



AI-Driven Green Chemistry: A Digital Innovation Framework for Developing Countries

* Dr. Anil Kumar¹, Ashwaraya Prakash²

¹ Head of Dept., P.G. Department of Chemistry, Sahibganj College, Sahibganj, S.K.M.U.-Dumka.

² P.G. Scholar, P.G. Department of Chemistry, Sahibganj College, Sahibganj, S.K.M.U.-Dumka.

Corresponding author: **Dr. Anil Kumar**

Head of Dept., P.G. Department of Chemistry, Sahibganj College, Sahibganj, S.K.M.U.-Dumka.

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Abstract

Artificial Intelligence (AI) is creating new opportunities for skill development and entrepreneurship, especially in India. In developing countries, many chemistry students and youth lack practical laboratory skills due to high costs, safety concerns and limited resources. Traditional chemistry education often depends on expensive chemicals and infrastructure, making it less accessible. Green Chemistry offers a sustainable solution by promoting eco-friendly reactions, safer solvents and waste reduction. AI can support this by predicting chemical reactions, suggesting greener methods and enabling skill-based learning. This paper highlights how AI-based tools, virtual labs and mobile platforms can train youth in green chemistry and support entrepreneurship. The study also discusses outcomes, challenges, government initiatives, ethical concerns and future scope.



Graphical Abstract: AI Tools & Apps for Green Chemistry

Keywords: AI in Green Chemistry, Entrepreneurship Skills, Skill Development, Sustainable Chemistry, Developing Countries.

I. INTRODUCTION

In progressive India, many students do not get the chance to learn chemistry in a practical way. This is mainly because schools and colleges often lack proper laboratories, chemicals are expensive and there are safety risks^[2]. So, students mostly study theory from books and do not get hands-on experience, which makes learning less effective.

Green Chemistry is a helpful approach here. It focuses on using safe, eco-friendly chemicals and reducing waste^[4,11]. This makes chemistry easier, cheaper and safer to practice, even in places with fewer resources.

At the same time, Artificial Intelligence (AI) is changing how students learn. AI tools can act like virtual labs where students can see experiments, understand reactions and learn step-by-step processes. They can also suggest safer and greener ways to carry out chemical reactions^[1,8].

When AI and Green Chemistry are combined, they can make learning more practical and interesting for students. It also opens doors for small business ideas like making herbal products, natural dyes, organic fertilizers and simple water purification systems. In this way, students not only learn better but can also use their knowledge to earn a living and support their communities^[5,15].

2. Objectives

The main objective of this study is to develop practical green chemistry skills among students using AI-based tools^[3,8], enabling them to understand concepts like solvent selection and reaction optimization in a simple and safe way. It also aims to promote entrepreneurship by encouraging youth to start small, eco-friendly businesses based on sustainable chemical processes^[5,16]. Another important goal is to reduce the gap between theoretical knowledge and practical application through virtual learning methods^[3]. Additionally, the study focuses on creating low-cost, mobile-based training models that are easily accessible to the students^[9], while promoting environmentally responsible and sustainable business practices^[10].

3. Experimental Mindset

This study is based on the use of AI tools and digital platforms for training in green chemistry. Machine learning-based tools are used for reaction prediction and green solvent selection^[8,13]. Virtual laboratories and simulations are used to provide practical experience without the use of real chemicals, making learning safe and cost-effective^[3,14].

Various AI tools and applications are included such as Unreal Chemist App for reaction simulation, AI4Green for sustainable solvent selection^[3,14], ChemCopilot for formulation development^[19] and DOZNTM (Sigma Aldrich) for evaluating chemical sustainability^[21]. These tools help students understand real-life chemical processes.

Mobile-based platforms are designed for such areas which have low internet connectivity. These platforms provide personalized learning modules, quizzes and case studies such as biofuel production and natural extraction techniques. AI is also used for entrepreneurship training by helping users generate business ideas, estimate costs and analyse market demand. Different AI tools are as follows^[7,17,18,20]: [Table 1]




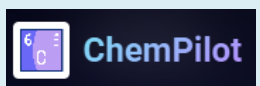


AI Tool	Symbolic Figure	Mode of Operation	Uses in Green Chemistry
AI4Green		Reaction input → AI analysis → Green solvent suggestion	Eco-friendly reaction design, solvent replacement, sustainability scoring
ChemCopilot		Data input → AI modeling (digital twin) → Optimization	Sustainable product formulation, emission reduction
ChemGPT		Molecule input → AI prediction → Green synthesis route	Designing safer synthesis pathways
ChemPilot		Reactants input → AI predicts pathways → Optimized reaction	Efficient, low-waste reaction development
DOZN TM Tool		Chemical input → 12 green principles evaluation → Score output	Sustainability assessment and green rating
Unreal Chemist		Virtual lab → Simulation → AI feedback	Safe practical training without real chemicals

