efficiency of mixed bio-fuel blends and amount levels of unburned hydrocarbons. These factors lead to more accurate accounting of emission profiles in the life-cycle inventory and for nonlinear interactions between e.g., oxygen content, fuel nitrogen, and combustion temperature. Under such an approach, the evaluation of environmental performance of bio-energy system during operation is better consistent and provide a more reliable estimate which extends beyond simple emission factors to site-specific predictions. In addition, corresponding real-time monitoring and control systems based on AI technology are able to vary operational parameters flexibly in order to achieve optimal combustion efficiency and minimize the generation of pollutants; therefore, they can enhance accuracy of LCA by accounting for actual operational conditions <sup>[13]</sup>. Hence, the use of such predictive models represent a significant improvement over static emission factors and can allow for a more accurate approximation of environmental footprints <sup>[3]</sup>. This iterative process forms a feedback loop in which data from operations fine-tune LCA models so as to increase the predictive capabilities of LCA towards future bioenergy projects <sup>[48]</sup>. Intelligent feedback loops of AI-powered digital twins optimize dynamic process control, by promoting generation systems that can automatically adapt the cultivation parameters in real time, according to bioenergy production efficiency and life cycle environmental impact reduction <sup>[49]</sup>. In addition to operational modifications, AI-based inferential sensors could enable on-line monitoring of renewable carbon content in co-processed fuels and can help overcome the difficulty in quantifying renewable carbon without costly offline analyses <sup>[50]</sup>.

### 4.5. Predicting LCA indicators directly

Some of the studies further expand applications of ML methods by considering LCA results as targets themselves. These models predict potential and cumulative impact indicators (GWP, CED etc.) using the design variables, feedstock properties and operational conditions. Macro-level methodologies have been introduced wherein previously published LCA case studies and detailed process simulation are used to learn machine learning (ML) models that can be used to obtain quick environmental assessments of new bio-energy designs. This has been implemented for the bio-oil pathways: food-waste-to-biofuels processes as well as other more general renewable-energy portfolios with biomass. Fast versus full LCA runs It gives a quick alternative for doing complete LCA's, very useful at an early-stage design or in comparative considerations. This predictive component enables fast screening of bioenergy system configurations, which are optimized in

terms of environmental impact, economic viability and technical performance <sup>[51]</sup>. For example, an integrated machine learning model could take databases of HTL, HTC and HTP gasification to integrate with a life cycle assessment (LCA) model to determine global warming potential and energy return on investment <sup>[4]</sup>. These models not only speed up the evaluation but they can also be used to explore high and low cases allowing for the isolation of key design parameters that affect environment performance <sup>[2]</sup>. This delivers a more flexible and iterative design process where the environmental aspects of different choices can be immediately checked and optimized, in support of sustainable bioenergy industry <sup>[52]</sup>.

## 5. Artificial intelligence models for pollution quantitation associated to bio-energy

Estimation of emissions rates and ambient pollutant concentrations are required to quantify pollution. In the case of bio-energy, these are direct stack emissions from biomass plants and system-level emissions for bio-energy being run alongside other generation. The chain of processes from pollution sources to exposure is fortified by AI methods with respect to the detection, and forecast, spatial characterization of pollutants. The **figure 5** illustrates the workflow of using deep learning to process satellite and IoT data for real-time emission tracking and forecasting. These outputs replace static metrics in Life Cycle Assessments (LCA), enabling more accurate environmental impact analysis and informed policy decisions.

