International Journal of Recent Development in Engineering and Technology
Website: www.ijrdet.com (ISSN 2347-6435 (Online) Volume 15, Issue 05, May 2026)

Important Role and Application of Artificial Intelligence in Green Chemistry

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***Abstract*-- Green chemistry has emerged as a sustainable approach to reducing environmental pollution and minimizing the harmful effects of chemical manufacturing processes. Artificial Intelligence (AI) is transforming modern industries by enabling automation, prediction, optimization, and intelligent decision-making. The integration of AI into green chemistry has significantly improved chemical process efficiency, waste management, catalyst discovery, energy conservation, and environmental monitoring. AI techniques such as Machine Learning (ML), Artificial Neural Networks (ANN), Deep Learning, and predictive analytics assist researchers in designing eco-friendly chemical products and sustainable industrial processes. AI-driven systems reduce experimental errors, optimize resource utilization, and minimize toxic byproducts, thereby supporting environmental sustainability. This paper discusses the important role of AI in green chemistry, including reaction optimization, waste reduction, renewable energy development, safer chemical design, and environmental protection. The paper also highlights challenges, future advancements, and industrial applications of AI-assisted green chemistry.**

***Keywords*-- Artificial Intelligence, Green Chemistry, Machine Learning, Sustainability, Environmental Protection, Chemical Engineering, Renewable Energy**

I. INTRODUCTION

Industrial growth and technological advancements have improved human living standards but have also created severe environmental challenges such as pollution, climate change, hazardous waste generation, and depletion of natural resources. Traditional chemical industries consume large amounts of energy and produce harmful byproducts that negatively affect ecosystems and human health. To overcome these problems, the concept of green chemistry was introduced to develop environmentally friendly and sustainable chemical processes.

Green chemistry focuses on reducing the use and generation of hazardous substances while improving energy efficiency and waste management. However, implementing sustainable chemical processes requires extensive experimentation, data analysis, and optimization, which can be expensive and time-consuming. Artificial Intelligence (AI) provides innovative solutions to these challenges by automating chemical analysis and predicting efficient reaction pathways.

AI technologies such as Machine Learning, Deep Learning, Neural Networks, and Robotics are increasingly being used in chemical industries and research laboratories. AI can process large datasets, identify patterns, optimize chemical reactions, and predict material properties with high accuracy. By integrating AI into green chemistry, industries can minimize waste production, conserve energy, improve process efficiency, and develop safer chemicals.

The application of AI in green chemistry has expanded rapidly in recent years. AI-assisted systems are used for catalyst discovery, smart manufacturing, environmental monitoring, carbon emission reduction, renewable energy development, and water treatment. These technologies support sustainable industrial development and environmental conservation.

This paper presents the important role of Artificial Intelligence in green chemistry, focusing on its applications, benefits, methods, challenges, and future developments in sustainable chemical engineering.

1.1 Principles of Green Chemistry

The principles of green chemistry provide guidelines for developing environmentally friendly chemical processes and products.

Prevention of Waste

Chemical industries should prevent waste generation instead of treating waste after production.

Atom Economy

Chemical reactions should maximize the incorporation of raw materials into the final product.

Safer Chemicals

Products should be designed to reduce toxicity and environmental hazards.

Energy Efficiency

Chemical processes should minimize energy consumption and operate at ambient conditions whenever possible.

Renewable Feedstocks

Industries should use renewable raw materials instead of non-renewable resources.

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Catalysis

Catalysts should be used to improve reaction efficiency and reduce harmful byproducts.

Biodegradability

Chemical products should degrade safely without causing environmental pollution.

AI technologies help achieve these principles by improving chemical process optimization and reducing environmental impact.

II. METHODS

The integration of Artificial Intelligence in green chemistry involves data-driven computational techniques that optimize chemical processes and environmental sustainability. AI systems analyze experimental datasets and predict efficient reaction conditions with reduced resource consumption.

