



Role of Artificial Intelligence in Green Analytical Technique

Saleem Javid^{1*}, Anamika anil², Diva Suresh.R², Heba Muhammed Haris², Mohammed Gulzar Ahmed³.

¹Department of Pharmaceutical Chemistry, Yenepoya Pharmacy College & Research Centre, Yenepoya (Deemed to be University), Mangalore 570 018, Karnataka, India.

²Department of Pharmacology, Yenepoya Pharmacy College & Research Centre, Yenepoya (Deemed to be University), Mangalore 570 018, Karnataka, India.

³Department of Pharmaceutics, Yenepoya Pharmacy College & Research Centre, Yenepoya (Deemed to be University), Mangalore 570 018, Karnataka, India.

Corresponding author Email: saleemjavid@yenepoya.edu.in

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ABSTRACT

Green analytical chemistry (GAC) has been accelerated by the growing necessity to mitigate environmental degradation and other health hazards posed by conventional analytical processes. The discipline is aimed at minimizing chemical waste and energy consumption and reliance on dangerous substances. The present review explains the usage of Artificial Intelligence (AI) in collaboration with GAC to enhance its sustainability, precision, and efficiency in its analytical operations. The article describes the twelve postulates of GAC, dwells upon the developments in the green chromatography, green spectroscopy, and green extraction techniques, new approaches to gauging of greenness, including GAPI, and the Analytical Eco-Scale. The AI innovation is more concentrated in such aspects as optimization of methods, automation, minimization of waste, and environmental observation. In green analytical chemistry, the application of AI presents a new direction of sustainable operations despite the drawbacks such as high costs, regulatory issues, and data availability. A combination of green principles and digital intelligence is not only enhancing the ability to make analyses but also uniting the chemical sciences in the process of building a greener, safer, and smarter world.

Keywords: Artificial intelligence, Analytical Eco-scale, Green Analytical Chemistry, Green Analytical techniques, Green Analytical Procedure index.

INTRODUCTION

Green analytical chemistry is an overall approach that strives to minimize or avoid toxic and dangerous solvents, reagents, and methods of the preparation, pre-treatment, and analysis stages of an analytical procedure.[1] The objective of the new branch of green analytical chemistry (GAC) is to neutralize the negative effects of chemical analysis on the environment and health in the past by incorporating the principles of green chemistry in the analytical procedures. GAC works to bring analytical protocols in harmony with the overall sustainability objectives by curbing the use of hazardous reagents, cut back on energy usage, and eradicate the creation of hazardous waste. 12 sustainability-based principles spanning waste avoidance to safer solvents and reaction conditions and energy consumption guide GAC discipline. These guidelines constitute a methodology paradigm of creating efficient and sustainable methodologies.[2]

DIFFERENCE BETWEEN GREEN ANALYTICAL CHEMISTRY AND GREEN CHEMISTRY

The main goal of Green Chemistry is to create safer ways of chemical syntheses and production, whereas the Green Analytical Chemistry (GAC) intends to offer greener testing and analysis procedures.

1. Goal: Green chemistry is supposed to make the chemicals not polluting. GAC will assist in reducing wastage and energy consumption during chemical analysis.
2. Management of Waste : Green Chemistry avoids waste during the synthesis process. GAC prefers direct methods of analysis in order to reduce amounts of waste and sample preparation.
3. Chemical Safety: Green Chemistry generates less harmful substances and processes.
4. Use of energy: Green chemistry makes the low energy processes more efficient in the way of energy use.
5. Reagents and Solvents: Green chemistry utilises less hazardous solvents and renewable feedstocks.
6. Green Chemistry attaches a lot of importance to the atom economy in terms of reaction and catalysis efficiency.[3]

The advantages of the green analysis techniques are as follows.

Environment:

- a)The majority of the chemicals enter the environment either during disposal, accidentally (e.g., in emissions during manufacturing) or deliberately, eughthed by using pesticides, etc. Green chemicals either break down to cause no harm or can be recycled to be used once again.
- b) Reduced toxicity of the environment on animals and plants.
- c) Less likelihood of global warming, depletion of ozone layer and smog.
- d)Reduced chemical interference with ecosystems.
- e) Reduced land-filling especially of hazardous waste.

Economy and Business:

- a) Chemical processes with lower amounts of feedstock to produce an equal amount of output yield higher.
- b) Reduced synthetic steps, which are more permissive of greater plant capacity, reduced energy, water usage, and faster production of products.
- c) permit a waste product to be used instead of a purchased feedstock.
- d) Improved performance, which includes using less product in order to attain the same objective.
- e) Increased disagreement between chemical producers and their clients.[4].

Green chemistry reduces environmental and socio-economic effects linked to chemical reactions in industries as well. The conventional methods of chemical manufacturing usually result in the production of hazardous wastes and the endangerment of the health of workers and the environment. Green chemistry is aimed at creating processes and products that do not include the use of harmful substances, or at least limit them, and solve the pollution problem at the design phase instead of dealing with it afterwards. The twelve principles of green chemistry provide guidance to promote safer and more sustainable operations of chemicals [5].