### 5.1. Emission plumes, remote sensing, and deep learning

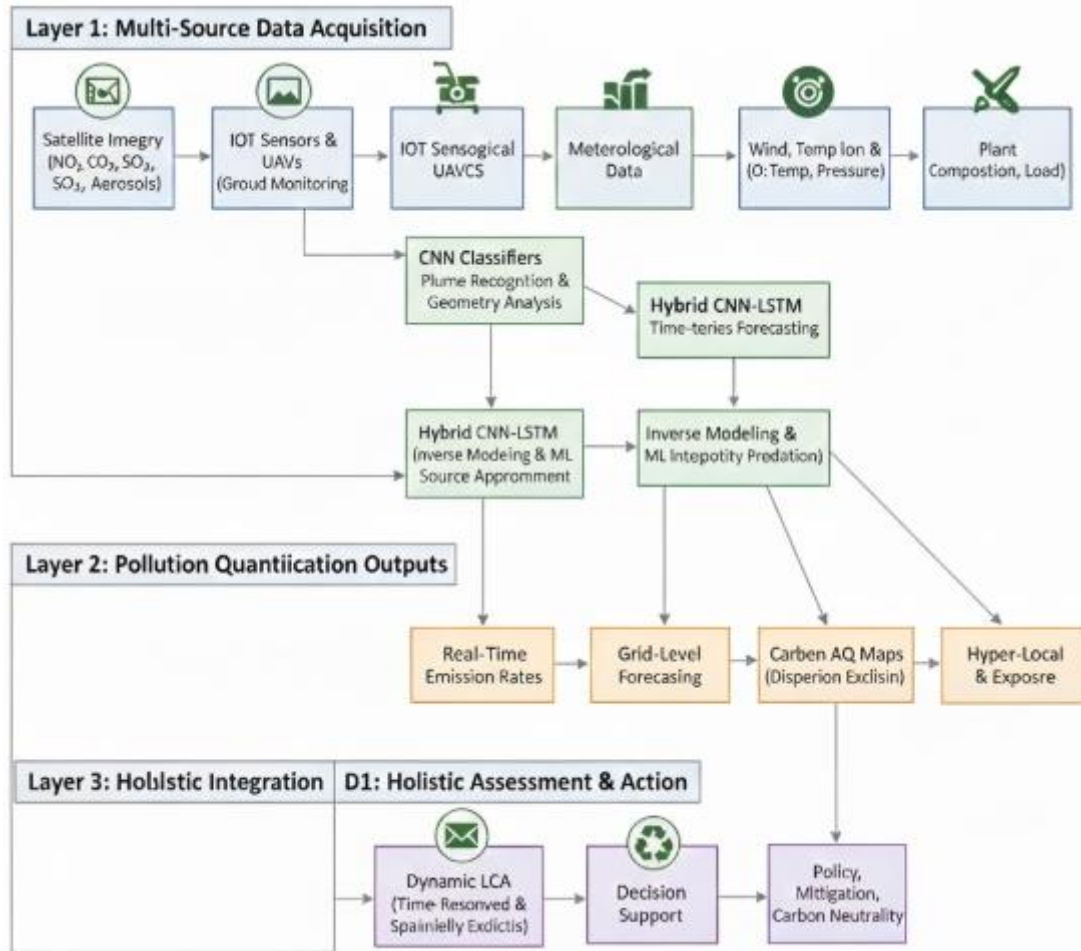
Satellite measurements map a wide range of atmospheric species (NO<sub>2</sub>, CO<sub>2</sub>, SO<sub>2</sub> and aerosols) with good spatial coverage. These datasets can be utilized with deep learning models to detect emission patterns and measure plume intensity. CNN classifiers can recognize plumes of smoke; pinpoint the locations of active combustion and capture features associated with plume behavior. Other approaches deploy CNNs trained on synthetic or field labelled datasets to predict emission flux from plume geometry, density and meteorology. Most research is concentrated on fossil-fuel plants, even though the same methods can be extended to biomass plants. Given plant type and fuel quality, DNNs can predict stack emissions in real time utilizable for emission monitoring over days or seasons. This will enable dynamic LCA on the basis of time-resolved profiles of bio-energy operations instead of static averages <sup>[2, 3, 53]</sup>. Deep learning combined with remote sensing enhances detection of the pollutant and prediction of air quality, as well as alleviates computational constraints associated with conventional inverse models <sup>[36, 54, 55]</sup>. These developments enhance source identification, facilitate targeted mitigation and support countries to build up towards carbon-neutral pathways <sup>[55, 56]</sup>. By combining simulated and measured data, the output CO<sub>2</sub> estimates from PP can be further adjusted and large emitting sources in all sectors are clearly identified <sup>[50]</sup>. Integration of AI and IoT sensors with satellite images is aiding in real-time industrial monitoring, carbon-stock assessment and environmental management decision <sup>[15, 57, 58]</sup>. The fusion of local IoT data with satellite monitoring enhances understanding of environmental (weather) conditions, and feeds multi-model systems for air-quality forecast <sup>[59–62]</sup>.

### 5.2. AI-Based carbon emission forecasting

Short-term carbon emission forecasts at the grid level are particularly useful to understand how different generation sources, including bio-energy, influence system wide emissions. Deep learning techniques, ie hybrid CNN–LSTMs models, have used to forecast the ins CO<sub>2</sub> emissions from past generation data, demand patterns and market signals for fuels.

The same set of forecasting tools can be used for future grid penetrations with significant bio-energy. They complement marginal emission factors in that they provide time-variant carbon intensities for bio-electricity, and are a useful tool to improve prospective LCAs with further spatial and temporal resolution. This contrasts with the commonly used time-invariant grid emission factors and presents a more appropriate image of the environmental burdens from bio-energy in transition power systems. Integration of AI and real-

time carbon monitoring provides a basis for the implementation of global climate decision support in emission control complexity and risk rebounding among industries [57]. This capacity is critical for investment and policy planning in the context of climate neutrality [63]. Integrated AI systems for surveillance and forecasting have been shown to yield higher accuracy over traditional techniques [62] which can lead to evidence-based management decisions, and in some instances automated decisions, that result in carbon savings [64].



