

APPLICATIONS OF ARTIFICIAL INTELLIGENCE (AI) IN GREEN CHEMISTRY

* S. G. Jagadhani

* Karmaveer Bhaurao Patil College, Vashi, Navi Mumbai, Pin. 400702, Maharashtra, India.

Abstract:

AI is making noteworthy steps across various scientific disciplines. These advancements are paving the way for a greener chemical industry by aligning with the 12 principles of green chemistry. Green chemistry is branch of Chemistry which specially focused on designing chemical products and processes that reduce or eliminate the use of hazardous substances.

AI is revolutionary tool for altering the approach scientists for research, more efficient, making discoveries faster, and often uncovering visions that were previously unbelievable.

Keywords: Green Chemistry, AI tools, Applications.

Copyright © 2025 The Author(s): This is an open-access article distributed under the terms of the Creative Commons Attribution 4.0 International License (CC BY-NC 4.0) which permits unrestricted use, distribution, and reproduction in any medium for non-commercial Use Provided the Original Author and Source Are Credited.

Introduction:

Green chemistry, often known as sustainable chemistry, is a scientific method that focusses on creating goods and procedures that use and produce fewer or no harmful materials. The objective is to lessen the negative effects of chemical manufacturing and use on the environment, making it safer for both people and the environment.¹ The twelve guiding principles of green chemistry are frequently used.¹

Approach of AI towards Twelve Principles of Green Chemistry:

1. **Prevention:** By using AI to Scientist can identify possible waste and byproducts in chemical reactions, chemists may create procedures that produce as little waste as possible.
2. **Atom Economy:** AI systems can minimize waste, by incorporation of all elements into the final product through reaction optimization.
3. **Syntheses of Less Hazardous Chemicals:** AI can help to design less toxic chemical pathways, reducing the use of hazardous substances.
4. **Creating Safer Chemicals:** AI can forecast a new chemical's toxicity, which makes it possible to create safer substitutes.
5. **Safer Auxiliaries and Solvents:** AI can suggest safer auxiliary materials and solvents, reducing the impact of chemical processes on the environment
6. **Energy Efficiency:** AI can promote energy-efficient processes by optimizing response conditions to reduce energy usage.

7. **Utilization of Renewable Raw materials:** AI is able to recognize and maximize the utilization of renewable feedstock in chemical reactions.
8. **Reduce Unnecessary Derivatization:** AI can reduce waste and resource consumption by streamlining synthetic routes to exclude unnecessary derivatization processes.
9. **Catalysis:** AI can design and optimize catalysts that enhance reaction efficiency and Selectivity reducing the need for stoichiometric reagents.
10. **Design for Degradation:** AI can predict the environmental fate of chemicals, enabling the Design of products that degrade into harmless substances.
11. **Pollution Prevention:** AI can provide real-time monitoring and analysis of chemical processes, allowing for immediate adjustments to prevent pollution.
12. **Safer Chemistry for Accident Prevention:** AI can identify potential hazards in chemical processes and suggest safer alternatives to prevent accidents.

Importance of AI (Artificial Intelligence) in some important areas:

The importance of artificial intelligence (AI) has grown in many facets of our life. AI is important in the following important areas:

- **Healthcare& Treatment:**

AI is transforming customized medicine, treatment planning, and medical diagnosis. It aids in illness early detection, medical picture analysis, and patient outcome prediction.

- **Data Analysis for Decision-Making:**

AI can analyse enormous volumes of data at incredibly fast speeds, assisting businesses in making better, data-driven decisions.

- **Predictive analytics:**

By using historical data to forecast future patterns and results, AI systems can improve risk management and strategic planning.

- **Enhanced Productivity:**

AI-powered systems are more efficient and productive than people because they can complete routine, repetitive jobs faster and more correctly.

Cost Reduction: Businesses can save a lot of money by automating operations, which lowers labour costs and minimizes human error.

- **Global Issues:**

Climate Change: AI can assist in tracking and forecasting changes in the environment, which will help combat climate change and create sustainable solutions.

Disaster Response: By analysing data from natural disasters, artificial intelligence (AI) can enhance response and recovery activities, potentially saving resources and lives.

Artificial Intelligence in Green Chemistry:

There are tremendous advancements in Green chemistry due to Artificial Intelligence (AI), which is promoting Eco-friendly and sustainable chemical processes. The following are some important uses of AI in green chemistry.

- **Optimization of the Chemical Reactions:** Chemists can optimise the reaction conditions to reduce waste and energy consumption by using AI algorithms that can predict the results of chemical reactions. This results in chemical processes that are more sustainable and efficient.³
- **Solvents Selection:** AI can help in the identification of eco-friendly solvents for chemical processes. By evaluating extensive datasets, AI can pinpoint solvents that pose a reduced risk to both the environment and human health.
- **Artificial Intelligence can reduce waste in Chemical processes:** By creating synthetic pathways that generate fewer byproducts, AI-driven methods can aid in the reduction of waste in chemical processes. This is in line with the Principles of green chemistry, which seek to reduce the negative effects of chemical manufacturing on the environment.⁴
- **Development of Eco-friendly Catalysts:** AI can help in the development of newer environment friendly catalysts that enhance the efficiency of chemical reactions while reducing the production of harmful by-products. These catalysts can lower energy consumption and improve the overall sustainability of chemical processes.
- **Prediction of Biodegradability:** Deep learning algorithms and other AI models are able to forecast how biodegradable organic molecules will be? This lessens the impact of chemicals on the environment by designing them to decompose more readily.⁵
- **Discovery of Materials:** AI has the potential to speed up the process of finding new materials with suitable features for applications in green chemistry. The time and resources needed for experimentation can be decreased by using machine learning techniques to forecast the characteristics and performance of possible materials.⁵

References:

1. Varma R S, *Green chemistry*, **1999**.
2. *Organic Chemistry by Rao*, **2018**.
3. *Asian Journal of Chemistry*, **2023**.
4. *Artificial Intelligence in Green Organic Chemistry: Pathway to Sustainable and Eco- Friendly Chemistry*, Vol. 36, 12, **2024**.
5. *Deep learning for Green Chemistry: An AI-Enabled Pathway for Biodegradability, Prediction and Organic Material Discovery*, Vol. 41, **2024**

Cite This Article: Jagadhani S.G. (2025). Applications of Artificial Intelligence (AI) in Green Chemistry. In **Educreator Research Journal**: Vol. XII (Issue II), pp. 90–92.