AI and ML are altering the state of green chemistry by enhancing productivity, minimizing waste, and promoting sustainable innovations. AI is more efficient in saving time and materials during research through prediction of material properties, optimization of the process of chemical reactions as well as discovering complex chemical interactions. It can be used to create biodegradable plastics, to come up with green energy sources, in creating pollution reduction strategies, and in producing sustainable hydrogen catalysts. Other uses of AI include wastewater treatment, whereby it forecasts levels of toxicity, and it can track the environment. The research can be simulated faster and more efficiently with the help of language models and data-driven algorithms. Working examples of pharmaceutical firms indicate that there is a substantial increase in the reduction of toxic waste. The

study concludes that despite the immense potential of AI, the collaboration of industry, policymakers and scientists will be paramount to realize all the benefits and help develop more environmentally friendly solutions.[6]

OBJECTIVES:

1. To give a full overview of green analytical chemistry.
2. To demonstrate the common green analytical methods and their evaluation standards.
3. To speak about how Artificial Intelligence(AI) helps and supports green analytical operations.
4. To comment on the application of AI in streamlining of experimental conditions and wastage reduction.
5. To comment on where AI has the potential to proceed to further make sustainable analytical chemistry even more groundbreaking.
6. To map current issues and obstacles of implementing AI and green analytical methods.

FUNDAMENTALS OF GREEN ANALYTICAL TECHNIQUES

The rapid development of green analytical chemistry (GAC) requires straightforward and transparent concepts that are going to aid in sustaining environmentally friendly laboratory operations[7].

The twelve principles have been developed to enhance waste prevention, increase the efficiency of atoms, and limit the utilization of hazardous reagents in chemical synthesis[8]. The principles also focus on the need to adopt solvents that are less hazardous, renewable materials, energy-saving processes and catalytic processes over stoichiometric ones.[9] Moreover, green chemistry promotes the production of chemical products that can be disintegrated into harmless substances when used. This is in order to reduce their long-term impact on the environment.[10].

The real-time analysis and the construction of less harmful chemicals are regarded as the key to avoiding pollution and minimizing the risks of chemical accidents[11]

GAC Follows 12 principles:

1. **Prevention:** It is better to prevent rather than to treat or clean up waste after it has been produced.[12]. Prevention is better than cure and it is better not to create waste than to remove or rectify it once it is created. In a bid to reduce the cost and resource consumption of waste disposal, the philosophy tries to develop chemical processes that result into minimal waste.
2. **Atom Economy:** To ensure that all the parts of the process are incorporated in the product in a maximum way, synthetic protocols must be developed. Atom economics aims at maximizing the use of the raw materials in the end product and minimizing the formation of byproducts.
3. **Reduced Generation of Toxic Chemicals:** Synthetic operations ought to be fashioned where possible to utilize and generate materials that are as reduced or completely detrimental to the environment and human body. This idea minimizes the risk to the environment and human health by selecting synthetic processes that have fewer dangerous chemicals.
4. **Designing Safer Chemicals:** The minimum level of toxicity can be achieved in designing chemicals and still remain functional. When coming up with safer chemicals, one should consider potential hazards of chemical products so as to create molecules which are inherently safer and effective.
5. **Solvents and Auxiliaries that are Safer:** Since solvents determine the effects that chemical reactions have on the environment, fewer auxiliaries should be used and safer versions applied when necessary. Two examples of them are solvents and separation agents.
6. **Design to be Energy Efficient:** To minimize the adverse effects on the economic and environmental setting, they should be designed to consume less energy. The best conditions of synthetic processes are at room

temperature and pressure. Economic and environmental costs are minimized by reducing the energy used in processes by efficient process design.

7. Renewable Feedstocks: whenever it can be technically and economically feasible, a raw material or a feedstock must be a few regenerative rather than a depleting one. Renewable feedstocks will decrease reliance on exhausted stocks and decrease the environmental impact.

8. Minimized Derivatives: Derivatives should be minimized or should not be used since unnecessary derivatization (use of blocking groups, protection/deprotection, and temporary physical/chemical process modification) may lead to wastage, and more reagents may be necessary. Less generation of waste and reagent wastages is saved by reducing derivatization.

9. Catalysis Catalytic reagents (as selective as practicable) are desirable above stoichiometric reagents. Catalysis reduces the amount of waste produced and the amount of energy used through reactions that are more efficient.

10. Degradation Design: When the chemical products have reached the end of their useful life period, they must be designed to break down into harmless breakdown products rather than to stay in the environment. Deteriorating environmental damage over the long term may be prevented by formulating chemical product to break down into safe molecules.

11. Prevention of pollution through real-time analysis: It is necessary to develop analytical methods that will allow real-time monitoring and control of the in-process before the emergence of the toxic elements. The real-time analysis prevents the formation of toxic compounds due to the possibility of monitoring and controlling chemical processes.

12. Safer Chemistry by Nature to Prevent Accidents: The materials used in a chemical process and how they are arranged should minimize the risk of the chemical accidents, i.e., fire, explosion, and leakage. This principle is related to the selection of materials and conditions, which contribute to the increase in the reliability of processes by reducing the risk of chemical accidents[13].