**Figure 5.** AI-Integrated Framework for Bio-energy Pollution Quantification and Dynamic LCA

### 5.3. Air quality monitoring and emission dispersion

Pollutants are emitted during the burning of garbage at a bio-energy plant including NO<sub>x</sub>, SO<sub>x</sub>, VOCs and particulate matter, all of which can contribute to local and regional air pollution. AI-based approaches integrate the ground monitoring, satellite observations and meteorological parameters to increase the spatial granularity and temporal frequency of pollutant estimation. ML interpolation models are used to bridge the gaps between the sparsely distributed monitoring centers. Prediction models are established to predict the short-term air-quality indices and estimate the major emission sources with atmospheric dynamic variations. Such AI-based methods can provide a high level of resolution in recognizing the source apportionment, i.e., distinguishing bio energy plants emissions from other industrial or natural related sources for targeted pollution control [64]. Additionally, advanced AI algorithms could use real time sensor data from UAVs and ground-based mobile lab sensor networks to generate hyper-localized AQ maps that are able to be evaluated immediately for any exceedances near bio-energy facilities. Data obtained from such granular analyses guide optimization of operational parameters for environmentally sound and regulatory-compliant oil production [65]. In addition, AI based models can predict the spread of pollutants in different atmospheric conditions that may



provide a predictive understanding of exposure pathways and help in designing more effective stacks heights and emission control devices [14, 57].

Inverse modelling and ML surrogates can help to estimate source strengths and identify hotspots more accurately. This information flow can enter then into LCIA steps characterizing human-health, and (eco) system impact potential, so that spatial exposure aspects are included in the assessment instead of only total emitted mass.

#### 5.4. Linking pollution quantification to LCA

The integration of environmental pollution quantification to LCA depends on a consistent harmonization between model outputs and inventory flows. Emissions estimated from remote sensing observations need to be linked to site life cycle stages that allow the separation of plant operation from upstream transportation or pre-treatment activities. Models may provide temporal profiles to be used for time-sensitive LCIs, for example related to short-lived climate pollutants or seasonal variability in biomass availability and combustion. By doing so, it provides the means to more holistically understand life cycle impacts in a bio-energy supply chain and overcome the static and rounded average approach. In addition, the penetration of machine learning in environmental impact assessments make it possible to predict environmental impacts, optimize land utilization and meet regulatory standards in the process of producing sustainable biomass [3]. This integrated characteristic facilitates the more informative attribution of environment burdens and benefits, thereby improving the credibility and applicability when the LCA study is used for policy-making or technology investment about bio-energy technologies. Such integration is especially important for accounting for non-climate change impacts such as eutrophication and acidification from fertilizer application, and damage categories related to loss of biodiversity which are neglected in conventional analyses [66]. In addition, the AI-guided pollution quantification seamlessly combines with LCA methods enabling spatial explicit characterization factors to be constructed so as to include regional differences in environmental damages, an aspect often overlooked in more general assessments [67]. As such this refined link therefore contributes to a more comprehensive approach on the environmental performance assessment of bio-energy systems, not only limited to simplified impact considerations [68].

**Table 3.** AI Models Used for Pollution Quantification in Bio-Energy Systems

Focus Area	AI Methods Used	Data Sources	Key Functions	Representative Outcomes	Relevance to Bio-Energy
Emission Plumes & Remote Sensing	CNNs, DNNs, Deep classifiers	Satellite data (NO <sub>2</sub> , CO <sub>2</sub> , SO <sub>2</sub> , aerosols), plume geometry	Detect emission plumes, estimate flux, map hotspots	Real-time stack emissions, dynamic LCA profiles, improved plume identification	Useful for biomass plants with variable operating loads
Carbon Emission Forecasting	CNN-LSTM hybrids, DL time-series models	Grid data, load profiles, fuel mixes, market signals	Short-term CO <sub>2</sub> forecasting, trend learning	Time-variant carbon intensities, better prospective LCA resolution	Supports future grids with high bio-energy penetration
Air Quality Monitoring & Dispersion	ML interpolation, UAV-sensor AI models, surrogate dispersion models	Ground sensors, UAV data, meteorology, satellite inputs	High-resolution AQ mapping, pollutant source apportionment	Hyper-local AQ indices, optimized stack design, improved emission control	Distinguishes bio-energy emissions from other sources
Linking Pollution Data to LCA	ML-LCA integration, spatial-temporal ML models	Emission inventories, remote sensing, plant operation data	Align pollution data with LCA flows; build time-sensitive LCIs	More accurate impact categories, regional differentiation, credible LCA outputs	Improves assessments for seasonal biomass and variable load conditions

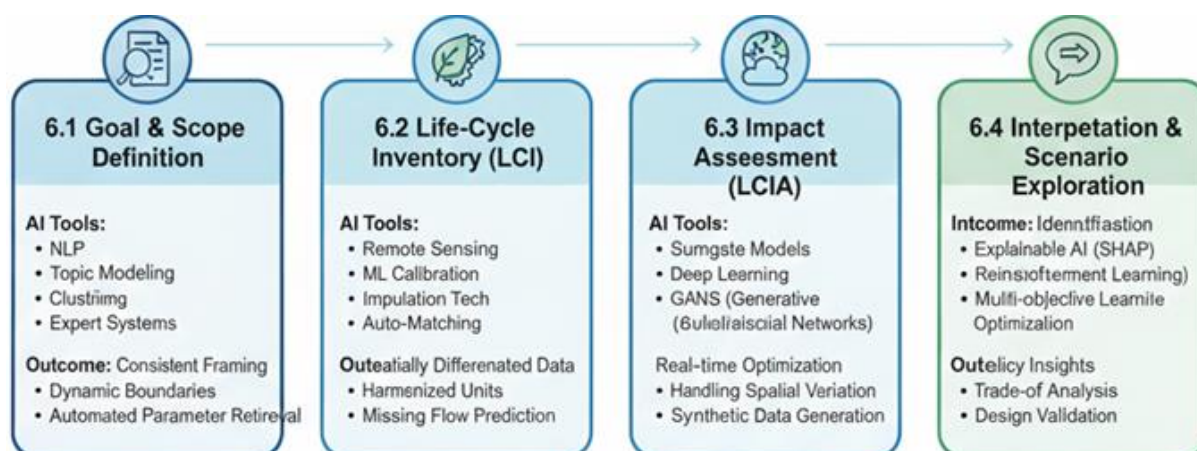
The **table 3** summarizes how different AI approaches support pollution quantification in bio-energy systems by detailing their data sources, functions, outcomes, and relevance to environmental assessment. It highlights the role of deep learning, forecasting models, air-quality mapping tools, and ML–LCA integration in improving emission estimation and impact evaluation.