Table 1: Different AI tools

3.1 Implementation

AI4Green is a web application that helps users manage chemical data and calculate sustainability metrics. It's built with Python (Flask) for the backend and JavaScript, HTML and CSS for the frontend. Users can enter chemical data using a chemical editor (MarvinJS) or formats like SMILES. The app dynamically calculates green chemistry metrics and generates reports that can be downloaded as PDF or CSV^[3,14].

The backend uses a Postgres database containing chemical and sustainability data from sources like PubChem and ChEMBL. The database organizes information into tables for users, groups, workbooks, solvents, hazards, compounds and reactions. Flask's structure makes it easy to add new features and the app can be hosted online or locally using Docker. Process of implementation is as follows:

1. Reaction Design: The chemical reaction is drawn in the AI4Green software. Phenol reacts with acetic anhydride to form phenyl acetate and acetic acid. The structures of reactants and products are clearly shown with a reaction arrow. This step is important because it defines what reaction is going to be performed. (Figure 1)

2. Reactants and Reagents Entry: All reactants and reagents are entered into the system. Details such as molecular weight, density, amount, volume and equivalents are filled. Phenol is selected as the limiting reagent; acetic anhydride is taken in excess and sulfuric acid is added as a catalyst. This helps the software understand the quantities used in the reaction. (Figure 2)

3. Summary of Reaction and Hazard Assessment: It includes all reactants, reagents and solvent details along with calculated values. The theoretical yield of the product (phenyl acetate) is also shown. This summary works like a ready-made lab report. The hazards of all chemicals are listed using H-codes. The software also shows hazard rating, exposure level and overall risk. In this case, the reaction has a high-risk rating due to harmful and flammable chemicals. This helps ensure safe handling in the laboratory. (Figure 3)

4. Solvent Guide: Ethyl acetate is selected as the solvent. The software gives ratings for safety, health and environmental impact. It also provides information like boiling point and flash point. This helps in choosing safer and eco-friendly solvents. (Figure 4)

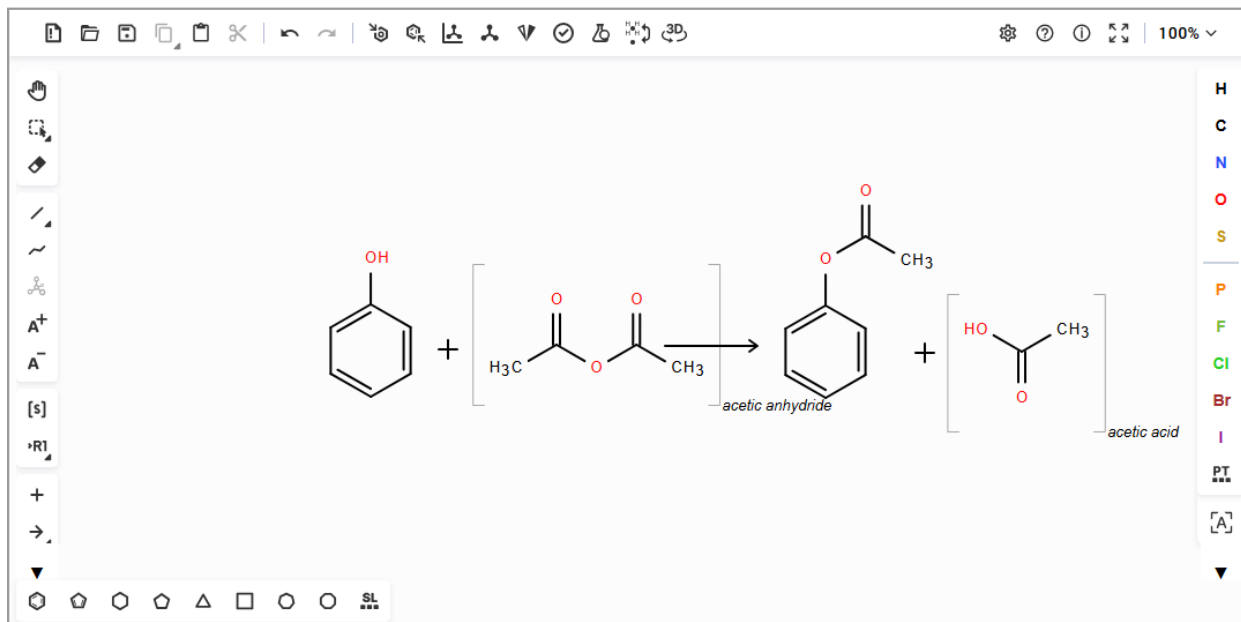
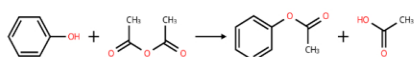


Figure 1. Users draw their reaction using the Marvin reaction sketcher.

