

Revolutionizing Green Chemistry through Artificial Intelligence and its Applications

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ABSTRACT

The integration of Artificial Intelligence (AI) into green chemistry has emerged as a transformative approach for developing sustainable and environmentally benign chemical processes. AI techniques such as machine learning, data analytics, and predictive modeling enable researchers to design eco-friendly synthesis pathways, optimize reaction conditions, reduce waste generation, and minimize energy consumption. By analyzing large chemical datasets, AI can identify greener solvents, catalysts, and reaction mechanisms that enhance efficiency while lowering environmental impact. Furthermore, AI-driven tools accelerate the discovery of sustainable materials and improve lifecycle assessment, supporting the principles of green chemistry. The application of AI also facilitates real-time monitoring and intelligent process control in industrial chemistry, leading to safer and more resource-efficient production systems. Despite challenges such as data availability, model transparency, and computational limitations, the synergy between AI and green chemistry holds significant potential for advancing sustainable innovation.

Keywords: Artificial Intelligence, Green Chemistry, Sustainable Chemistry, Machine Learning, Eco-friendly Synthesis, Waste Reduction, Chemical Process Optimization.

INTRODUCTION: ROLE OF ARTIFICIAL INTELLIGENCE IN GREEN CHEMISTRY

Green chemistry has emerged as a fundamental approach to designing chemical products and processes that minimize environmental impact and promote sustainability. The concept focuses on reducing the use of hazardous substances, preventing waste generation, improving energy efficiency, and promoting the use of renewable resources. With the growing global concern regarding climate change, environmental pollution, and depletion of natural resources, the need for sustainable chemical practices has become more important than ever. In this context, green chemistry provides a scientific framework that encourages safer and more environmentally friendly chemical innovations.

In recent years, Artificial Intelligence (AI) has become a powerful technological tool that is transforming various scientific disciplines, including chemistry. AI refers to computational systems capable of performing tasks that typically require human intelligence, such as pattern recognition, prediction, and decision-making. Techniques such as machine learning, deep learning, and data-driven modeling enable scientists to analyze large and complex chemical datasets efficiently. These capabilities make AI particularly valuable for accelerating research and improving efficiency in chemical sciences.

The integration of AI with green chemistry has opened new possibilities for designing sustainable chemical processes. AI can predict optimal reaction pathways, identify environmentally benign solvents and catalysts, and optimize reaction conditions to reduce waste and energy consumption. By analyzing large experimental and computational datasets, AI models can assist chemists in selecting greener alternatives that follow the principles of green chemistry. Additionally, AI-driven simulations can reduce the need for extensive laboratory experimentation, thereby saving resources, time, and materials.

Furthermore, AI technologies are increasingly being applied in the development of sustainable materials, environmental monitoring, and industrial process optimization. In pharmaceutical, materials, and chemical industries, AI helps in designing eco-friendly synthesis routes and improving process efficiency while maintaining safety and productivity. The use of AI also supports lifecycle analysis and environmental impact assessment, which are essential components of sustainable chemical development.

Despite its significant potential, the application of AI in green chemistry also faces certain challenges, including limited availability of high-quality datasets, model interpretability issues, and computational resource requirements. However, continuous advancements in computational power, data science, and collaborative research are helping to overcome these limitations.

Therefore, the integration of AI with green chemistry represents a promising pathway toward achieving sustainable chemical innovation. By combining advanced computational techniques with the principles of environmentally responsible chemistry, AI has the potential to significantly enhance the development of greener chemical processes and contribute to global sustainability goals.

Role of Artificial Intelligence in Green Chemistry

The principles of green chemistry provide guidelines for developing safer and more sustainable chemical processes. AI contributes to many of these principles by assisting scientists in making informed decisions during chemical design, synthesis, and industrial production.

1. Waste Prevention

AI helps researchers design reaction pathways that generate fewer by-products. By predicting reaction outcomes and optimizing conditions before performing experiments, AI reduces unnecessary trials and chemical waste.

2. Atom Economy

Machine learning models analyze reaction mechanisms and recommend pathways in which most of the atoms from the starting materials are incorporated into the final product. This improves the efficiency of chemical synthesis and minimizes material loss.

3. Less Hazardous Chemical Synthesis

AI systems can evaluate the toxicity and reactivity of chemicals using existing databases. This allows scientists to select safer reagents and reaction conditions that reduce risks to human health and the environment.

