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Next-Wave Science and Technology: Research Advancements

Editors:
Dr. Manish P. Tirpude
Dr. Md Dilwar Alam Khan
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PREFACE

It gives us immense pleasure to present the book *Next-Wave Science and Technology: Research Advancements*, a comprehensive volume that explores the emerging frontiers shaping the future of scientific inquiry and technological innovation. In an era defined by rapid transformation, interdisciplinary integration, and global connectivity, science and technology continue to redefine the boundaries of knowledge and societal progress.

This book brings together diverse contributions that reflect cutting-edge research across life sciences, physical sciences, chemical sciences, computational technologies, and applied engineering. The "next wave" signifies not only advanced tools and methodologies but also a paradigm shift toward sustainable development, digital transformation, precision technologies, and intelligent systems. From artificial intelligence–driven analytics and nanotechnological breakthroughs to biotechnological innovations and renewable energy solutions, the chapters collectively highlight the dynamic evolution of modern research.

A key strength of this volume lies in its interdisciplinary perspective. Contemporary challenges—such as climate change, healthcare innovation, food security, and smart infrastructure—demand collaborative solutions that transcend traditional academic boundaries. The contributors to this book have successfully integrated theoretical foundations with experimental insights, offering both conceptual clarity and practical relevance.

We believe this book will serve as a valuable resource for researchers, academicians, industry professionals, and postgraduate students seeking to understand current trends and future directions in science and technology. It is our hope that the ideas presented herein will inspire new research initiatives, foster innovation-driven thinking, and contribute meaningfully to global scientific advancement.

We sincerely acknowledge all authors, reviewers, and contributors whose dedication and scholarly efforts have made this publication possible. May this volume stimulate curiosity, encourage collaboration, and pave the way for transformative discoveries in the years to come.

- Editors

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BIOFUELS AND HYDROGEN ENERGY IN SUSTAINABLE DEVELOPMENT

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Abstract

The escalating global energy demand coupled with the imperative to mitigate climate change necessitates a paradigm shift towards sustainable energy sources. This chapter explores into the pivotal roles of biofuels and hydrogen energy in achieving sustainable development. It examines the various types of biofuels, their production pathways, and diverse applications in transportation, power generation, and industrial processes. Similarly, the chapter explores hydrogen production methods, its versatility as an energy carrier, and its potential in fuel cells for clean power. Challenges associated with the widespread adoption of both energy forms, such as scalability, cost-effectiveness, infrastructure development, and environmental impacts, are critically discussed.

1. Introduction

The relentless pursuit of economic growth over the past century has been closely linked to the extensive use of fossil fuels such as coal, oil, and natural gas. These energy sources have played a central role in industrial expansion, urbanization, and technological progress. However, their continued dominance has resulted in severe environmental consequences, including rising greenhouse gas emissions, global warming, ocean acidification, and widespread air pollution [1, 2]. The increasing frequency of extreme weather events and growing public health concerns have further highlighted the unsustainability of the current energy paradigm. Scientific assessments and international climate agreements consistently stress that limiting global temperature rise requires a rapid reduction in fossil fuel consumption and a decisive shift toward low-carbon energy systems [3].

In response to these challenges, sustainable energy alternatives have gained significant global attention, with biofuels and hydrogen energy emerging as key candidates for decarbonization. Biofuels, produced from renewable biological materials such as crops, agricultural residues, and organic waste, offer a viable pathway to reduce emissions in transportation and industrial sectors while supporting rural economies [4]. Hydrogen energy, particularly green hydrogen produced using renewable electricity, is recognized for its potential to provide clean energy across multiple sectors, including power generation, transport, and heavy industry, without emitting carbon dioxide at the point of use [5]. Despite their promise, both biofuels and hydrogen face notable challenges, such as high production costs, technological limitations, land-use concerns, and the need for extensive infrastructure development [6]. This chapter examines the roles of biofuels and hydrogen energy in the global transition toward sustainability, analyzes the technical and economic barriers to their adoption, and evaluates their long-term prospects in shaping a resilient and sustainable energy future.

2. Biofuels: A Renewable Path to Decarbonization

Biofuels are liquid, solid, or gaseous fuels derived from biomass. They offer a renewable alternative to fossil fuels, and their carbon neutrality (in an ideal lifecycle) makes them attractive for mitigating climate change.