No	Reactants	Limiting Reagent?	Mol.Wt	Density (g/mL)	Conc. (M)	Equiv.	Amount (mmol)	Volume (mL)	Mass (mg)	Physical Form	Hazards
1	Phenol	●	94.11	1.06	-	1	10.00	0.89	941	Dense solid	H301-H311-H314-H331-H341-H373
2	Acetic Anhydride	○	102.09	1.08	-	1.2	12.0	1.13	1225	Volatile liquid (70°C ≤ b.p. ≤ 130°C)	H226-H302-H314-H332
Catalysts/reagents											
3	Sulfuric Acid	○	98.08	1.841	-	0.1	1.00	0.05	98.1	Non-volatile liquid (b.p. > 130°C)	H314
Solvents											
4	Ethyl Acetate	○			2.00			5		Volatile liquid (70°C ≤ b.p. ≤ 130°C)	H225-H302-H314-H371
Product											
5	Phenyl acetate	●	136.15			1	10.00	1361		Unknown	H302-H315-H319
6	Acetic Acid	○	60.05			1	10.00	600		Volatile liquid (70°C ≤ b.p. ≤ 130°C)	H226-H314

Summary

Figure 2. A partially complete reaction table. Users can get proper idea about the reaction. Users are directed to provide some information about reaction (highlighted in red). Reagents, solvents and novel compounds can be added or removed. Some information such as molecular weight and hazard codes are automatically taken from the PubChem database.



No	Reactants/catalysts/reagents	Mol.Wt	Equiv.	Density (g/mL)	Conc. (M)	Amount (mmol)	Volume (mL)	Mass (mg)
1	Phenol	94.11	1	1.06		10.00	0.89	941
2	Acetic Anhydride	102.09	1.2	1.08		12.0	1.13	1225
3	Sulfuric Acid	98.08	0.1	1.841		1.00	0.05	98.1
Solvents								Volume (mL)
4	Ethyl Acetate						5	
Product		Mol.Wt	Equiv.	Theoretical Yield (mg)		Unreacted (mg)	Product Mass (mg)	% Yield
5	Phenyl acetate	136.15	11	1361				
6	Acetic Acid	60.05		600				

Hazards	Hazard Rating	Exposure Potential	Risk Rating
1 H301 Toxic if swallowed, H311 Toxic in contact with skin, H314 Causes severe skin burns and eye damage, H331 Toxic if inhaled, H341 Suspected of causing genetic defects, H373 Causes damage to organs through prolonged or repeated exposure	H	L	M
2 H226 Flammable liquid and vapor, H302 Harmful if swallowed, H314 Causes severe skin burns and eye damage, H332 Harmful if inhaled	H	M	H
3 H314 Causes severe skin burns and eye damage	H	L	M
4 H225 Highly Flammable liquid and vapor, H302 Harmful if swallowed, H319 Causes serious eye irritation, H371 May cause damage to organs	H	M	H
5 H302 Harmful if swallowed, H315 Causes skin irritation, H319 Causes serious eye irritation	H	M	H
6 H226 Flammable liquid and vapor, H314 Causes severe skin burns and eye damage	H	M	H

Figure 3. Part of the Summary Table showing information about the hazards of the reactions and various green and sustainability metrics and considerations.

Solvent Guide

About the Solvent Guide | Solvent Surfer

Choose up to two solvents from the classes below to compare them!

- Acids
- Alcohols
- Amines
- Aprotic polar
- Esters
- Ethers
- Halogenated
- Hydrocarbons
- Ketones
- Miscellaneous
- Water

Ethyl acetate
Recommended

CAS: 141-79-6
Family: Esters
Boiling Point / °C: 77
Flash Point / °C: -4
Safety: 5
Health: 3
Environment: 5
Worst H3xx: H319
Worst H4xx: 0

Issues: na
Possible Substitution(s): No Substitutions Found

Figure 4. Solvent Guide where users can explore different solvent options for their reaction.