## 6. Methodological basis for AI-Supported LCA in Bio-Energy

Current research In recent work we introduced structured methods for incorporating AI within LCA and thus enable more detailed, data-rich and adaptive LC These libraries integrate AI tools into the various components of an LCA workflow, including environmental modelling and remote sensing combined with optimization and interpretability. The **figure 6** illustrates the integration of artificial intelligence technologies across the four standard phases of the ISO 14040 LCA framework to enhance bio-energy analysis. It details how specific tools—such as NLP for scoping, remote sensing for inventory data, and surrogate models for impact assessment—automate data retrieval and accelerate complex calculations. The workflow culminates in an iterative interpretation phase where explainable AI and optimization algorithms facilitate proactive design improvements for more sustainable energy systems.

### 6.1. Function-oriented golden rules during AI-Assisted goal and scope definition

The early stages of LCA, in particular, may be helped through the use of AI tools text analysis of existing literature and reports and databases. Clustering and topic-modelling reveal common system boundaries, recurring functional units and frequently cited hotspots across comparable bio-energy studies. Such techniques enable a clear and consistent framing of the assessment, for example, with respect to different types of feedstock or multi-step conversion chains. Additionally, natural language processing algorithms may support the automated retrieval of relevant parameters and assumptions from unstructured text as part of LCA initialization <sup>[1]</sup>. Furthermore, AI-based expert systems could assist practitioners in navigating complex methodological choices (e.g., allocation procedures for co-products) by advising on best practices inferred from the agenda setting identified throughout past case studies and regulatory debates <sup>[7]</sup>. By this means a less variable and stronger LCA scope determination is obtained compared to bio-energy system analyses <sup>[1]</sup>. 1475AI can also define the boundaries of an LCA by automatically retrieving and completing missing data, hence leading to more dynamic models <sup>[1]</sup>. Also, machine learning methods can quickly spot influential parameters and data gaps affecting LCA outcomes so that to optimize resource-distribution process of data framework-making for the model <sup>[2]</sup>. Such an automatic identification procedure guarantees the importance of LCA data points measured in terms of equivalent CO<sub>2</sub> emission and helps reduce time-consuming and resource-intensive efforts normally required for collection of full LCA dataset <sup>[6]</sup>.



**Figure 6.** Framework for AI-Integrated Life Cycle Assessment (LCA) in Bio-Energy

## 6.2. AI-Assisted life-cycle inventory

Machine learning has already proven to be beneficial for the life-cycle inventory phase. (Machine-) models calibrated on inventory database, own process-based experimental data, could be used to estimate missing inventory flows (energy input, emission factor or material use). Remote-sensing-based proxies—like land cover change, the crop or pasture biomass production or soil related emissions—are integrated as direct input values in LCIs replacing large averages by spatially differentiate data. Thus more stable upstream stocks are obtained for the stages of cultivation, transport and processing. AI methods also enrich data generation for things we have difficulty measuring directly (e.g., to predict: biomass, biofuel properties or to optimize supply chains) [8]. For example, based on spectral data, machine learning algorithms can predict calorific value or elemental composition of various types of biomass feedstock without the requiring extensive laboratory analysis. In addition, more complex AI models can also help to reconcile different data sources and endpoints (through automatic matching and cleaning of the data), find inconsistencies between datasets or even propose imputation techniques for improving inventory quality with minimum human intervention [39]. These and similar developments not only simplify the inventory process but also improve the resolution and accuracy of data, creating a more solid basis for further impact assessments [5]. Furthermore, machine learning approaches can connect LCA outcomes with additional relevant data (e.g. economic or social) and offer the possibility to directly harmonize inventory information into a common unit, harmonizing between different formats of collected fields by reference databases [9]. This is a highly attractive feature as it cuts down the workload of costly manual data harmonization which often becomes a bottleneck in full-scale LCA studies [69]. The use of AI in LCI also aims for the automated selection of relevant background processes and their related elementary flows, thereby minimizing manual work required for building a complete inventory [70].