4. Designing Safer Chemicals

Predictive AI tools can estimate the toxicity, biodegradability, and environmental persistence of newly designed molecules. This helps chemists create chemical products that perform their intended function while causing minimal ecological harm.

5. Safer Solvents and Auxiliaries

Solvents are widely used in chemical processes but many are hazardous. AI can screen large solvent databases and recommend greener alternatives that maintain reaction efficiency while reducing environmental impact.

6. Energy Efficiency

AI-driven optimization techniques help determine reaction conditions that require lower temperatures and pressures. This reduces energy consumption in chemical processes and contributes to sustainable industrial practices.

7. Use of Renewable Feedstocks

AI assists in identifying renewable and bio-based raw materials as alternatives to fossil-based Feedstocks. It can analyze the feasibility of these materials for various chemical reactions and industrial applications.

8. Catalysis

Catalysts play a crucial role in improving reaction efficiency. AI accelerates the discovery of new catalysts by predicting their activity, selectivity, and stability, which helps reduce energy use and unwanted by-products.

9. Real-Time Analysis for Pollution Prevention

AI can be integrated with monitoring systems and sensors to analyze chemical processes in real time. This allows early detection of harmful emissions and helps prevent environmental contamination.

10. Inherently Safer Chemistry for Accident Prevention

AI-based simulations can predict potential hazards in chemical reactions or industrial processes before they occur. This improves safety by allowing researchers to design safer chemical systems and avoid dangerous conditions.

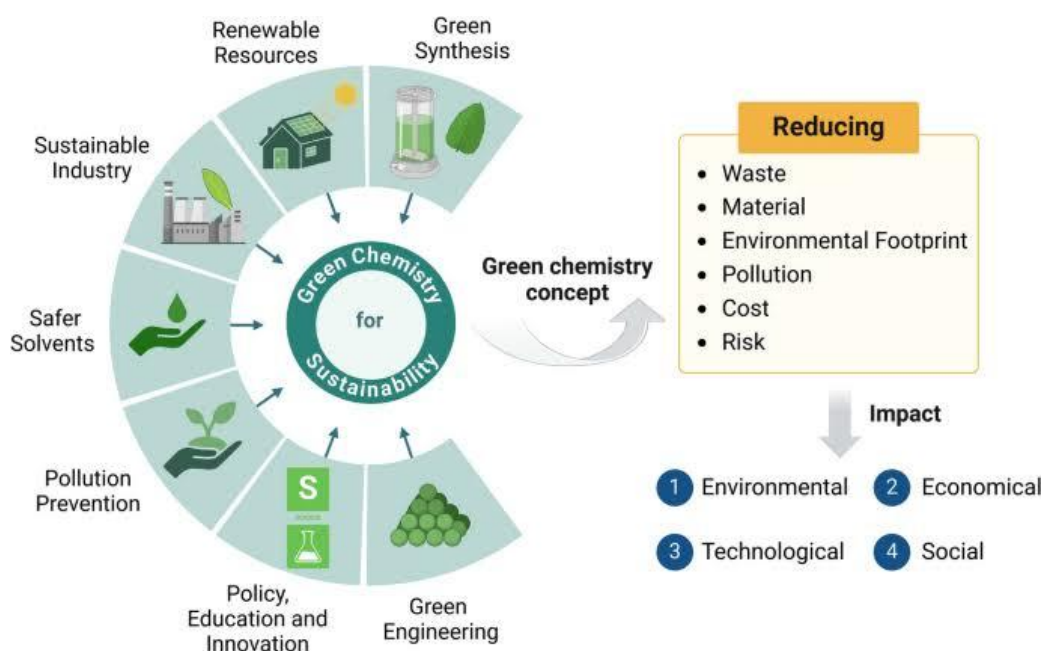


Fig. 1 The Role of AI in Green Chemistry with their Principles

Recent Trends in AI Applications in Green Chemistry

1. Machine Learning for Sustainable Chemical Design

Machine learning algorithms are widely used to analyze chemical structures and reaction datasets. These models can predict the behavior, reactivity, and toxicity of chemical compounds before they are synthesized in laboratories. This approach reduces unnecessary experimentation, saves resources, and supports the development of environmentally friendly chemicals.

2. AI-Assisted Reaction Optimization

AI-based systems are now being used to optimize chemical reactions by determining the best reaction conditions such as temperature, pressure, catalysts, and solvents. Through predictive modeling and automated experimentation, AI can quickly identify conditions that maximize product yield while minimizing waste and energy consumption.

