

ADVANCEMENTS IN THERMOCHEMICAL BIOMASS CONVERSION: A SYSTEMATIC REVIEW OF AI AND ML TECHNIQUES (2014-2024)

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ABSTRACT

Artificial Intelligence (AI) and Machine Learning (ML) algorithms have emerged as transformative tools for enhancing efficiency and sustainability in biomass thermochemical conversion processes such as pyrolysis, gasification, and hydrothermal liquefaction. These processes produce valuable energy products like bio-oil, syngas, and biochar, significantly reducing greenhouse gas emissions and promoting energy security. This systematic review evaluates 830 articles on the use of AI and ML in these processes, ranging from 2014 to 2024, sourced from multiple academic databases. The review identifies trends in algorithm usage, effectiveness, and geographical distribution. Key findings reveal that Neural Networks (ANN), Support Vector Machines (SVM), and Random Forests (RF) are predominant, optimizing processes like pyrolysis and gasification. These algorithms have improved efficiency, reduced costs, and promoted sustainability in bioenergy, renewable energy, water treatment, and pollution control sectors. Despite these advancements, challenges remain in practical implementation and economic analysis within industrial settings. Future research should focus on bridging this gap by incorporating economic assessments and fostering greater collaboration with industries to scale up AI-driven biomass conversion technologies, ensuring they deliver sustainable and economically viable solutions to global energy challenges.

Keywords: Biomass. Thermochemical conversion. Artificial Intelligence. Machine Learning. Bioenergy.

1 INTRODUCTION

The urgent global demand for sustainable and renewable energy has amplified interest in biomass thermochemical conversion processes such as pyrolysis, gasification, and hydrothermal liquefaction. These processes transform biomass into valuable energy products like bio-oil, syngas, and biochar, significantly reducing greenhouse gas emissions and promoting energy security¹. However, their complexity necessitates advanced predictive and optimization techniques to maximize efficiency and output.

In recent years, the landscape of energy production has shifted dramatically with the urgency of climate change mitigation. Artificial Intelligence and Machine Learning have emerged as transformative tools in industrial applications and academic research. AI and ML excel at handling complex, nonlinear relationships in biomass conversion, enabling precise modeling, prediction, and optimization². These technologies can revolutionize industries by optimizing processes, reducing costs, and improving sustainability. AI and ML algorithms can analyze vast datasets to identify patterns, make predictions, and automate decision-making processes, enhancing productivity and innovation across various sectors. Despite significant advancements, integrating AI and ML into industrial settings poses challenges. The need for extensive datasets, computational resources, and practical implementation of predictive models hinders widespread adoption³. Moreover, aligning academic research with industrial applications is crucial to demonstrating tangible economic and environmental benefits.

This study provides a comprehensive systematic review of predictive modeling techniques in biomass thermochemical conversion over the past decade. By analyzing 830 articles from multiple academic databases, it was identified trends in algorithm usage, evaluated their effectiveness across various industrial applications, and highlighted the geographical distribution of research contributions. This review underscores the necessity for future research to bridge the gap between academic advancements and industrial implementation, ensuring AI-driven biomass conversion technologies deliver practical, sustainable, and economically viable solutions to the global energy crisis.

2 MATERIALS AND METHODS

To conduct a systematic review on the use of predictive modeling techniques in biomass thermochemical conversion over the last ten years, searches were performed across Scopus, Web of Science, ScienceDirect, PubMed, and SpringerLink platforms. Boolean operators were used with search strings such as "biomass" AND "thermochemical conversion" AND ("predictive modeling" OR "machine learning" OR "artificial intelligence") NOT "review", to ensure only experimental research papers. Python scripts utilizing the CrossRef API and web scraping techniques were developed to extract metadata from 830 articles, including the country of origin, keywords, publication year, and citation count. Tools BeautifulSoup, Selenium, and Requests facilitated data retrieval and processing. The first author's country of affiliation was used for geographical analysis. The references were organized into data processing software to provide insights into publication trends, keyword usage, and geographical distribution.