GREEN ANALYTICAL TECHNIQUES

1. Green Chromatographic Techniques

In green analytical chemistry, green chromatographic techniques are very important. They minimize the use of solvents, minimize the formation of toxic waste and enhance energy consumption without reducing the quality of analysis [14].

Green chromatography resolves this problem by applying less toxic agents such as water, ethanol, ethyl lactate, or supercritical CO₂. As an example, the supercritical fluid chromatography (SFC) employs CO₂ as the primary mobile phase. The biggest challenge on enhancing sustainability in gas chromatography has been on the reduction or total elimination of the use of harmful gasses and solvents. In this regard, hydrogen can be used as a carrier gas as opposed to conventional helium, which reduces environmental hazards and curbs the challenge of rising prices as well as the scarcity of helium. Besides, due to the lower viscosity of hydrogen and greater diffusivity, as compared to helium, hydrogen is advantageous to chromatography, which includes faster analysis and increased resolution rate[15][16].

2. Microwave-Assisted Extraction (MAE):

The technique operates on microwave power to rapidly heat polar solvents and sample matrices. This aids in mass transfer and enhances the extraction efficiency.[17]. The microwave-assisted extraction (MAE) is an extraction method that produces heat through molecular interactions and directs the microwave energy to the extract material. Compared to conventional techniques used to extract oil, MAE requires less energy, thus it is cheaper. It reduces the need to use solvents thereby aiding in reducing pollution of the environment caused by excessive use of solvents. In addition, the process can be conducted in the absence of solvents thus reducing wastage and solvents

dumping issues. To give an example, dry MAE can be used to extract essential oils without solvents in plant materials[18].

3. Solid-Phase Microextraction(SPME)

Solid phase microextraction (SPME) is regarded as a non-pollutant technique of analysis. It can do this without solvents or with significantly less solvent and still be highly analytically sensitive[19]. Traditional methods of analysis usually use dangerous chemicals and cause a lot of waste that may cause environmental pollution. Green analytical chemistry is focused on coming up with alternatives that are environmentally friendly. Microextraction (SPME) in solid phase is emerging as a promising technique. The SPME is applicable in numerous sample preparation cases and demonstrated usefulness in food, forensic, environmental, pharmaceutical, and biological analyses. The technique is a good way of removing water, soil, and food contaminants, drugs and pharmaceuticals. Besides having eco-friendly analysis, SPME is also instrumental in drug development of the pharmaceutical and biomedical sectors. It enables the analysis of drugs and metabolites in biological specimen samples[20].

4. Pressurised Liquid Extraction (PLE)

Accelerated Solvent Extraction An environmentally friendly and efficient method of extracting bioactive compounds of plant materials is Pressurized Liquid Extraction (PLE) which involves high temperatures and pressure of solvents. Under this technique the pressure maintains the solvent in a liquid form at a temperature higher than its usual boiling point. This enhances solubility and mass transfer besides reducing the time of extraction. It is generally carried out at moderate temperatures (40-60 °C) and pressures (10-15 MPa), which enables the solvents such as ethanol, hydroalcoholic mixtures or water to enter the plant matrices. In one study on *Momordica charantia* leaves, the scholars optimized PLE using various solvents, temperatures and flow rates. When operating with a 50% hydroalcoholic solvent, they found that the maximum phenolic and flavonoid content was obtained with 60 °C and at a flow rate of 2g/min. Antioxidant activity was also found to be strong in the extracts with 24 phenolic compounds being identified using HPLC-DAD-ESI-MSn. Altogether, the PLE provides a long-term substitute to conventional extraction processes. It reduces the amount of solvents and energy consumption and has high extraction efficiency, which promotes the targets of Green Analytical Chemistry.[21]

5. Stir-bar Sorptive Extraction

Stir bar sorptive extraction (SBSE) is considered to be an analysis method with environmental friendliness. It is solvent-free, highly efficient in recovery, and minimized steps required in the sample preparation process[22]. The objective of SBSE was to exclude and isolate volatile analytes and water. Its applications were expanded in the future to encompass the examination of the headspace of liquid and solid samples, gaseous samples and other forms of sample. It is also a non-volatile analyte that is combined with HPLC. SBSE employs sorptive extraction like SPME. Rather than a fiber, it carries analytical materials into a polymer, such as polydimethylsiloxane which winds around a magnetic stir rod.[23].

6. Dispersive liquid-liquid microextraction (DLLME)

The dispersive liquid-liquid microextraction (DLLME) is a novel type of sample preparation method that provides large enrichment factors with limited volumes of water samples. Its simplicity, low cost, and ease of development make it popular with its usage being observed in almost all the analytical laboratories. It is a method used in pre-concentrating metal ions and is available in a number of variants. In a few words, we will summarize the various applications of DLLME to various types of analytes, such as phenols, medicines, insecticides, and other substances.[24] In comparison to the classical liquid-liquid extraction, DLLME offers shorter extraction periods, superior extraction rate, and increased sensitivity to the analysis [25].

7. Ultrasound Assisted Extraction

Sound waves with a frequency exceeding the auditory range of a human being and falling between 16 and 18 kHz, make up ultrasound. Propagation in gas takes place at frequencies up to 5 MHz and propagation in liquids and

solids at frequencies up to 500 MHz. The fundamental principle of ultrasound is the transformation of electric energy into mechanical energy with the help of transducers that generate mechanical vibrations with frequencies higher than 20 kHz.