3. Discovery of Green Catalysts

Catalysts play an important role in improving reaction efficiency and reducing harmful by-products. AI technologies help scientists discover and design new catalysts by predicting their performance and stability. This accelerates catalyst development and contributes to cleaner and more efficient chemical processes.

4. Green Solvent Selection

Solvents are widely used in chemical synthesis but many traditional solvents are toxic and harmful to the environment. AI tools can analyze chemical databases to identify safer and environmentally friendly solvent alternatives. These recommendations help industries adopt greener solvent systems in chemical manufacturing.

5. AI in Sustainable Materials Development

Recent research shows that AI is being applied to develop sustainable materials such as biodegradable polymers, eco-friendly coatings, and renewable energy materials. By analyzing molecular properties and material performance, AI can accelerate the discovery of materials that are both efficient and environmentally safe.

6. Real-Time Monitoring and Smart Manufacturing

I-driven sensors and automated monitoring systems are being integrated into chemical industries to track reaction progress and environmental emissions in real time. These intelligent systems help detect potential hazards, control pollution, and improve the safety of industrial processes.

Review of Literature

Green chemistry has become a central framework for addressing environmental challenges associated with chemical manufacturing and industrial processes. Since the introduction of the twelve principles of green chemistry, researchers have increasingly focused on designing chemical reactions and products that minimize waste, reduce toxicity, and improve energy efficiency. In recent years, the integration of artificial intelligence (AI), machine learning (ML), and data-driven computational methods has significantly accelerated research and innovation in this field. AI has emerged as a powerful tool for optimizing chemical processes, predicting reaction outcomes, and discovering sustainable materials.

Recent literature demonstrates that AI and data science are transforming green chemistry by enabling the analysis of large chemical datasets and facilitating predictive modelling. According to the review by Yadav et al. (2025), AI-based algorithms such as machine learning and deep learning can analyze complex chemical information to predict molecular properties, reaction mechanisms, and optimal reaction pathways. These capabilities significantly reduce the need for traditional trial-and-error experimentation and enable faster discovery of environmentally friendly chemical processes.

A major focus in the literature is the application of AI in reaction prediction and synthesis planning. Traditional chemical synthesis often requires extensive experimental screening of reagents, catalysts, and reaction conditions. However, AI models can analyze historical reaction data and predict reaction yields, selectivity, and possible by-products. Studies indicate that machine learning models can optimize reaction parameters such as temperature, solvent selection, and catalyst loading, leading to more efficient and sustainable chemical transformations. This approach helps minimize waste generation and reduces energy consumption in chemical laboratories and industrial production systems.

Another significant research direction involves the use of AI in catalyst discovery and molecular design. Catalysts play a crucial role in green chemistry because they enhance reaction efficiency while reducing energy requirements and harmful by-products. AI-based molecular modelling techniques allow researchers to explore vast chemical spaces and identify potential catalysts with improved activity and selectivity. Advanced machine learning models are increasingly used to establish relationships between catalyst structures and their catalytic performance, enabling faster development of environmentally friendly catalytic

AI also contributes significantly to sustainable materials discovery, including the development of green catalysts and functional materials. For instance, machine learning-assisted approaches are being used to design advanced two-dimensional catalytic materials for pollutant degradation and environmental remediation. These computational methods enable the rapid screening of thousands of material candidates before experimental validation, thereby reducing laboratory waste and resource

Furthermore, several studies highlight the role of AI in green process development and environmental applications. Machine learning models are increasingly used to optimize wastewater treatment processes, adsorption systems, and advanced oxidation processes used in pollution control. AI algorithms can predict pollutant degradation efficiency under varying conditions such as pH, catalyst concentration, and reaction time, enabling more efficient environmental management strategies. These applications demonstrate the ability of AI to support sustainable chemical engineering and environmental protection.

Another emerging research area involves the integration of computational chemistry and machine learning to improve biomass conversion and renewable feedstock utilization. Computational models combined with machine learning are being used to study complex systems such as ionic liquids for lignin processing and biomass valorization. These approaches provide predictive insights into molecular interactions and reaction mechanisms, facilitating the design of greener solvents and sustainable chemical processes.