4. AI Tools Applications in Green Chemistry

AI plays a key role in the different application of AI tools in Green Chemistry [Figure 5]

- 1. Reaction Prediction and Optimization:** AI predicts chemical reactions and suggests ideal conditions (temperature, solvent, catalyst) to increase yield while reducing waste and energy consumption^[1,8].
- 2. Selection of Eco-friendly Solvents:** AI tools recommend green solvents that are less toxic, biodegradable and safer for both humans and the environment^[4,10].
- 3. Waste Reduction Strategies:** AI identifies cleaner reaction pathways and helps minimize harmful by-products, supporting pollution control and sustainability^[12].
- 4. Process Simulation and Modelling:** AI enables virtual testing of chemical processes, reducing the need for real experiments, saving cost, time and resources^[8].
- 5. Designing Sustainable Chemical Products:** AI helps in designing eco-friendly products that are efficient, safe and aligned with green chemistry principles^[5].
- 6. Energy Efficiency Optimization:** AI suggests low-energy reaction routes and optimal conditions to reduce power consumption in chemical processes^[1].
- 7. Green Catalyst Design:** AI assists in discovering and optimizing catalysts that are non-toxic, reusable and highly efficient^[13].
- 8. Life Cycle Assessment (LCA):** AI evaluates the environmental impact of chemicals and processes from production to disposal^[5].
- 9. Real-time Process Monitoring:** AI uses sensors and data analytics to monitor reactions and control emissions during manufacturing^[8].
- 10. Green Drug Design:** AI supports the development of pharmaceuticals with reduced toxicity and environmental impact^[6,11].
- 11. Supply Chain Optimization:** AI improves raw material selection, logistics and reduces carbon footprint in chemical industries^[5].

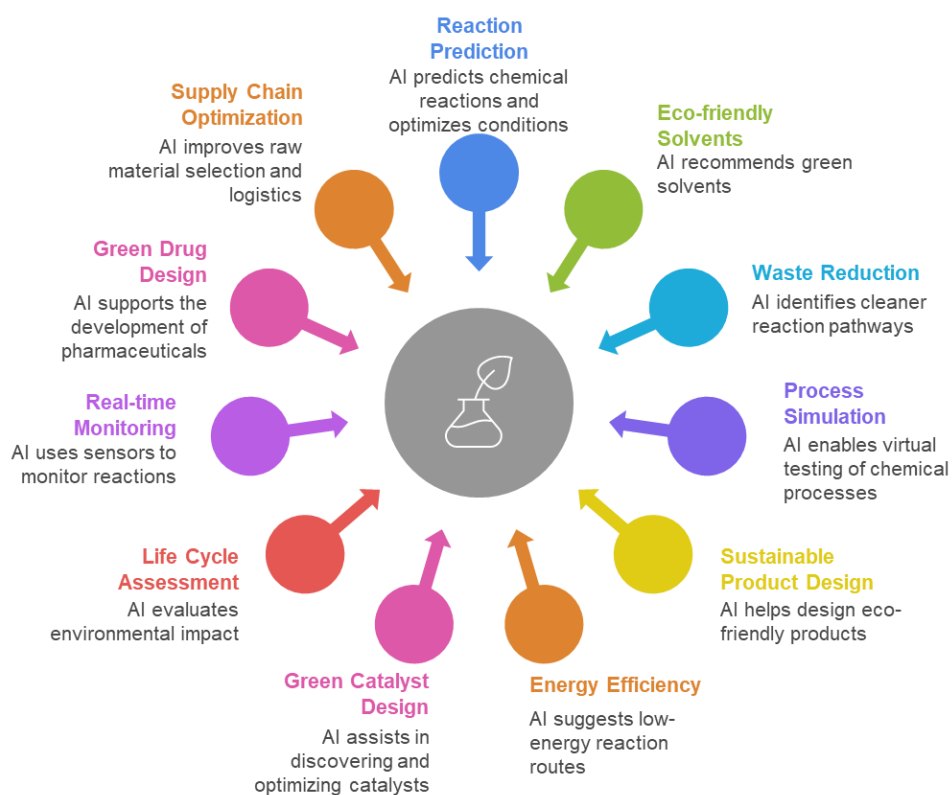


Figure 5: Application of AI Tools in Green Chemistry

5. Advantages

Artificial Intelligence-based green chemistry training offers several important benefits for education and entrepreneurship, as explained below:

1. **Low-cost Skill Development:** AI-based platforms reduce the need for expensive chemicals and laboratory setups, making training affordable for students^[3].
2. **Safe Learning Environment:** Virtual labs allow students to perform experiments without handling hazardous chemicals, reducing risks and accidents^[14].
3. **Promotes Sustainability:** AI encourages the use of eco-friendly methods, reducing pollution and supporting green chemistry principles^[12,15].
4. **Encourages Self-employment:** Learners can use their skills to start small businesses such as natural product making, eco-dyes and water purification systems^[5].
5. **Accessible through Mobile Devices:** AI tools and apps can be accessed through smartphones, making learning possible even in remote areas^[9].
6. **Personalized Learning:** AI provides customized learning paths based on the student's level, improving understanding and skill development.
7. **Time-efficient Learning:** AI speeds up the learning process by providing quick solutions, simulations and real-time feedback.

6. Disadvantages

AI-based green chemistry training also has some limitations, especially in rural settings, as explained below:

1. **Dependence on Technology:** Continuous access to devices and software is required; system failures or lack of devices can interrupt learning^[2].
2. **Limited Internet Connectivity:** Many areas have slow or unstable internet, which affects access to online tools, updates and cloud-based simulations^[2].
3. **Lack of Awareness and Digital Literacy:** Students and teachers may not be familiar with AI tools, reducing effective usage and adoption^[9].
4. **Initial Training Requirement:** Users need basic training to operate AI platforms, which may require time, resources and expert support.
5. **Cost of Devices and Maintenance:** Although training is low-cost, smartphones, computers and their maintenance can still be expensive for some learners.

7. Challenges

AI-based green chemistry training faces several practical challenges in some areas, as explained below:

1. **Digital Divide:** Unequal access to internet, smartphones and computers limits the reach and effectiveness of AI-based learning platforms^[2].
2. **Language Barriers:** Most AI tools are available only in English, making it difficult for students to understand and use them properly^[9].
3. **Lack of Trained Instructors:** There is a shortage of teachers who have expertise in both artificial intelligence and green chemistry, affecting quality training^[2].
4. **Limited Infrastructure:** In many areas often lack proper laboratories, electricity supply and technical resources, which restricts implementation of AI-based education.
5. **Low Awareness and Adoption:** Many students and institutions are not aware of AI tools and their benefits, leading to slow adoption in education systems.

8. Ethical Consideration

The use of AI in green chemistry must follow ethical principles to ensure safe and fair use, as explained below:

1. **Responsible Use of AI Tools:** AI should be used only for educational and sustainable purposes, avoiding harmful or unethical chemical practices^[10].
2. **Data Privacy and Security:** Personal and research data used in AI platforms must be protected from unauthorized access and misuse.
3. **Avoid Misuse of Chemical Knowledge:** AI-generated chemical information should not be used for harmful activities such as toxic substance development.
4. **Equal Access to Technology:** All students should have fair access to AI tools to avoid inequality in learning opportunities.
5. **Transparency and Accountability:** AI systems should provide clear information about how results are generated and users should be responsible for their application.

9. Expected Outcome

The use of AI in green chemistry must follow ethical principles to ensure safe and fair use, as explained below:

1. **Responsible Use of AI Tools:** AI should be used only for educational and sustainable purposes, avoiding harmful or unethical chemical practices.
2. **Data Privacy and Security:** Personal and research data used in AI platforms must be protected from unauthorized access and misuse.
3. **Avoid Misuse of Chemical Knowledge:** AI-generated chemical information should not be used for harmful activities such as toxic substance development.
4. **Equal Access to Technology:** All students should have fair access to AI tools to avoid inequality in learning opportunities.
5. **Transparency and Accountability:** AI systems should provide clear information about how results are generated and users should be responsible for their application.

10. Scope for Future Work

AI-based green chemistry training can be further improved by developing platforms in regional languages to make learning more accessible for students^[9]. Integrating these modules into college and ITI curricula will provide structured and practical education. This approach can also be expanded to other scientific fields like environmental science and biotechnology^[5]. Additionally, government-supported free training programs can help in reaching a larger population and ensuring equal opportunities for skill development and sustainable entrepreneurship^[10].

11. Conclusion

AI-enabled green chemistry training has the potential to transform education and entrepreneurship in India. It provides safe, affordable and practical learning opportunities. By integrating AI with sustainable chemistry, youth can develop innovative business ideas and contribute to environmental protection. Collaboration between educational institutions, government and technology providers is essential for successful implementation^[1,5,15].

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