Acoustic streaming can be caused by ultrasound when it is used in liquids. When the liquid has gas bubbles, compress and rarefaction cycles can be used on them resulting in collapse. The bursting of microbubbles is referred to as acoustic cavitation and may be either symmetrical or not. During a symmetric collapse, shock propagation establishes agitation as well as imparts energy to the media. This is a process which aids in dissolving the intermolecular interactions of the target compounds in the matrix, i.e. carbohydrates, lipids and proteins. Conversely, asymmetrical burst can produce microjets which can destroy or tear cell walls.

Cavitation may be termed as either a stable or transient. To achieve stable cavitation, we require bubbles to be created at u-sounds with higher frequencies (hundreds of kHz) with less collapse. Transient cavitation, in contrast, happens at lower frequencies (lower than hundreds of kHz) and leads to violent bubble collapse.[26].

METRICS FOR ASSESSING GREENNESS

1. Analytical eco-scale

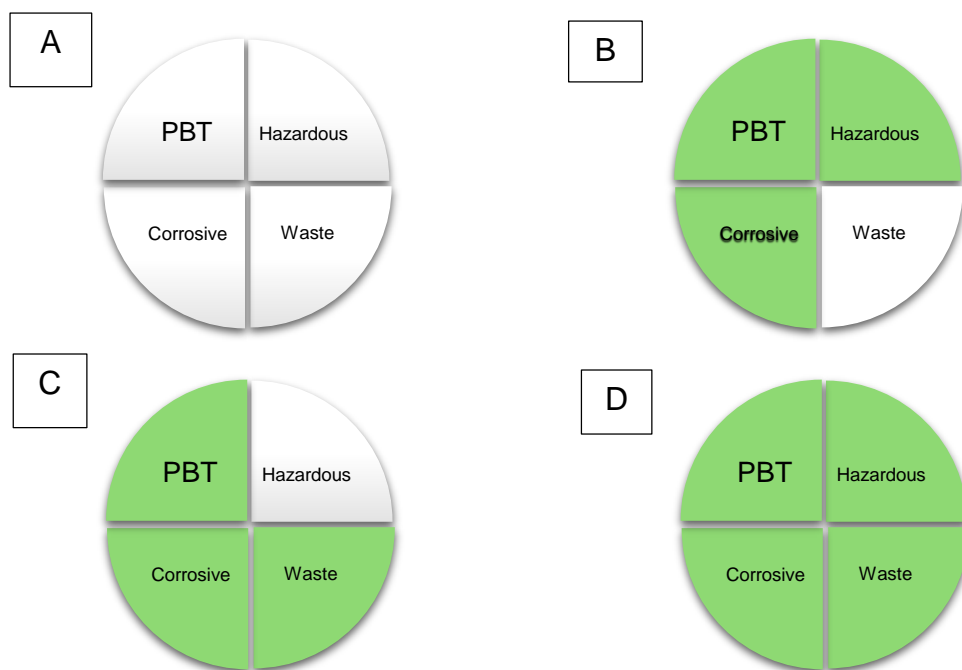
The Analytical Eco-Scale is an active instrument to assess the sustainability of environmental friendliness of the analytical processes by giving penalty points (PPs) to those segments of the process not environmentally friendly. The processes initially begin with a score of 100 out of which PPs are subtracted based on factors like the type and amount of solvents and reagents used, their toxicity or hazard classification, energy use, waste production and occupational hazards. The end score is the total greenness indicator: above 75 shows great green analysis, 50-75 is acceptable and below 50 is not enough. This is a measure which is easy to use and is fast to implement and provides a single value to compare between various approaches. Neither does it show the actions that have the most influence on the environment nor does it consider the parameters of analytical performance[27].

2. Index of National Environmental Method(NEMI).

The National Environmental Methods Index (NEMI) is one of the first evaluation instruments of green analytical chemistry (GAC), which was initiated in 2002. The pictogram is a circle that is subdivided into four quadrants with each quadrant representing a criterion including chemicals non-persistent and non-toxic, non-hazardous solvents, sample pH of 2 to 12, and less than 50 g of waste generation. Where one of the criteria is satisfied by a method, the quadrant is filled in with green. NEMI is simple to operate and gives a fast visual evaluation, however it does not give detailed data, and does not make a comprehensive approach to comparing methods. Ten systems of greenness ratings, including the National Environmental Method Index (NEMI), are initially analyzed, published and practiced [28].

Quadrant	Green criteria
Green-filled Quadrant	Met green criteria
Empty Quadrant	Does not meet green criteria

Quadrant representing the greenness



A: Does not meet any green criteria B: Only waste criteria does not meet C: Hazardous solvents used D: Methods met all criteria of Green Chemistry

Figure 1: The typical output pictogram of NEMI

3. Advanced NEMI

In order to overcome the weaknesses of NEMI, advanced NEMI was created. It does not incorporate a simple system of green and blank but adopts a color scale of traffic lights (green, yellow, red) to demonstrate various rates of adherence to the same standards. This improvement adds advanced semi-quantitative ability to NEMI, which makes it more informative and suitable in comparison of analytical procedures. Nonetheless, it is yet to cover the entire issue of method greenness.