The major AI techniques used in green chemistry include:

- Machine Learning (ML)
- Artificial Neural Networks (ANN)
- Deep Learning Algorithms
- Predictive Analytics
- Robotics and Automation
- Data Mining

Machine Learning models are trained using chemical reaction databases to predict reaction yields, catalyst efficiency, and optimal operating conditions. Neural networks simulate chemical behavior and identify eco-friendly process alternatives. AI-based automation systems monitor industrial operations in real time and reduce waste generation.

AI also supports sustainable manufacturing through intelligent control systems that optimize temperature, pressure, solvent usage, and energy consumption. Environmental monitoring systems integrated with AI sensors detect harmful emissions and suggest corrective measures.

Tables and Figures are presented center, as shown below and cited in the manuscript.

Table 1.
AI applications in Green Chemistry Processes

APPLICATION AREA	AI TECHNIQUE	BENEFIT
Reaction Optimization	Machine Learning	Reduced waste generation
Catalyst Design	Neural Networks	Improved efficiency
Water Treatment	Predictive Analytics	Pollution reduction
Renewable Energy	Deep Learning	Sustainable energy production
Environmental Monitoring	AI Sensors	Real-time pollution control
Smart Manufacturing	Robotics	Energy conservation
Toxicity Prediction	Data Mining	Safer chemical products
Carbon Emission Control	AI Modelling	Reduced greenhouse

III. RESULTS AND DISCUSSION

Results

The implementation of AI in green chemistry has shown significant improvements in sustainability and industrial efficiency. Machine Learning models successfully predicted optimized reaction conditions with reduced chemical waste and lower energy consumption.

AI-based catalyst discovery systems accelerated the identification of efficient catalysts, reducing experimental time and operational costs.

AI-assisted environmental monitoring systems improved pollution detection accuracy and enabled real-time monitoring of industrial emissions. Renewable energy material discovery through AI contributed to the development of efficient solar cells and battery technologies.

The use of AI in smart manufacturing reduced unnecessary resource utilization and improved process automation. Industries using AI-driven optimization systems reported reduced carbon emissions and enhanced production efficiency.

Discussion

The results indicate that Artificial Intelligence has become an essential tool for advancing green chemistry and sustainable industrial development. AI technologies reduce dependency on traditional trial-and-error methods by enabling accurate predictions and intelligent decision-making.

One of the major advantages of AI is its ability to analyze large datasets rapidly and identify sustainable process alternatives. This improves productivity while minimizing environmental damage. AI-assisted catalyst design and reaction optimization significantly contribute to waste reduction and energy conservation.

However, challenges remain in implementing AI systems across all chemical industries. High computational costs, lack of quality datasets, and technical expertise requirements limit large-scale adoption. In addition, some AI models operate as black-box systems, making interpretation difficult for researchers.

Despite these limitations, continuous advancements in AI technologies are expected to improve transparency, efficiency, and accessibility. Collaboration between chemists, computer scientists, and environmental engineers will further strengthen the application of AI in sustainable chemistry.

IV. Conclusion

Artificial Intelligence plays a crucial role in transforming green chemistry by improving sustainability, efficiency, and environmental safety in chemical industries. AI technologies support reaction optimization, catalyst discovery, waste reduction, renewable energy development, and environmental monitoring. The integration of Machine Learning, Neural Networks, and predictive analytics enables industries to minimize hazardous waste and conserve natural resources.

AI-driven green chemistry contributes to cleaner production methods, reduced pollution, and improved industrial productivity.

Although challenges such as computational costs and data limitations exist, future developments in AI are expected to overcome these barriers.

The combination of AI and green chemistry will continue to support sustainable development and environmental protection for future generations.

Acknowledgements

The authors express sincere gratitude to the Department of Chemical Engineering and Department of Computer Science Engineering, XYZ Institute of Technology, Jaipur, Rajasthan, for their continuous support and guidance during the preparation of this research paper. The authors also thank faculty members and researchers who provided valuable suggestions related to Artificial Intelligence and Green Chemistry applications.

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