Despite these promising developments, the literature also identifies several limitations and challenges. One of the most significant issues is the availability of high-quality and standardized chemical datasets required for training AI models. Many chemical databases remain incomplete or inconsistent, which can limit the accuracy of predictive models. Additionally, the interpretability of AI algorithms remains a challenge, as complex machine learning models often function as “black boxes,” making it difficult for chemists to understand the underlying decision-making processes. Researchers therefore emphasize the importance of interdisciplinary collaboration between chemists, computer scientists, and data analysts to fully realize the potential of AI in sustainable chemistry.

Overall, the existing literature suggests that artificial intelligence has the potential to significantly transform green chemistry by enabling data-driven discovery, improving reaction efficiency, and supporting the development of environmentally sustainable chemical processes. As computational capabilities continue to evolve and larger chemical datasets become available, AI is expected to play an increasingly important role in advancing sustainable chemical research and industrial applications.

Research and Methodology

The methodological framework of this research is designed to critically investigate how AI-driven technologies are revolutionizing green chemistry by enabling more efficient, sustainable, and data-driven chemical innovation. This approach combines systematic scientific analysis, critical evaluation of contemporary literature, and interdisciplinary interpretation of technological developments within the fields of computational chemistry and sustainable chemical engineering.

The study relies primarily on a comprehensive and methodologically structured review of peer-reviewed scientific literature obtained from internationally recognized academic databases. Authoritative research sources were collected from platforms such as Google Scholar, Science Direct, SpringerLink, Web of Science, and Scopus, which collectively provide extensive coverage of high-impact publications in chemistry, materials science, and artificial intelligence. The literature search strategy employed a combination of targeted keywords and Boolean search expressions including “artificial intelligence in sustainable chemistry,” “machine learning-assisted reaction optimization,” “AI-driven green process design,” “data-driven catalysis,” and “sustainable chemical manufacturing through machine learning.” To ensure the relevance and contemporary significance of the research, the literature survey focused primarily on studies published between 2015 and 2025, a period characterized by rapid advancements in AI-enabled chemical research.

Following the identification of potential sources, a rigorous screening and selection procedure was implemented to ensure the scientific credibility and relevance of the analyzed literature. Publications were

included if they provided empirical evidence or computational demonstrations of AI applications in areas such as sustainable reaction design, catalytic optimization, solvent selection, molecular property prediction, and environmentally responsible materials discovery. Studies lacking methodological transparency, experimental validation, or relevance to green chemistry principles were systematically excluded. Through this evaluation process, only high-quality peer-reviewed articles and review papers with strong methodological foundations were incorporated into the analytical dataset.

The analytical component of the research focuses on evaluating the role of advanced AI methodologies, particularly machine learning algorithms, deep neural networks, and predictive modeling frameworks, in optimizing chemical reactions and minimizing environmental impact. These computational approaches allow chemists to analyze large experimental datasets, identify correlations between molecular structures and reaction outcomes, and predict optimal reaction conditions with significantly reduced experimental trials. Such predictive capabilities are particularly valuable in green chemistry because they enable the design of synthetic pathways that minimize hazardous reagents, reduce solvent usage, and enhance atom economy while maintaining high reaction efficiency.

In addition to predictive modeling, the methodological framework also examines how AI-based systems contribute to intelligent reaction planning and automated process optimization. By analyzing case studies reported in recent scientific publications, the research evaluates examples where AI algorithms have been applied to accelerate catalyst discovery, design biodegradable materials, and optimize pharmaceutical synthesis using environmentally safer methodologies. These case studies demonstrate that AI can significantly reduce the time and resource requirements associated with traditional experimental workflows while simultaneously improving sustainability metrics such as energy efficiency and waste minimization. The methodology therefore incorporates comparative evaluation between conventional trial-and-error experimental strategies and AI-assisted data-driven approaches to highlight the efficiency gains achieved through computational technologies.

Furthermore, this research integrates conceptual insights from multiple scientific disciplines, including computational chemistry, chemical engineering, and environmental science, in order to provide a holistic understanding of AI-driven sustainable innovation. Particular emphasis is placed on the emerging role of automated laboratories, intelligent reaction optimization platforms, and digital chemical databases that facilitate rapid data analysis and predictive experimentation. These technological developments illustrate how AI can transform traditional chemical research environments into highly efficient and environmentally responsible systems capable of continuously improving reaction performance while adhering to the core principles of green chemistry.