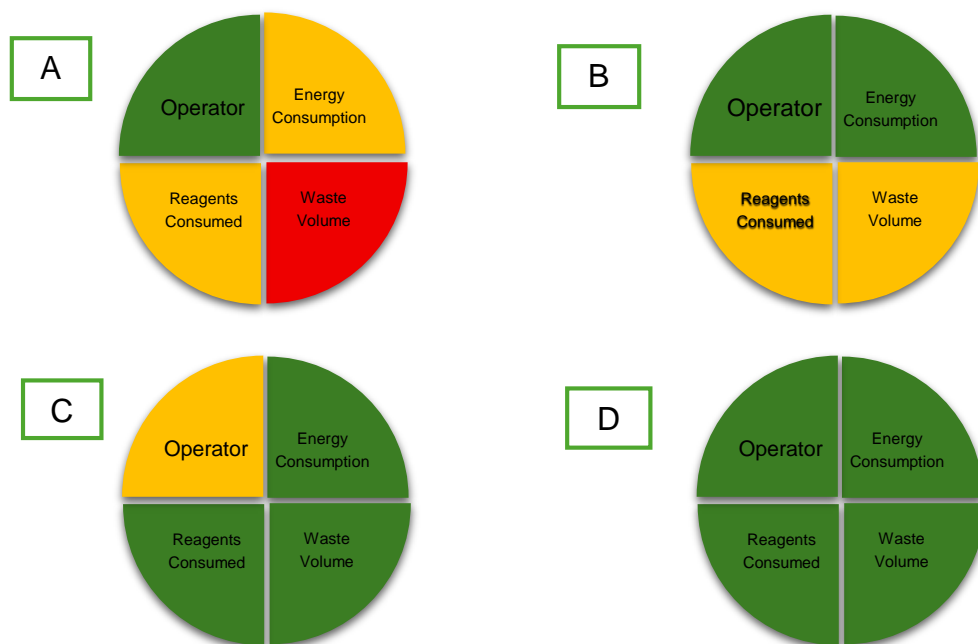


Figure.2. The typical output pictogram of advanced NEMI

4. Green Profile Assessment AGP is a development that widens the assessment into five groups namely environment, waste, energy, health and safety. It has a pictogram of the same shape, but each sector has an assigned color (green, yellow, red) based on the scores and dosage levels required by NFPA. The NEMI or the advanced NEMI does not allow the analytical chemistry as well-balanced analysis of the environmental and safety factors as is possible in AGP.

5. Green Analytical Procedure Index(GAPI) The GAPI measure, invented by Płotka-Wasyłka, is to evaluate the green nature of an entire analytical process between sampling and the wastes. The symbol consists of five pentagrams which depict a stage of the analytical process. The low, medium and high environmental health effect are represented as green, yellow, or red.

Pentagram 1 (Sampling): The assessment of sample collection, preservation, transportation and storage. In-line collection preservation need not In-line collection with no preservation requirement is illustrated in green, and off-line collection with chemical/physical preservation and special storage is illustrated in red.

Pentagram 2 (Method type): Takes into account the sample processing requirements and no processing is green, easy processing is yellow, and additional extraction is red. The pentagram circle represents the presence of both qualitative and quantitative outputs in the method.

Pentagram 3 (Sample processing): Contains extraction scale (nano-, micro-, or macro-scale), solvent type (green, solventless, or non-green), and the need of additional preparation procedure.

Pentagram 4 (Reagents/solvents): Checks the quantity of solvents, health risks (revealed by NFPA health rating), and safety risks (as regards instability and flammability). Green demonstrates less toxicity and minimal use of solvents and red demonstrates risky and high usage of solvents.

Pentagram 5 (Last factors): takes into account the utilization of energy, risks associated with work, quantity of waste and waste disposal. Sealed low-energy systems with little or no waste, and with recycling are all environmentally friendly[29].

OVERVIEW OF ARTIFICIAL INTELLIGENCE IN ANALYTICAL CHEMISTRY

The application of Artificial Intelligence (AI) and Machine Learning (ML) and artificial neural networks, in particular, has experienced upsurges and downturns in the field of molecular sciences. In the recent past, there has been a resurgence of new ML techniques in the scientific world. They have become very successful in computer vision, speech recognition, and natural language processing (NLP) and this has motivated chemists and biologists to use it in solving problems in natural science. This has advanced because of modern and powerful Graphics Processing Unit (GPU), big datasets, better algorithms, and software libraries. The reason is that ML techniques can be used to provide results much faster and in some cases more accurate than other methods that rely on Quantum Mechanical (QM) calculations, Density Functional Theory (DFT) or Molecular Mechanics (MM) calculations. The methods have been useful in numerous fields such as in drug discovery, quantum energies, new molecule design, molecular dynamics simulations, the study of materials and in designing synthetic pathways to organic compounds[30].