## 6.3. Surrogate model assisted impact assessment

Advanced impact assessment techniques such as (that of) climate forcing, ecosystem change and toxicity generally involve intensive computation. Simplified models for the coefficients trained using full LCIA simulations have been demonstrated to reproduce those results at only a fraction of computational expense. This supports rapid assessment of thousands of design options, augmented with comprehensive sensitivity analysis and makes Monte Carlo analysis of uncertainty realistic for large scale bio-energy systems. The second one Enable on line system optimization and a change in the design of these systems paving way for more sustainable and profit-making bio energy solutions [1]. Moreover, AI-based methods are able to identify primary impact categories and hotspots in the life cycle of bio-energy, allowing the prioritization of mitigation options for improving ecological efficiency of bio-energy systems [5]. Additionally, the integration of AI might contribute to enhancing the precision of impact assessment in view of space-time variation in pollution burdens and regional emissions that the classical LCA methods have been tending to over-simplify [1,9]. They allow taking into account dynamic parameters (price and policy) in order to estimate a full and adapted environmental impact [1]. The machine learning methodology, particularly deep learning, may also benefit from complex dose-response relationship and the capability of extrapolating environmental impact to larger ecosystems for the complete landscape analysis of any bio-energy system effect. Generative adversarial networks could also help to produce synthetic but non-limited environment impact data in order to address data scarcity in emerging bio-energy technologies [71].

## 6.4. Interpretation and scenario exploration

Interpretability is enlightening, with an assist from explainable AI. Methods such as those in SHAP provide insight into which factors most drive large impacts and can help researchers and policy makers to understand the ways in which process changes impact environmental performance. Reinforcement learning and multi-objective optimization generalize the idea, suggesting alternatives to this design. An agent evaluates candidate designs and is given rewards or punishments based on the estimated LCA performance, enabling the

exploration of a process design space for optimized cost-efficient environmentally benign processes. This AI-driven iterative optimization enables to find the optimal routes for an economically and ecologically viable production of bio-energy. This kind of paradigm shift from rule based to AI-based interpretation and optimization enables bio-energy systems to be designed in anticipation of lower environmental footprints and higher resource utilization [72]. Moreover, AI applications may improve the cross-referencing of different databases (such as economic models, social impact assessment methodologies or regulatory databases) and even overcome human bias which might provide a more complete treatment than assessing bioenergy technologies [1]. Doing that kind of «rich» analytics leads to obtaining a detailed map of trade-offs and synergies across sustainability dimensions, rather than relying on standard single-objective optimization.

These methodologies are also becoming a part of bio-energy research. Research combines process optimization and environmental performance indicators, comparison of alternative biomass conversion pathways and analysis of portfolios of bio-energy projects in larger renewable energy systems. Through infusing AI-enabled applications in the LCA process, these methods enable more granular and interpretable appraisals which can better respond to developments in data and technology.

**Table 4.** Dataset Size and Validation Practices in AI-Based Bio-Energy LCA Studies

Life-Cycle Stage / Application	Typical Dataset Size	Validation Strategy	Key Performance Metrics	Real-World Relevance
Feedstock assessment and land-use analysis	$10^3$ – $10^5$ samples	Spatial or temporal hold-out validation	$R^2$ , RMSE	Regional and satellite-based studies
Conversion and upgrading processes	50–300 samples	k-fold cross-validation	$R^2$ , RMSE, MAPE	Laboratory and pilot-scale systems
Direct prediction of LCA indicators	$10^2$ – $10^3$ cases	Cross-validation; external testing	$R^2$ , relative error	Early-stage design screening
Plant-level emission prediction	$10^3$ – $10^4$ time-series points	Rolling-window temporal validation	MAE, RMSE	Sensor-assisted operational plants
Remote sensing-based pollution monitoring	$10^5$ – $10^6$ pixels	Spatial and temporal validation	Precision, recall, RMSE	Satellite-supported emission tracking

**Table 4** explains the typical dataset sizes and validation practices reported in AI-based studies across key life-cycle stages of bio-energy systems. It shows that upstream feedstock assessment and pollution monitoring rely on large, data-intensive sources, while conversion-stage models are often trained on smaller experimental datasets. The table also highlights the dominant use of cross-validation and temporal testing to assess predictive robustness. Overall, it provides insight into the practical reliability and transferability of AI approaches used in life-cycle assessment and pollution quantification.

## 7. Key challenges and research gaps

Although AI-driven approaches offer significant advantages for bio-energy LCA, several challenges restrict broader adoption. Current research highlights persistent issues related to data quality, transparency, system boundaries, uncertainty treatment and integration of wider sustainability dimensions. Addressing these gaps is essential for developing AI-enhanced LCAs that are robust, credible and suitable for decision-making.

### 7.1. Data quality, representativeness and bias

The performance of AI in bio-energy LCA depends largely on the quality, quantity, and representativeness of the training data. Most datasets are of small scale, site-specific in geography, and show a bias towards well-instrumented and performing plants, thus limiting generalization ability across climates and management practices, as well as emerging technologies. Data limitations, uncertainty and limited access to high-quality inventories continue to constrain robust modelling. Better data curation is needed, as well transparent reporting of model limits, thorough validation and sensor/real time data integration. Advanced



imputation, generative models and data fusion as well as open-source efforts such as federated learning provide partial solutions that need to be carefully validated for its real-world relevance [73,74].