To ensure methodological robustness, the selected literature was critically evaluated based on factors such as reproducibility of experimental results, reliability of computational models, and relevance to sustainability objectives. Studies demonstrating clear validation of AI predictions through experimental verification were given greater emphasis, as such work provides strong evidence of the practical applicability of AI in chemical research. By synthesizing insights from diverse yet complementary research domains, this methodological approach enables a comprehensive understanding of how artificial intelligence is reshaping the conceptual and practical foundations of green chemistry.

Overall, the research methodology integrates systematic literature analysis, interdisciplinary knowledge synthesis, and critical scientific evaluation to investigate the revolutionary influence of artificial intelligence on sustainable chemical innovation. Through this rigorous methodological framework, the study highlights how AI-driven technologies can significantly enhance the design of environmentally friendly chemical processes, reduce resource consumption, and accelerate the transition toward sustainable industrial chemistry. The findings derived from this approach contribute to a deeper scientific understanding of how artificial intelligence can function as a powerful catalyst for advancing the global objectives of green chemistry and sustainable technological development.

AI in Green Process Development

Artificial Intelligence (AI) has become an influential tool in the development of environmentally sustainable chemical processes, often referred to as green process development. In traditional chemical manufacturing,

designing efficient processes requires extensive experimentation, high energy input, and large quantities of raw materials, which can lead to significant waste generation and environmental pollution. AI helps overcome these challenges by using advanced computational techniques such as machine learning, predictive modeling, and data analytics to design and optimize chemical processes more efficiently. By analyzing vast chemical datasets, AI can identify optimal reaction pathways, select safer reagents and solvents, and determine reaction conditions that minimize energy consumption and waste formation.

In green process development, AI-driven models can predict reaction yields, catalyst performance, and process efficiency before laboratory-scale experiments are conducted. This predictive capability reduces the need for repeated trial-and-error experimentation, saving both time and resources. AI can also assist in discovering greener catalysts and environmentally friendly solvents that enhance reaction selectivity while reducing the production of harmful by-products. Furthermore, AI technologies integrated with real-time monitoring systems enable continuous control of chemical processes, ensuring that reactions operate under optimal and safe conditions.

Another important contribution of AI is its ability to support process intensification and resource optimization in industrial manufacturing. AI algorithms can analyze operational data from chemical plants to identify inefficiencies and recommend improvements that reduce energy consumption and emissions. This approach not only improves the sustainability of chemical production but also enhances economic efficiency. As research in computational chemistry and data science continues to advance, AI is expected to play an even more significant role in green process development, helping scientists and industries design cleaner, safer, and more sustainable chemical manufacturing systems that align with the principles of green chemistry.



Fig. 2 AI-Driven Green Technologies

AI-Assisted Electrocatalysis: A Case Study in Advancing Green Chemistry

A significant case study demonstrating the impact of artificial intelligence in sustainable chemical innovation is the application of AI in electrocatalysis for environmentally friendly energy and chemical production. Electrocatalysis has become a central area of research in Green Chemistry because it enables chemical transformations driven by electricity rather than fossil-fuel-intensive thermal processes. However, identifying highly efficient and stable electrocatalysts through conventional experimentation is often slow and resource-intensive. Artificial intelligence has emerged as a powerful tool to accelerate the discovery and optimization of electrocatalytic materials by analyzing large datasets and predicting catalyst performance before laboratory synthesis.

In recent research, machine learning algorithms have been employed to design advanced electrocatalysts for reactions such as hydrogen evolution, oxygen reduction, and carbon dioxide reduction. One notable study applied machine learning models trained on thousands of experimentally reported catalytic materials to predict

the activity of transition metal catalysts for hydrogen production. The AI system evaluated structural descriptors such as electronic configuration, binding energy, and surface adsorption properties, allowing it to rapidly screen numerous catalyst candidates. The model successfully identified several non-precious metal catalysts capable of exhibiting catalytic activity comparable to traditional platinum-based catalysts. This discovery is particularly significant because replacing rare and expensive metals with abundant alternatives can greatly improve the sustainability and economic feasibility of clean energy technologies.

Another example highlights the application of deep learning methods to discover electrocatalysts for carbon dioxide conversion. In this case, researchers developed AI models capable of predicting how different catalyst surfaces interact with CO₂ molecules during electrochemical reduction. By analyzing complex reaction intermediates and adsorption energies, the model identified promising copper-based alloy catalysts that enhance the selectivity of CO₂ conversion into useful fuels such as carbon monoxide and formic acid. These AI-guided predictions were subsequently validated through experimental testing, confirming that the predicted catalysts demonstrated improved efficiency and lower energy requirements compared with conventional materials. Such findings illustrate how AI can reduce the need for extensive laboratory screening while simultaneously improving catalytic performance.