Artificial intelligence has contributed significantly to analytical chemistry especially in handling diverse and complex information. Previously, it required much time and skills to analyze such data. It is now easy and quick to extract the relevant information with the help of AI algorithms. In spectroscopy AI has been used to decompose and analyze complex spectra and this greatly enhances the detection of a compound. Even with such developments, there are challenges associated with the use of AI in the field of analytical chemistry. Studies are ongoing regarding the problem of interpreting AI models, large-scale training requirements, and multi-source data combinations. The development of AI in analytical chemistry over the decades has been admirable and consistent. AI has in the recent past proved to be a game changer in most aspects of technology and science. AI facilitates data analysis, which improves productivity and the accuracy and reliability of the results. Also, the application of AI to enhance the work of experiments has an enormous potential to significantly accelerate the development of the sphere of innovation [31].

SMART SOLVENT SELECTION AND GREEN SOLVENT DISCOVERY THROUGH AI

Chemicals processes cannot be carried out without solvents and using of greener, safe, and efficient solvents is critical in developing green chemical processes. In the modern world, new methods are used to find and study green solvents, and one of them, the artificial intelligence (AI) can become more and more significant in predicting their physical and chemical characteristics. The ability to explore chemical space of green solvents, it is also possible to use AI to screen perceived solvents and design new solvents in an inverted way. This review presents the use of AI assisted green solvent design, which is the intensification methods in the green solvent design and property prediction processes. To begin with, the techniques of quantitative structure property relations (QSPR) intensification techniques that are utilized in the solvent property prediction process are characterized, such as the optimization and intensification of feature extraction, ensemble learning, uncertainty analysis, and interpretability modeling.[32].

ADVANTAGES OF GREEN ARTIFICIAL INTELLIGENCE (AI)

1. Environmentally Friendly: Green AI is also less carbon footprint and it uses less energy compared to traditional AI systems.
2. Cost effective it does not incur high costs to buy cloud servers and instead researchers can carry out good quality research using normal computers.
3. Inclusive and Accessible: Allows researchers to do top-notch AI research and development, regardless of their economic status.
4. Energy-Saving Algorithms: The purpose of doing this is to create machine learning models that consume less power and use less energy.

5. Promotes Eco-Friendliness With AI: It implements AI-based technologies to aid environmental friendliness in all industries.

6. Performance Without Compromise: Produces proper and high-quality results without raising the cost of computing or harming the environment.[33].

APPLICATIONS OF AI IN GREEN ANALYTICAL CHEMISTRY

1. Method development and optimization

Artificial intelligence (AI) is transforming the field of analytical chemistry by accelerating the method development and optimization of HPLC. Traditionally, chromatographic methods development has been based on trial-and-error, which has been very expensive in terms of experimental effort and experience. However, by considering several variables, AI tools can produce, be predictive, and optimize the separation conditions at an accelerated rate. The separation was done in a single separation using HPLC parameters predicted by AI of amlodipine, hydrochlorothiazide, and candesartan. The comparison of the AI-generated and empirically optimized approaches revealed that although AI makes the process faster and more efficient and spares testing, the input of human expertise is still needed to refine it and make it resilient. Above all, by saving solvent consumption and increasing efficiency, also this inclusion of AI predetermines the development of more environmentally-safe and sustainable processes[34]. ML can be applied to learn the patterns and rules behind a dataset by assessing a subset of the given data and subsequently predict the behavior of a system, and this has been applied in the field of molecular and materials science to discover and predict the performance of new materials.6,7 It has also been described as a rapidly expanding field of study [35].

2. Automation and Miniaturization

Analytical chemistry is important in most applications and the monitoring of chemical species is necessary, although complex sample matrices tend to interfere with accurate detection. In a bid to focus the analytes and remove interferences therefore, sample preparation is essential. Decades ago, the conventional techniques of liquid-liquid extraction (LLE) and solid-phase extraction (SPE) were used, which are time-consuming, prone to error, and need extensive quantities of solvents. Microscale methods including dispersive liquid-liquid microextraction (DLLME), solid-phase microextraction (SPME), stir bar sorptive extraction (SBSE) and micro extraction by packed sorbent (MEPS) reduced the amount of solvents and sample used, but otherwise most procedures were still laborious. The online SPE, multidimensional LC-based systems and automated SPME took the field into the modern age through automation. Such methods along with artificial intelligence (AI) offer more effective, quicker, and environmentally-friendly methods of analysis to the environment[36].

3.Live Monitoring of Waste Products.

The monitoring of industrial waste can be done immediately with the help of AI-powered sensors and analytical systems. It assists in determining pollutants in a short time and changing analysis techniques when necessary. It minimizes overuse of chemicals that is usually used in conventional batch tests and a fast response that prevents environmental pollution[37].

4. Data-Driven Waste Reduction

The AI is used to develop more sustainable chemical processes through the analysis of enormous data sets in search of patterns and links not noticeable by humans. As an example, predictive models may propose less risky solvents, reduced reaction times, or reduced amounts of chemicals. This assists in reducing the generation of harmful waste at the laboratories and the industrial facilities.[38].