## **7.2. Transparency, interpretability and reproducibility**

The more we use sophisticated ML models, the more it becomes important to explain how they work. LCA demands transparent documentation of assumptions, allocation methods and impact models – an expectation that should also be valid when AI drives the results of such assessment. XAI tools can shed light on feature importance and model behavior, yet interpretation of the tool itself should be careful in not overstating causal connections. Reproducibility also requires sharing of the code, the data sets, and trained models when possible. Without these conventions it is hard to assess the robustness of LCA results supported by AI. What's more, some state-of-the-art AI models (or in particular deep learning architectures) are “black-box” and these black boxes identities of rationale for impact prediction. For this lack of interpretability it may have an impact on trust with stakeholders and regulatory authorities, making therefore required more sophisticated types of explainable AI techniques tailored to the requirements of Environmental Impact Assessment [1]. Researchers are seeking to address this by developing means of communication from complex model outcomes to policy-relevant insights, typically interactive visual tooling and simplified explanations [75]. On the other hand, the validation of such models with real environmental data is fundamental to their credibility and acceptance by the LCA community [1]. However, the strong validation bases for AI models in LCA are relatively underdeveloped, especially in terms of generalization over a wide diversity of geographical and technological conditions [9].

## **7.3. System boundaries and double counting**

When the LCA models are embedded into AI-based pollution quantification tools, detailed boundary definition is necessary. For instance, resource-based emissions estimates could correspond to the fall of the emissions on emissions already considered in inventory emission units. Misaligned, this is double-counting (or else incoherent across life-cycle stages). A similar challenge arises when co-products or carbon sequestration pathways are treated differently across multiple data sources. This would imply that AI outputs and LCA unit processes are in a one-to-one relationship to maintain consistency. Such integration is based on elaborate ontological framework and standard formats for data sharing to ensure reliable mapping across studies, and to eliminate methodological ambiguities [1]. Furthermore, the dynamic nature of bio-energy systems (e.g. supply chain variations and variable operation conditions) suggests parameterized boundary setting that enables adequate capture of full life-cycle impacts without over or under estimating environmental burdens or benefits [76-80]. The issue of defining system boundaries becomes even more complicated by evolving bio-energy technology development and the intricate agricultural/industrial systems interlinking in turn may demand for detailed multi-scale modelling to represent all relevant flows [11]. This issue becomes more severe in complex bio-refineries where several co-products and energy carriers are produced, which require to be neat accounted to avoid both misses and over counting [81-85]. Consequently, it is important that strong AI-supported strategies are available to adequately keep and continuously identify system boundaries across the various bio-energy pathways for obtaining trustworthy LCA results [11]. In addition, clash between what is feasible in practice in terms of realizations and timescales at different spatial/temporal scales from the AI methodologies compared to the LCA elucidates much of the lack of agreement seen here and underscores that more sophisticated spatiotemporal aggregation methods are necessary [86-94]. Furthermore, the subjectiveness in determination of system boundaries for LCA, which is often influenced by study purposes or policy orientation, might lead to inconsistency of AI-interpreted environmental data [95-99].

## **7.4. Uncertainty and temporal dynamics**

AI models typically result in output that is probabilistic or time-dependent rather than the static emission factors which are used in reliance on standard LCAs. The propagation of these time-varying and uncertain

figures through impact assessment begs a methodological question. Trade-offs will have to be made concerning time horizon, characterization factors and discounting, in particular when considering short-lived climate pollutants or operations of seasonal biomass. An interesting avenue for the future is to also develop stochastic LCA frameworks that can handle ML outputs. Therefore, these probabilistic and time-series predictions should be integrated into the life cycle assessment model at large (the dynamic LCA models) in order to more accurately represent the actual environmental consequences of the biogenic carbon cycles and temporal variation in renewable sources <sup>[100-109]</sup>. Such integration is essential for informed decisions in bio-energy systems, since both short-term variations as well as long-term upward or downward trends have substantial effects on sustainability indicators <sup>[110]</sup>. Bayesian approaches provide computationally expensive but systematic ways to quantify the uncertainties through combining expert opinions with observed data <sup>[111]</sup>. Probabilistic graphical models can also improve the characterization of uncertainty by modelling complex dependencies between different factors along the bio-energy supply chain <sup>[9]</sup>. Furthermore, there are no standardized sustainability criteria for these processes and bio/geophysical interactions are ever-changing – factors that complicate the LCA into a traditional procedural framework <sup>[112-114]</sup>. This is additionally challenging considering the paucity of comprehensive biochar emission datasets as well as the limited scope and applicability of experimental measures generally obtained from single-site studies in a controlled environment, bearing high uncertainties in representing regional differences and incomparability of results elsewhere. Hence, it is highly desirable that state-of-the-art AI methods (e.g. deep learning) quantify and manage these uncertainties at different spatio-temporal scales in bio-energy systems <sup>[115-128]</sup>. Explainable AI methods can cover the challenge of interpretability by giving transparent explanations about decisions made by non-transparent models, thus building trust and encouraging acceptance from stakeholders <sup>[129]</sup>.