2.1 Types of Biofuels

Biofuels are broadly categorized into generations based on their feedstock and production technologies:

i. **First-Generation Biofuels**: Produced from food crops such as corn (ethanol), sugarcane (ethanol), and vegetable oils (biodiesel). While readily available, concerns about "food vs. fuel" competition and land-use change impacts persist [7].

ii. **Second-Generation Biofuels**: Derived from non-food biomass, including lignocellulosic materials (agricultural residues, forestry waste) and dedicated energy crops (e.g., switchgrass, jatropha). These offer higher greenhouse gas reduction potential and alleviate food security concerns [8].

iii. **Third-Generation Biofuels:** Produced from algae, which can yield high amounts of oil and biomass without competing for arable land or fresh water. Research in this area is ongoing, focusing on optimizing cultivation and extraction processes [9].

iv. **Fourth-Generation Biofuels:** Focus on genetically engineered organisms or advanced biorefinery concepts to produce biofuels with enhanced properties or capture carbon dioxide during production, leading to net carbon negative emissions [10].

2.2 Production Pathways

Various technologies are employed for biofuel production:

i.**Bioethanol Production:** Bioethanol is one of the most widely used biofuels and is primarily produced through the fermentation of sugars by microorganisms such as Saccharomyces cerevisiae. In first-generation bioethanol production, starch-rich crops like sugarcane, maize, and wheat are processed to release fermentable sugars, which are then converted into ethanol. Although this method is technologically mature, it raises concerns related to food security and land use. Second-generation bioethanol addresses these issues by utilizing lignocellulosic biomass such as agricultural residues, grasses, and woody materials. This process involves pretreatment, enzymatic hydrolysis, and fermentation, making it more complex but environmentally sustainable due to the use of non-food feedstocks [11].

ii. Biodiesel Production: Biodiesel is produced through a chemical process known as transesterification, in which vegetable oils or animal fats react with an alcohol, typically methanol or ethanol, in the presence of a catalyst. This reaction converts triglycerides into fatty acid methyl esters (FAME), which can be used directly in diesel engines or blended with conventional diesel. Biodiesel offers several advantages, including biodegradability, reduced greenhouse gas emissions, and lower particulate emissions compared to fossil diesel. However, challenges such as feedstock cost, cold flow properties, and large-scale availability remain important considerations for its widespread adoption [12].

iii. Biogas Production: Biogas is generated through the anaerobic digestion of organic materials such as animal manure, food waste, sewage sludge, and agricultural residues. This biological process occurs in the absence of oxygen and involves multiple stages, including hydrolysis, acidogenesis, acetogenesis, and methanogenesis. The resulting biogas mainly consists of methane and carbon dioxide and can be used for cooking, heating, electricity generation, or upgraded to biomethane for use as a vehicle fuel. Biogas production not only provides renewable energy but also helps in waste management and reduces methane emissions from uncontrolled decomposition [13].

iv. Biorefineries: Biorefineries are advanced, integrated systems designed to convert biomass into a wide range of biofuels, biochemicals, and value-added bioproducts. Similar to petroleum refineries, biorefineries aim to maximize resource efficiency by utilizing every component of the biomass feedstock. This integrated approach improves economic viability and reduces waste generation while supporting the transition to a circular bioeconomy. By producing fuels, chemicals, materials, and energy simultaneously, biorefineries enhance sustainability and play a crucial role in reducing dependence on fossil resources [14].

2.3 Applications of Biofuels

Biofuels find diverse applications across various sectors:

i. Transportation: Biofuels play a crucial role in decarbonizing the transportation sector, which is a major contributor to greenhouse gas emissions. Ethanol is commonly blended with gasoline (such as E10, E20, or higher blends) to improve fuel oxygen content, enhance combustion efficiency, and reduce carbon monoxide emissions. Biodiesel and biodiesel blends are used in diesel engines with little or no engine modification, offering reduced particulate matter and sulfur emissions. Additionally, sustainable aviation fuels (SAFs), derived from biomass and waste feedstocks, are emerging as a promising alternative to conventional jet fuel, helping to significantly lower lifecycle carbon emissions in the aviation sector, where electrification remains challenging [15].