5. Environmental Monitoring

Environmental monitoring is a tool that is significant in gathering data on pollution, enhancing the health of the ecosystem, and conservation. The evolution of intelligent analytical systems has given way to advancement of dealing with environmental issues. Such technologies offer autonomous trace pollutant examination and gather data in real-time, which enhances efficiency in monitoring and decreases the harm to the environment. The

scientists are able to react to environmental changes very fast considering that real-time sensor is used to monitor the soil, water, and air. Green analytical platforms will be able to forecast high-risk zones, identify patterns of pollution, and enhance decision-making when used together with machine learning. Above all, the technologies have enabled sustainability through energy consumption reduction and waste minimization, which reinforce conservation and promote environmentally friendly monitoring practices [39].

7. Artificial Intelligence-based Sustainability in Catalysis.

Green organic chemistry has to be promoted by catalysis. Artificial Intelligence (AI) is highly important in ensuring that this process is more sustainable. With the forecasting of catalytic behavior and the selection of systems that are environmentally friendly, AI aids in the development of more efficient catalysts that can decrease energy consumption and decrease the number of harmful byproducts. This was demonstrated in the works of Kalikadien et al. (2024) who used machine learning (ML) to enhance Rh-based chiral catalysts to catalyze the enantioselective hydrogenation of olefins. Their computational frameworks added quantum chemistry descriptors and ML models to ascertain catalytic selectivity and catalytic reactivity. Although predictions were more accurate in the field of training, predicting smaller or more diverse datasets in terms of enantioselectivity was an issue. The study emphasizes the role of AI in accelerating the identification of catalysts, reducing the amount of waste in the laboratory, and facilitating the process of developing green catalysts in a sustainable way [40].

8. Enhancement of Analytical Priorities.

Determining the most advantageous experimental conditions can be boosted by the machine learning (ML) or other artificial intelligence (AI) algorithms and enhance analytical methods in green chemistry. The AI models may be used in waste management to calculate the minimal solvent amounts, optimal pH, temperature, and flow rates in the chromatographic or spectroscopic procedures. This makes the use of chemicals and production of hazardous wastes to be minimized. This method has a firm correlation with the fundamentals of green analytical chemistry.[41].

CASE STUDIES

1.AI-Driven Catalyst Design:

- AI Designed Hydrogen Production Catalyst

The development of AI-based hydrogen generation catalysts will enable producing hydrogen fuel by hydrogen electrons through a similar approach. The advancement of AI-based hydrogen generation catalysts will make it possible to generate hydrogen fuel by hydrogen electrons in a similar fashion. In 2023, IBM Research presented an artificial intelligence-based model that discovered an effective catalyst to hydrogen generation. The innovation contributed to the trend to sustainable energy, as the reaction efficiency was increased, and energy consumption was shortened by 20 percent. Hydrogen fuel is becoming sustainable and more affordable with the help of AI.

- AI for Carbon Capture at Stanford University

Stanford University AI on Carbon Capture: In 2022, a team of researchers at Stanford created a platform, which uses AI to identify efficient catalysts to capture CO₂. These catalysts minimize emissions in industries by hastening the process of converting CO₂ to useful products. The development of catalysts, which is facilitated by AI, is a significant step towards carbon neutrality.

2.Solvent Choice Greener Processes AI.

- AI for Solvent Choice for Greener Process

The AI Model of Solvents in the University of Edinburgh: In 2023, University of Edinburgh Researchers created an AI algorithm with the highest standings at 87 per cent accuracy in predicting the eco-friendly solvents. This resulted in the reduction of 30% of solvent wastes because industry replaced the use of solvents that were hazardous. AI selects safer solvents, and more chemical production that is green.

3.Optimization of Processes Artificial Intelligence.

- Machine Learning: A Pharmaceutical Production Case Study:

In 2023, Pfizer and Merck made use of AI to streamline the process of producing medicine, using 25% less energy. AI maximized the effectiveness of production and reduced waste via reaction optimization. It is a program that reduces the environmental impact of producing drugs.

- AI in Biofuel Production;

The University of Toronto increased the volume of fuel by 35 percent by maximizing the production of algae-based biofuels. AI reduced the energy use by one-third through the adjustment of light exposure and nutrition levels. Biofuel optimization via AI facilitates the transition to green power.

4. AI in Discovery of Green Materials.

- The Biodegradable Discovery Driven by AI Plastic by MIT.

In 2023, MIT researchers discovered bio-degradable polymers after scanning one million polymer forms using AI. Bio plastics developed by AI will help to eliminate plastic pollution by degrading at a rate 50 times higher than the existing plastics. The increasing growth of environmentally safe consumer goods and packaging is made possible by AI.

- Google DeepMind An AI-Powered Eco-Friendly Packaging.

Google DeepMind, Unilever and Nestle, collaborated in an effort to develop future generation biodegradable packaging in 2024. Polymer blends were also discovered by AI and can be degraded in the environment within a relatively short period of time without affecting the stability. This action should make a significant contribution to plastic waste reduction in the world[42].

CHALLENGES

1. Creation and upkeep of AI models are expensive. These costs are added by high-performance computing, software licenses, and professional trained persons. These costs can be greater than the short-term advantages of AI use in many labs because of the nature of sustainability-oriented smaller academic or industrial labs, [43].