Artificial intelligence has also been used to optimize the operational conditions of electrocatalytic systems. Through data-driven analysis, AI models can determine the optimal voltage, electrolyte composition, and reaction temperature required to maximize catalytic efficiency while minimizing energy consumption. This capability is particularly valuable in large-scale electrochemical processes where small improvements in efficiency can lead to substantial reductions in energy usage and greenhouse gas emissions. By combining predictive catalyst discovery with intelligent process optimization, AI significantly enhances the environmental benefits of electrocatalytic technologies.

Overall, the integration of artificial intelligence with electrocatalysis represents a transformative advancement for sustainable chemical research. AI-assisted catalyst design enables rapid exploration of complex chemical spaces, allowing scientists to identify environmentally benign catalytic materials that support clean energy generation and carbon recycling. These developments demonstrate that AI not only accelerates catalyst discovery but also contributes directly to the broader objectives of green chemistry, including reduced reliance on toxic materials, improved energy efficiency, and the development of sustainable chemical processes.

Impact of Artificial Intelligence on Green Chemistry Development

1.Improving Efficiency in Chemical Research

One of the major advantages of AI is its ability to analyze large volumes of chemical data quickly and accurately. Traditional chemical research often involves numerous experimental trials, which require significant time, materials, and energy. AI algorithms can predict reaction outcomes, molecular properties, and optimal reaction conditions before laboratory experimentation. This reduces the need for repeated experiments and improves the efficiency of chemical research.

2.Reduction of Chemical Waste

Waste generation is a major issue in chemical industries. AI plays an important role in reducing chemical waste by predicting reaction pathways that produce fewer unwanted by-products. Machine learning models can suggest efficient synthesis routes that follow the principle of waste prevention in green chemistry. By optimizing reactions and minimizing material loss, AI contributes to cleaner and more sustainable chemical production.

3.Development of Safer Chemicals

Another important contribution of AI in green chemistry is the development of safer and less toxic chemical substances. AI systems can analyze chemical structures and predict toxicity, biodegradability, and environmental persistence of compounds. These predictions help scientists design chemicals that perform their intended function while causing minimal harm to the environment and human health.

4. Energy Conservation and Process Optimization

Chemical manufacturing often requires high energy input due to extreme temperatures and pressures. AI-based optimization tools can analyze process data and determine conditions that require less energy while maintaining high product yield. By improving energy efficiency, AI helps reduce greenhouse gas emissions and promotes environmentally sustainable industrial practices.

5. Discovery of Sustainable Catalysts and Materials

Catalysts are essential for improving reaction efficiency and reducing waste formation. AI accelerates the discovery of new catalysts by predicting their activity, selectivity, and stability. Similarly, AI helps researchers design sustainable materials such as biodegradable polymers and environmentally friendly coatings. These innovations support the development of greener chemical technologies.

6. Real-Time Monitoring and Pollution Prevention

AI technologies can be integrated with sensors and monitoring systems to track chemical reactions and industrial emissions in real time. These systems can detect harmful pollutants and process irregularities at early stages. Early detection allows industries to control emissions and prevent environmental contamination, which aligns with the pollution prevention principle of green chemistry.

7. Supporting Sustainable Industrial Development

AI-driven technologies enable industries to adopt sustainable manufacturing practices by improving resource management and reducing environmental impact. Through predictive modeling and data-driven decision-making, industries can develop processes that use fewer raw materials, generate less waste, and consume less energy. This contributes to sustainable economic development and environmental protection.

8. Encouraging Innovation and Future Research

The integration of AI with green chemistry encourages interdisciplinary research involving chemists, data scientists, and environmental scientists. AI-driven tools open new opportunities for discovering innovative chemical processes and materials that were previously difficult to design using conventional methods. As computational technologies continue to advance, the role of AI in green chemistry is expected to expand further.