To ensure in-depth trend analysis, 50 articles of the total were proportionally selected from each year between 2014 and 2024. For example, 27 articles were published in 2014 and approximately 2 articles were selected, calculated as $(27/830) * 50 \approx 2$ articles. This process was repeated for each year, with random DOI selection ensuring unbiased sampling. The selected articles were analyzed using the PRISMA methodology⁴. Data categorization focused on key aspects such as study titles, thermochemical

conversion techniques, study objectives, results, industrial application sectors, algorithms used and environmental and economic impacts. The systematic review aimed to identify common predictive modeling techniques, evaluate their effectiveness in different thermochemical processes, and assess their industrial applicability. It also explored the integration of AI and ML algorithms in the biomass conversion industry, highlighting key trends, adoption phases, future directions, and challenges. All graphs and visualizations were created using the Python libraries Matplotlib and Seaborn, and the R library Circlize, chosen for their efficiency and effectiveness in generating detailed charts. The codes for the visualizations, metadata extraction, web scraping, and DOI selection are available in the first author's GitHub repository SR-thermochemicalML.

3 RESULTS AND DISCUSSION

The systematic review conducted gathering experimental articles about biomass thermoconversion with help of machine learning and artificial intelligence between 2014 and 2024 yielded a total of 830 articles across multiple academic databases, duplicates excluded. Specifically, 215 articles were identified in Scopus, 36 in Web of Science, 521 in ScienceDirect, 21 in PubMed, and 37 in SpringerLink. This collection underscores the extensive research interest in the application of predictive modeling techniques in biomass thermochemical conversion. Over the past ten years, research in this area has received contributions from 62 countries. Notably, China leads with 267 publications, followed by the United States of America with 87, and India with 68. Other major contributors include Spain (29), United Kingdom (29), Malaysia (28), Iran (26) and Turkey (25), as illustrated in Figure 1.

The total number of publications has shown a steady increase from 2014 to 2024, as depicted in the annual publications and cumulative publications total graph (Figure 2). The cumulative total citations, 19,735 until June 2024 (Fig. 1), further indicate the growing impact and relevance of this research field. The significant rise in publications, particularly from 2021 onwards, underscores the accelerating interest and advancements in utilizing AI and ML techniques in biomass conversion processes.

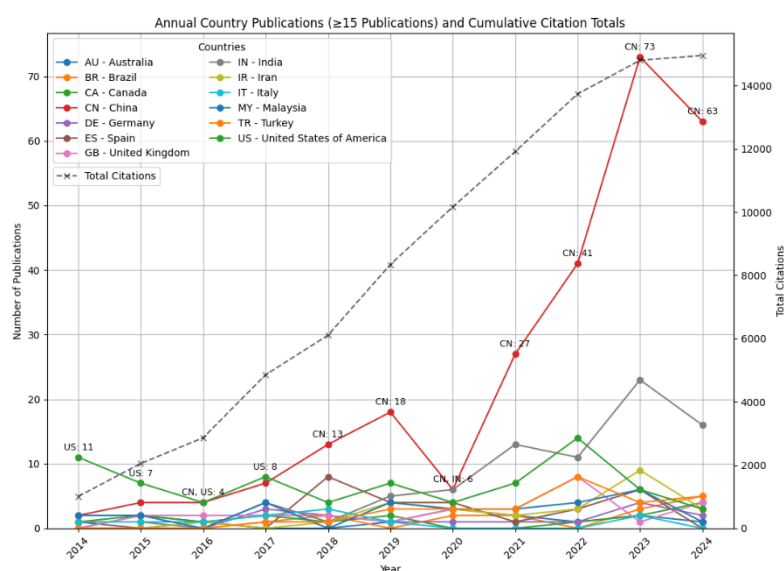


Figure 1. Yearly publication, from 2014 to 2024, count of countries with at least 15 publications in biomass thermochemical conversion using AI and ML techniques (colored lines), alongside the cumulative citation totals (grey line).