## 7.5. Integration of social and economic dimensions

While most AI based LCAs concentrate on environmental factors, they largely neglect social and economic effects. Factors such as land-tenure changes, the food/fuel debate and rural employment/regional growth also demand analytical instruments to deal with different datasets. Socio-economic modelling using machine learning approaches There are available some ML methods for socio-economic modelling (but rarely these are connected to bio-energy LCA workflows. Integration of AI–LCA into multi-criteria sustainability assessment: A potential good way forward in tools that address biodiesel’s holistic impact frame. This level of integration at a more macro scale is required to support sustainability in a holistic sense, not just confined to environmental indicators but also the dynamic interaction of social justice and economic viability <sup>[130-135]</sup>. The idea of such a holistic picture argues for AI systems that would learn to interpret interactive qualitative and quantitative socio-economic data together with environmental readings - including natural language processing in interpreting policy effects and sentiment among stakeholders <sup>[136]</sup>. This also means such gap must be extended to available Life Cycle Costing and Social Life Cycle Assessment methods, as well as their integration into a LCA-based comprehensive Life Cycle Sustainability Assessment framework <sup>[137]</sup>. To overcome these challenges will need integrated solution where both technological advancements; regulation ergonomic interventions and stakeholder involvement together with environmentally sound management practices must be considered <sup>[138]</sup>. The identification of robust indicators and profiles to assess the social economic and sustainable development dimensions on BECCS projects is still a barrier that requires further research for comprehensive assessment <sup>[139-145]</sup>.

Moreover, dealing with the difficulties in the harmonization of diverse impact categories and data comparability between multiple bio-energy systems is also a main issue that should be tackled when developing comprehensive and generally applicable sustainability assessments. The fundamental challenge of combining sustainability indicators across environment, social and economic dimensions is a central methodological issue in holistic assessments of bioenergy approaches.

## 8. Future directions

Recent studies suggest several directions where AI can significantly extend the capabilities of LCA for bio-energy and pollution quantification. These directions focus on tighter integration between models and data, operational decision support, and better treatment of spatial, temporal and socio-technical complexity.

### 8.1. Hybrid physics-informed and data-driven models

Black-box data-driven models tend to be limited when the data is scarce, noisy or not a good representation of future operational scenarios. Hybrid methods which combine first-principles models with machine learning provide a possible path forward. In these models, the mass and energy balances, thermodynamic relations and fundamental reaction kinetics are based on process models and only uncertain (or highly nonlinear) parts of the system dynamics are identified based on data. A prototypical example is that of physics-informed neural networks. They incorporate conservation laws or governed equations in the loss function, which enables the network to discover sub-models of chemical reaction kinetics, decay rates or heat/mass transfer coefficients that were previously unknown without contraventions of underlying physical principles. For bio-energy processes, it may be possible to reduce the quantity of experimental data needed and increase the ability to extrapolate to new feedstocks or scales or operating conditions. The resulting hybrid models can then be used as better surrogates of LCA, particularly in early-stage design tasks or for new technologies.

### 8.2. Digital twins of bio-energy systems

These digital twins take this concept one step further, using in real-time. A digital copy of a bio-energy plant will integrate sensor streams, process simulations and ML-based surrogates to reflect the physical system throughout. If LCA modules, or calibrations to impact surrogates (see below) have been inserted in the twin it is also possible to look for environmental indicators combined with technical and economic performance. Larger biomass power plants, CHP units or integrated bio refineries might use such twins to monitor time-varying emissions and resource use and key impact indicators for decisions making under real-life operating conditions. They also allow what-if analysis; for example, operators can see how changes in feedstock mix, load factor or control strategies would influence emissions and LCA results. This moves LCA away from a single-point design exercise to a living tool for operational performance optimizations.

### 8.3. Generative and large language models for scenario design

New methods of building and exploring scenarios generative methods like large language models are providing new tools. They can also take information from technical reports, policies and datasets to assist in sketching out plausible future pathways: mixes of feedstocks, technologies, scales, sittings and regulatory environments. They can also contribute in building the input datasets, documenting assumptions and identifying key uncertainties. Connected to LCA engines with programmable interfaces, generative models allow for automatic generation of scenario families, batch triggering and summarizing outcomes. For bio-energy, this may hasten the examination of alternatives to cascading biomass use, combination with other renewables or regionally attractive resource mixes comprising residues, energy crops and waste streams. The problem is how to maintain the transparency and keep up the generated scenarios physically and socio-economically plausible?

### 8.4. Interactive AI-Driven LCA dashboards

A further positive is the use of interactive dashboards to combine the AI models with easy user interfaces. Written using the likes of Python, Streamlet and scikit-learn, these platforms take care of data ingestion, pre-processing, inventory completion, impact calculation and rudimentary sensitivity analysis. For facility operators, regulators or project developers, those dashboards could offer near instantaneous feedback on how

changes in feedstock sourcing and plant operation or technology choices are impacting an environmental performance index. To researchers, the framework provides a mean to communicate and disseminate AI enhanced LCA models in a transparent and reproducible manner. In the future, commonly used dashboards could enable benchmarks across plants and transfer of best practices in the bio-energy industry.