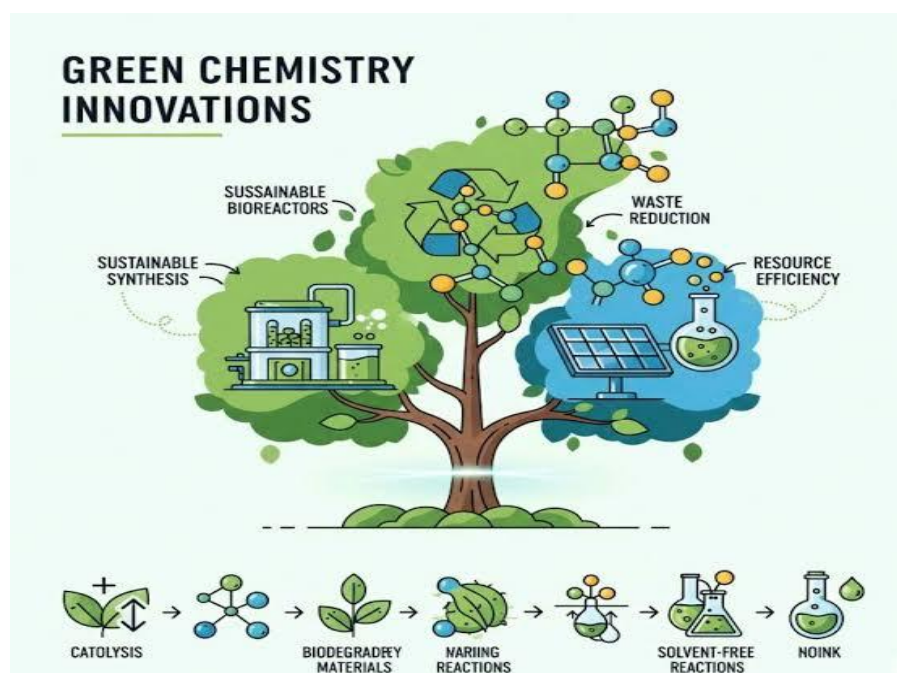


Fig.3 Enhancing Green Chemistry through Artificial Intelligence

Future Directions and Opportunities of Artificial Intelligence in Green Chemistry

The combination of Artificial Intelligence (AI) and green chemistry is creating new opportunities for developing sustainable chemical technologies. As environmental challenges such as pollution, climate change, and resource depletion increase, the need for cleaner and more efficient chemical processes has become essential. AI provides powerful computational tools that can analyze complex chemical systems, predict outcomes, and optimize processes. Future developments in AI are expected to further strengthen the application of green chemistry principles in research and industrial practices.

1. Development of Advanced Predictive Models

One important future direction of AI in green chemistry is the development of more accurate predictive models. These models can analyze molecular structures and reaction mechanisms to predict properties such as toxicity, stability, and environmental impact. Improved predictive capabilities will help chemists design safer chemicals and sustainable processes before performing laboratory experiments, reducing time, cost, and environmental risks.

2. Integration with Automated and Robotic Laboratories

The integration of AI with automated laboratory systems represents a promising opportunity for green chemistry research. AI-controlled robotic systems can perform multiple experiments simultaneously and analyze results in real time. This automated approach can rapidly identify optimal reaction conditions, reducing the consumption of chemicals, energy, and laboratory resources.

3. Expansion of Sustainable Chemical Databases

High-quality data is essential for training AI models. Future research will focus on creating large, well-organized databases containing information on chemical reactions, environmental toxicity, biodegradability, and energy efficiency. These databases will improve the accuracy of AI predictions and support the discovery of environmentally friendly chemical processes.

4. AI in Renewable Resource Utilization

Another promising direction is the use of AI to identify and develop renewable feedstocks for chemical synthesis. AI tools can analyze biological and agricultural resources to determine their potential as sustainable alternatives to fossil-based raw materials. This approach supports the development of bio-based chemicals and sustainable industrial practices.

5. Design of Eco-Friendly Materials

AI has the potential to accelerate the discovery of environmentally friendly materials such as biodegradable polymers, green solvents, and sustainable catalysts. By analyzing molecular structures and material properties, AI can suggest new compounds that meet both performance and environmental safety requirements. This will help reduce the environmental impact of industrial materials and chemical products.

6. Real-Time Environmental Monitoring

Future AI systems may be integrated with environmental sensors and monitoring technologies to track pollutants and emissions in real time. These intelligent monitoring systems can detect harmful substances and suggest corrective actions immediately. This approach will improve pollution control and support safer chemical manufacturing processes.

7. Promotion of Circular Chemical Economy

AI can support the development of a circular chemical economy, where resources are reused and recycled instead of being discarded as waste. AI-driven models can identify efficient recycling methods, optimize

material recovery processes, and suggest sustainable alternatives for waste management. This will help reduce environmental pollution and improve resource efficiency.