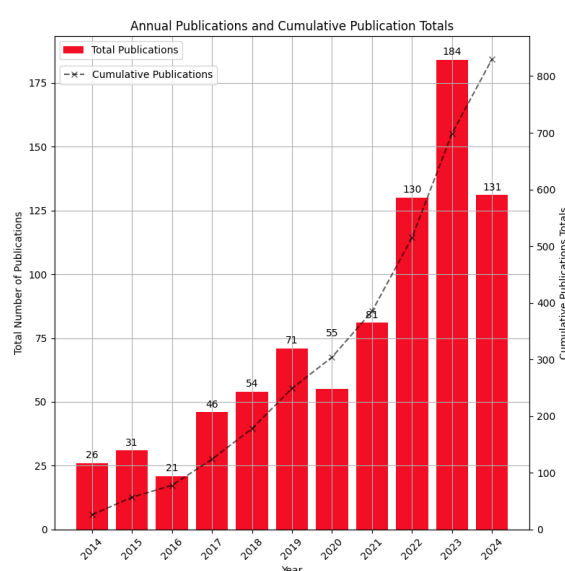


Figure 2. Yearly (red bars) and cumulative (grey line) total number of publications related to biomass thermochemical conversion using AI and ML techniques.

A detailed keyword analysis identified the most frequent terms and their correlations within the literature. The heatmap of keyword occurrences (Fig. 3) shows central themes such as "biomass," "model," "machine learning," "pyrolysis," and "prediction." The chord diagram (Fig. 4) illustrates the interconnectedness of these keywords, revealing clusters like conversion products, thermochemical process, data analysis and optimization and ML techniques.

The analysis of the selected articles provided deeper insights into trends, commonly used algorithms, research phases, and future directions in AI and ML integration in biomass thermochemical conversion. Neural Networks (ANN), used in 43.75% of studies, demonstrated robust performance in modeling complex, nonlinear relationships, improving processes like hydrolysis and pyrolysis. Support Vector Machines (SVM) and Random Forest (RF) were also prominent, accounting for 14.58% and 16.67% of studies, respectively, excelling in classification, regression tasks, and handling large datasets. Optimization algorithms like Genetic Algorithms (GA) and Particle Swarm Optimization (PSO) significantly improved process efficiency and output quality. GA aided in predicting biochar aromaticity and optimizing biomass conversion, while PSO enhanced kinetic modeling of pyrolysis and hydrogen production. Fuzzy Logic, Gaussian Process Regression (GPR), and ensemble methods further contributed by handling uncertainties and combining multiple learning algorithms for better predictive performance.

From 2014 to 2024, advancements in biomass thermoconversion techniques have been marked by significant integration of AI and optimization algorithms. It was identified three main phases in the trends. At the initial phase (2014-2017), studies primarily focused on applying AI to predict and optimize processes such as gasification, enzymatic hydrolysis, and pyrolysis. Techniques like Model Predictive Control and ANN were used to enhance process stability and predict sugar yields, achieving remarkable accuracy and operational improvements. The second phase (2018-2021) could be identified because of a diversification of AI techniques, including Support Vector Machines, Convolutional Neural Networks, and Particle Swarm Optimization, applied to processes like pyrolysis and gasification. This period highlighted improvements in prediction accuracy and generalization, with

algorithms such as RF and ensemble methods being used to optimize thermal decomposition and biochar yield, significantly advancing process efficiency.

From 2022 to 2024, a notable trend emerged towards integrating multivariate optimization techniques and combined models like XGBoost, GPR, and LightGBM. These models were widely used to optimize bio-oil and hydrogen production, with explainable AI enhancing prediction transparency and robustness. The application of these algorithms spans various industries: bioenergy (29.17%), renewable energy (27.08%), water treatment (12.5%), waste management (10.42%), chemical engineering (8.33%), pollution control (6.25%), and the biochar industry (6.25%). This diverse applicability underscores the broad impact of AI in enhancing efficiency and sustainability across sectors.