ii. Power Generation: Bioenergy sources such as biogas and solid biomass are widely used for electricity and heat generation. Biogas produced from anaerobic digestion can be directly used in gas engines or turbines to generate power, while the waste heat can be recovered through combined heat and power (CHP) systems, improving overall efficiency. Solid biomass, including wood pellets, agricultural residues, and energy crops, can be combusted in dedicated biomass power plants or co-fired with coal in existing thermal power plants. These applications contribute to renewable energy generation while providing effective waste management solutions [16].

iii. Industrial Processes:

In industrial applications, biofuels serve as a sustainable substitute for fossil fuels in boilers, kilns, and furnaces used in sectors such as cement, steel, textiles, and food processing. The use of biofuels for process heat helps reduce carbon dioxide emissions and dependence on non-renewable energy sources. Biomass-based fuels and biogas are particularly suitable for industries requiring continuous thermal energy. By integrating biofuels into industrial energy systems, industries can move toward cleaner production processes and improved environmental performance [17].

2.4 Challenges and Opportunities for Biofuels

Despite their potential, biofuels face several challenges:

i. Sustainability Concerns: While biofuels are often promoted as environmentally friendly alternatives to fossil fuels, their sustainability depends heavily on how and where the biomass feedstocks are produced. Large-scale cultivation of energy crops can lead to land-use change and deforestation, resulting in loss of biodiversity and carbon sinks. High water requirements for certain crops also raise concerns about water footprints, particularly in water-stressed regions. Additionally, indirect land-use change (ILUC) occurs when agricultural land previously used for food production is diverted to biofuel crops, pushing food cultivation into forested or grassland areas. These factors can offset the greenhouse gas reduction benefits of biofuels, making comprehensive life-cycle assessments essential for evaluating their true sustainability [18].

ii**. Technological Maturity and Cost:** Advanced biofuels, particularly second- and third-generation biofuels derived from lignocellulosic biomass and algae, offer significant sustainability advantages over first-generation biofuels. However, these technologies are still in the developmental or early commercialization stages. Complex processing steps such as pretreatment, enzymatic hydrolysis, and advanced conversion pathways increase capital and operational costs. As a result, the production cost of these biofuels often remains higher than that of conventional fossil fuels. Continued research, technological innovation, and policy support are required to improve efficiency, achieve economies of scale, and make advanced biofuels commercially competitive [19].

iii. Infrastructure: The widespread adoption of biofuels also depends on the availability of suitable infrastructure for storage, transportation, and dispensing. Existing fuel distribution systems are largely designed for petroleum-based fuels and may require modifications to handle higher biofuel blends due to issues such as material compatibility and fuel stability. Establishing dedicated infrastructure, including blending facilities, pipelines, and refueling stations, involves substantial investment and coordination among stakeholders. Inadequate infrastructure can limit market penetration and slow the transition toward bio-based energy systems, highlighting the need for integrated planning and supportive policies [20].

However, opportunities exist in:

- Advanced Feedstock Development: Research into high-yielding, low-input energy crops and waste-to-energy technologies.
- Policy Support and Incentives: Government policies, mandates, and tax incentives are crucial for driving biofuel adoption [21].
- Biorefinery Integration: Developing integrated biorefineries can enhance economic viability and resource efficiency.

3. Hydrogen Energy: The Clean Energy Carrier of the Future

Hydrogen is considered a versatile energy carrier due to its high energy content per unit mass and its clean combustion products (water). It can play a crucial role in decarbonizing hard-to-abate sectors.

3.1 Hydrogen Production Methods

Hydrogen production pathways are often categorized by their carbon intensity:

- **Grey Hydrogen:** Grey hydrogen is the most commonly produced form of hydrogen today and is primarily generated from fossil fuels, especially natural gas, using the steam methane reforming (SMR) process. In this method, methane reacts with steam at high temperatures to produce hydrogen and carbon monoxide, which is further converted into carbon dioxide. Although grey hydrogen is relatively inexpensive and technologically mature, it results in significant CO_2 emissions and contributes substantially to climate change. As a result, despite its widespread use in industries such as ammonia and petroleum refining, grey hydrogen is considered environmentally unsustainable in the long term [22].
- **Blue Hydrogen:** Blue hydrogen is produced using the same fossil-fuel-based processes as grey hydrogen, but it incorporates carbon capture, utilization, and storage (CCUS) technologies to reduce carbon dioxide emissions. In this approach, a large portion of the CO_2 generated during hydrogen production is captured and either stored underground or utilized in industrial applications. While blue hydrogen offers a transitional pathway toward lower-carbon hydrogen, its overall sustainability depends on the efficiency of carbon capture systems and the control of methane leakage during natural gas extraction and transport. Consequently, blue hydrogen is viewed as an intermediate solution rather than a fully carbon-neutral option [23].