2. Green analytical chemistry is related nearer to the environment and safety regulations. New solvents, reagents, or procedures that have not been standardized or approved by regulatory agencies may be suggested by AI-assisted methods. This poses problems in the adoption of industrial implementation and mass application in controlled settings [44].

3. Integrating AI into the already existing analytical labs is very infrastructure, software, and training intensive. In many developing green chemistry laboratories, the required computing facilities or expertise might not be available and therefore integrating them is not easy. One of the significant technical challenges is to ensure that AI systems have a smooth communication with the conventional lab equipment. [45]

4. Multi-component systems, environmental situations or biological samples frequently feature in green analytical chemistry. The non-linear nature of interactions and variability of these complex systems may make AI algorithms unable to predict results or enhance processes in such systems, due to this phenomenon and their complexity [46].

5. Ethical and Safety Issues AI generated suggestions can promote emerging solvents, chemicals or techniques that, theoretically, are eco-friendly. Nevertheless, they may be potentially toxic or harmful to the environment. The use of AI to predict without human supervision can result in unsafe experiments[47].

6. Computational and Energy Interestingly, AI models might consume a significant amount of computing storage and power. Otherwise, this may offset the environmental gains of green chemistry. It should be noted that to minimize this impact, one should employ effective algorithms and cloud-based solutions[48].

FUTURE PERSPECTIVES

The AI has an enormous potential in green organic chemistry as it can enhance the process of chemicals, produce environmentally friendly materials, and decrease waste. These advantages promote sustainability policies. Nonetheless, AI tools are not easily applicable due to their user-friendliness and accessibility. The AI solutions on the cloud will reduce the expenses of infrastructure and offer small businesses and laboratories with flexible solutions. The creation of open-access databases of high quality is necessary to ensure that AI becomes available to all people. Moreover, the energy consumption of the AI systems is also of concern because of the energy required to train high-demand models. The future of AI should be concerned with enhancing the efficiency of algorithms in order to bring energy consumption and environmental gains into balance. This concept is defined and outlined, as well as the advantages of the broader green AI methodology and the necessity of a collective effort in the given field. The explanation is justified by scientific studies in various disciplines, such as computer science, social and environmental science, and urban studies[49].

Global regulation is lacking a big problem to AI in sustainable chemistry. The existing AI technologies tend to be black boxes and raise concerns about transparency and safety. This would make regulatory bodies focus on such issues. Governments and international organizations need to develop policies that put explanatory, data protection, and safety standards at their forefront. This would assist in minimizing the environmental hazards and addressing such challenges. These standards should be created through the collaboration between chemists, AI researchers, legislators, and environmental groups all over the world. This collaboration can be assisted by such groups as the WEF and UNEP so that AI technologies usage could be ethically sustainable. Although AI has a promising future in the field of green chemistry, its international implementation and long-term positive environmental and social impacts depend on addressing the concern with the accessibility, energy-efficiency, and regulation.[50]

CONCLUSION

Green analytical chemistry is fast becoming transformed by artificial intelligence (AI). It achieves this through efficiency enhancement, lessening waste, and developing environmentally sustainable materials and techniques. Green Analytical Chemistry (GAC) is interested in sustainability in order to reduce the adverse effects of chemical analysis on the environment and human health. It focuses on such values as waste minimization, reduced use of solvents, energy consumption, and instant monitoring. The AI can contribute to these objectives by simplifying such processes as creation, optimization, automation, miniaturization, and precise environmental surveillance. It also assists in determining the existence of sustainable resources and more intelligent ways of waste disposal. Even though it is an innovative idea, there remains the problem of high cost of implementation, legal limitations, absence of experience, and energy consumption of AI models. To realize ethical, open and accessible AI application in sustainable chemistry, researchers, businesses, lawmakers and international organizations will have to cooperate. Green analytical techniques might become more effective, sustainable, and popular due to continuous innovation and the application of AI-based solutions. This will eventually lead to improved environment and sustainable industrial practices.

Conflicts of interest:

The authors declare that they have no conflicts of interest with the article's contents.

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ABBREVIATIONS

AGP – Assessment Of Green Profile

AI – Artificial Intelligence

DFT – Density Functional Theory

DLLME – Dispersive Liquid Liquid Micro Extraction
GAC – Green Analytical Chemistry
GAPI – Green Analytical Procedure Index
GPU – Graphics Processing Units
HPLC – High Performance Liquid Chromatography
kHz – Kilo Hertz
LC – Liquid Chromatography
LLE – Liquid Liquid Extraction
MAE – Microwave Assisted Extraction
MEPS – Micro Extraction By Packed Sorbent
MHz – Mega Hertz
ML – Machine Learning
MM – Molecular Mechanics
NEMI – National Environmental Method Index
NFPA – National Fire Protection Association
NLP – Natural Language Processing
PBT – Polybutylene Terephthalate
PLE – Pressurised Liquid Extraction
PP – Penalty Points
QM – Quantum Mechanical
QSPR – Quantitative Structure Property Relationship
SBSE – Stir Bar Sorptive Extraction
SFC – Supercritical Fluid Chromatography
SPE – Solid Phase Extraction
SPME – Solid Phase Micro Extraction
UNEP – United Nations Environmental Programme
WEF – World Economic Forum

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