### **8.5. Stronger coupling of remote sensing, Air-Quality models and LCIA**

Advanced remote-sensing platforms together with deep learning further enables spatially explicit LCAs that connect emissions to exposure. Satellite (or aircraft) based emission estimates along with chemical transport or dispersion models can provide concentration and exposure fields for pollutants such as PM<sub>2.5</sub>, NO<sub>2</sub> and ozone. AI models contribute to extracting emission fluxes from remote sensing, as well as the acceleration of dispersion calculations via surrogates. Using such spatially explored exposure metrics directly in LCIA methods for human health and ecosystems, LCIA could assess these location specific impacts rather than based on globally or regionally averaged outcomes. This is particularly relevant for bio-energy plants in or close to population centers or where sensitive ecosystems may be affected and for major utilization of residues that could alter regional burning practices, air quality and other patterns.

### **8.6. Standardisation and guidelines for AI-Enhanced LCA**

With the increasing application of AI-based approaches in LCA, demand for methodological recommendations and sector-specific standards is rising. General frameworks to incorporate AI into LCA already exist, but bio-energy is unique in its strong connection to land-use change, soil carbon dynamics, co-product markets and region-specific supply chains.

Future recommendations should focus on:

- AI model documentation (architecture, training data, validation);
- treatment of spatial and temporal variability in biomass systems;
- consistent accounting of co-products, negative emissions (e.g. BECCS, biochar) and indirect land-use effects;
- Uncertainty analysis procedures when applying ML outputs.

This guidance would facilitate the comparison between studies, decrease the likelihood of misapplication of AI tools and increase confidence in AI-driven bio-energy LCAs employed for policy or investment decisions.

## **9. Conclusion**

This review reveals that artificial intelligence is transforming the approach to bio-energy systems environmental impact assessment through all life cycle stages. Classical LCA approaches are handicapped by long-lasting limitations due to little availability of data, outdated inventories, unclear system boundaries, and lack of attention to fluctuation over space and time. Many of these problems associated with inventory compilation can be addressed by AI models that can predict the missing data in inventories, develop more refined feedstock and process modelling, better estimation of emission rates and spatially dynamic assessments. The combination of remote sensing, deep learning, and real-time sensing for richer data model of pollution quantification may result in more reliable impact assessments. At the same time the requirement for transparent, interpretable and reproducible models is still at the core of a quantitatively robust handling of uncertainty. The next steps are likely to be on hybrid physics-guided models, digital twins, generative scenario tools and standardized frameworks that can underpin rigorous and policy-relevant LCAs for emerging bio-energy technologies.



## Abbreviation

Abbreviation	Full Form
AI	Artificial Intelligence
ML	Machine Learning
DL	Deep Learning
ANN	Artificial Neural Network
CNN	Convolutional Neural Network
RNN	Recurrent Neural Network
LSTM	Long Short-Term Memory
SVM	Support Vector Machine
RF	Random Forest
XGBoost	Extreme Gradient Boosting
GPR	Gaussian Process Regression
BN	Bayesian Network
XAI	Explainable Artificial Intelligence
SHAP	SHapley Additive exPlanations
LIME	Local Interpretable Model-Agnostic Explanations
LRP	Layer-wise Relevance Propagation
LCA	Life-Cycle Assessment
LCI	Life-Cycle Inventory
LCIA	Life-Cycle Impact Assessment
ISO	International Organization for Standardization
GHG	Greenhouse Gas
GWP	Global Warming Potential
CED	Cumulative Energy Demand
NO <sub>x</sub>	Nitrogen Oxides
SO <sub>x</sub>	Sulfur Oxides
CO	Carbon Monoxide
CO <sub>2</sub>	Carbon Dioxide
PM	Particulate Matter
PM <sub>2.5</sub>	Particulate Matter with diameter $\leq 2.5 \mu\text{m}$
VOC	Volatile Organic Compounds
IoT	Internet of Things
UAV	Unmanned Aerial Vehicle
LUC	Land-Use Change
BECCS	Bioenergy with Carbon Capture and Storage
MAE	Mean Absolute Error
RMSE	Root Mean Square Error
MAPE	Mean Absolute Percentage Error
R <sup>2</sup>	Coefficient of Determination

## Author Contributions

**Madhuri Karad** and **Puja Gholap** contributed to the conceptualization of the study, literature survey, and overall structure of the review. **Ashwini Dhumal** and **Vilas Suresh Mane** were involved in data curation, analysis of AI methodologies, and drafting sections related to machine learning techniques. **N. Alangudi**

**Balaji** and **Kunal Ingole** contributed to the investigation of life-cycle assessment frameworks and pollution quantification approaches. **Rahul N. Patil** and **Shital Yashwant Waware** assisted in manuscript writing, figure preparation, and critical revision of the content. **Anant Sidhappa Kurhade** supervised the study, provided methodological guidance, reviewed and edited the manuscript, and finalized the version for submission. All authors read and approved the final manuscript.

## Acknowledgments

The authors would like to express their sincere gratitude to Dr. D. Y. Patil Institute of Technology and DPGU, School of Technology and Research - Dr. D. Y. Patil Unitech Society, Pimpri, Pune for providing the necessary support and research infrastructure.

## Conflict of interest

The authors declare no conflict of interest

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