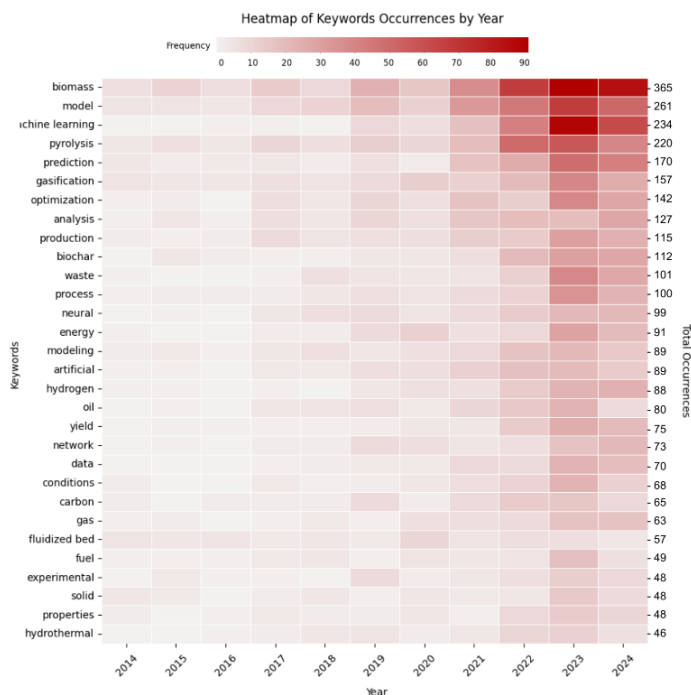


Figure 3. Frequency of keywords related to biomass thermochemical conversion using AI and ML techniques from 2014 to 2024.

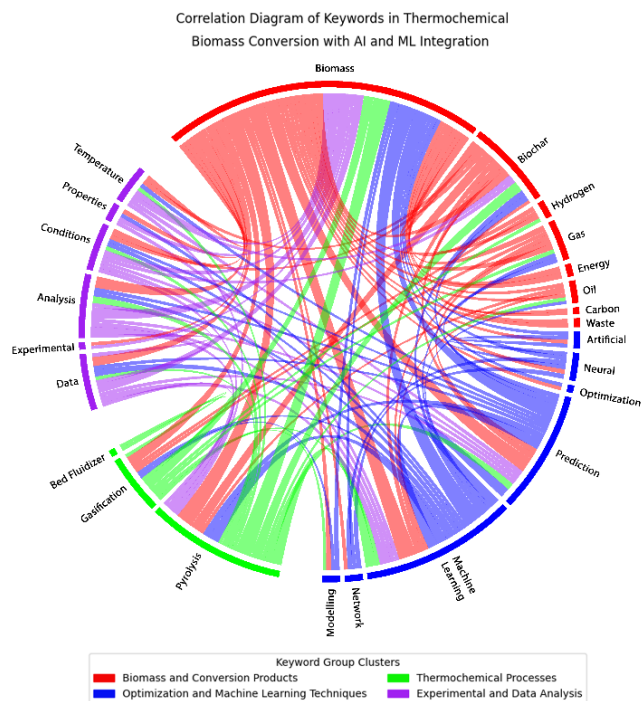


Figure 4. Interconnections between frequently occurring keywords, highlighting clusters related to biomass thermochemical conversion using AI and ML techniques from 2014 to 2024.

Despite these advancements, the practical application and economic analysis of these technologies in industrial settings remain limited. Future research should focus on bridging this gap by incorporating detailed economic assessments and industrial case studies, ensuring AI-driven biomass conversion technologies deliver practical, sustainable, and economically viable solutions.

4 CONCLUSION

This systematic review highlights significant advancements in the application of AI and ML algorithms in biomass thermochemical conversion from 2014 to 2024. Neural Networks (ANN), Support Vector Machines (SVM), and Random Forests (RF) have demonstrated robust performance in optimizing processes like pyrolysis, gasification, and bio-oil production, enhancing efficiency, reducing costs, and improving sustainability across sectors such as bioenergy, renewable energy, water treatment, and pollution control. Despite these advancements, practical implementation and economic analysis in industrial settings remain limited, underscoring the need for future research to bridge the gap between academic advancements and industrial application. Incorporating economic assessments and case studies will facilitate broader adoption of AI-driven biomass conversion technologies, ensuring they deliver practical, sustainable, and economically viable solutions to global energy challenges.

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