8.Strengthening Interdisciplinary Collaboration

Future progress in AI-driven green chemistry will depend on collaboration between chemists, computer scientists, environmental experts, and engineers. Interdisciplinary research will help develop more reliable AI tools and innovative solutions for sustainable chemical production.

9.Addressing Ethical and Technological Challenges

As AI becomes more widely used in chemical research, it will be important to address challenges related to data quality, transparency of AI models, and responsible use of technology. Future research should focus on developing interpretable AI systems and ensuring that AI technologies are applied ethically and responsibly in environmental and chemical research.

Challenges in the Role of Artificial Intelligence in Green Chemistry in Current Chemical Industries

The integration of Artificial Intelligence (AI) into green chemistry has created significant opportunities for developing sustainable and environmentally friendly chemical processes. However, despite its potential benefits, several challenges limit the widespread adoption of AI in current chemical industries. These challenges arise from technical limitations, data-related issues, economic factors, and the complexity of chemical systems.

1.Limited Availability of High-Quality Data

AI systems rely heavily on large and reliable datasets to make accurate predictions. In many chemical industries, experimental data are incomplete, inconsistent, or not standardized. Many chemical reactions and industrial processes have limited publicly available data, which makes it difficult to train effective AI models. Without sufficient high-quality data, AI predictions may become unreliable.

2.Complexity of Chemical Processes

Chemical reactions and industrial processes are often highly complex and involve multiple variables such as temperature, pressure, catalysts, and reaction mechanisms. These complex interactions are difficult for AI models to fully capture and predict accurately. As a result, developing reliable AI systems for industrial-scale chemical processes remains challenging.

3.Integration with Existing Industrial Systems

Many chemical industries operate using traditional manufacturing technologies that were developed long before AI applications became common. Integrating AI-based tools with these existing systems requires significant modification of infrastructure, which can be technically difficult and time-consuming.

4.High Implementation Cost

The adoption of AI technologies often requires advanced computational infrastructure, specialized software, and skilled professionals such as data scientists and computational chemists. These requirements can lead to high implementation costs, making it difficult for small or medium-sized chemical industries to adopt AI-based solutions.

5.Lack of Interdisciplinary Expertise

The successful application of AI in green chemistry requires collaboration between chemists, computer scientists, engineers, and environmental experts. However, many industries lack professionals who possess expertise in both chemistry and artificial intelligence. This knowledge gap slows the development and implementation of AI-driven sustainable technologies.

6. Difficulty in Interpreting AI Models

Many AI systems, especially deep learning models, function as “black boxes,” meaning their decision-making process is not always easy to interpret. For chemical researchers and engineers, understanding how AI arrives at its predictions is important for verifying the reliability and safety of chemical processes.

7. Data Privacy and Industrial Confidentiality

Chemical industries often treat experimental data and production methods as confidential information. Sharing such data for AI training can raise concerns related to intellectual property and industrial security. This limitation restricts the availability of large datasets needed for developing effective AI models.

8. Environmental and Ethical Considerations

Although AI supports sustainable chemical practices, the development and use of AI technologies themselves require computational resources and energy. High computational demands may lead to increased energy consumption, which could indirectly impact environmental sustainability if not managed properly.

9. Regulatory and Standardization Issues

The use of AI in chemical industries is still evolving, and regulatory frameworks for AI-driven chemical processes are not fully established in many regions. Lack of clear guidelines and standardization can slow down industrial adoption of AI technologies.

CONCLUSION

In conclusion, Artificial Intelligence (AI) has emerged as a powerful and transformative tool in advancing the goals of green chemistry. By integrating data-driven technologies such as machine learning, predictive modeling, and computational analysis, AI enables researchers to design safer chemicals, optimize reaction conditions, and develop more sustainable industrial processes. It helps reduce chemical waste, minimize energy consumption, and improve resource efficiency while supporting the discovery of environmentally friendly materials and catalysts. In addition, AI-driven monitoring and automation systems contribute to pollution prevention and safer chemical manufacturing. Although challenges such as limited datasets, computational complexity, and the need for interdisciplinary expertise still exist, ongoing technological advancements are gradually overcoming these limitations. Overall, the combination of AI and green chemistry offers significant potential for promoting sustainable scientific innovation and environmental protection. As research in this field continues to grow, AI is expected to play a crucial role in shaping the future of environmentally responsible chemical processes and contributing to global sustainability goals.

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