- **Green Hydrogen:** Green hydrogen is produced through the electrolysis of water using electricity generated from renewable energy sources such as solar, wind, or hydropower. This process splits water into hydrogen and oxygen without producing carbon emissions, making green hydrogen the most environmentally sustainable form of hydrogen production. When used as a fuel or energy carrier, it emits only water vapor, resulting in near-zero greenhouse gas emissions across its life cycle. Although currently more expensive due to high electricity and electrolyzer costs, green hydrogen is expected to play a vital role in achieving long-term climate and energy goals as renewable energy becomes more affordable [24].
- **Turquoise Hydrogen:** Turquoise hydrogen is an emerging production pathway based on methane pyrolysis, a process in which methane is thermally decomposed into hydrogen and solid carbon rather than carbon dioxide. By avoiding direct CO_2 emissions, this method has the potential to significantly reduce the carbon footprint of hydrogen production. The solid carbon by-product can be stored or used in industrial applications, further enhancing sustainability. However, turquoise hydrogen is still at the research and pilot stage, and challenges related to scalability, energy requirements, and economic viability must be addressed before it can be widely adopted [25].

3.2 Applications of Hydrogen Energy

Hydrogen's versatility allows for a wide range of applications:

- **Fuel Cells:** Hydrogen fuel cells generate electricity through an electrochemical reaction between hydrogen and oxygen, producing only water and heat as byproducts. This clean and efficient energy conversion makes fuel cells highly attractive for a wide range of applications, including fuel cell electric vehicles (FCEVs), stationary power generation, and backup power systems. Fuel cells offer high efficiency, quiet operation, and zero local emissions, making them particularly suitable for urban transport and critical infrastructure. Their ability to provide continuous power as long as hydrogen is supplied further enhances their reliability and versatility [26].
- **Industrial Feedstock:** Hydrogen plays a vital role as a feedstock in several industrial sectors, most notably in ammonia production for fertilizers, methanol synthesis, and petroleum refining processes such as hydrocracking and desulfurization. Currently, most industrial hydrogen is produced using fossil fuels, leading to significant carbon emissions. Replacing grey hydrogen with green or blue hydrogen in these applications presents a major opportunity for industrial decarbonization. Such a transition can substantially reduce greenhouse gas emissions while maintaining the essential chemical functions hydrogen provides in these industries [27].

- **Energy Storage:** Hydrogen serves as an effective medium for large-scale and long-duration energy storage, particularly in energy systems with high shares of renewable power. Excess electricity generated from solar or wind sources during periods of low demand can be used to produce hydrogen through electrolysis. This stored hydrogen can later be converted back into electricity or used directly as a fuel, helping to balance the intermittent nature of renewable energy sources. As a result, hydrogen enhances grid stability and supports the integration of renewable energy into the power system [28].
- **Heating**: Hydrogen can contribute to decarbonizing the heating sector by being blended with natural gas in existing pipeline networks or used directly in hydrogen-compatible boilers and industrial heating systems. Blending hydrogen reduces carbon emissions without requiring major changes to infrastructure or end-use appliances in the short term. In the long term, dedicated hydrogen heating systems can provide low-carbon heat for residential, commercial, and industrial applications. However, safety, infrastructure adaptation, and cost considerations remain important factors for large-scale deployment [29]. * Transportation: Beyond FCEVs, hydrogen is being explored for heavy-duty trucks, trains, ships, and even aviation [30].
- **Transportation**: Beyond its use in fuel cell electric vehicles, hydrogen is increasingly being explored as a fuel for hard-to-electrify transport sectors. These include heavy-duty trucks, trains, maritime transport, and potentially aviation, where high energy density and fast refueling are critical advantages. Hydrogen-based propulsion systems can significantly reduce emissions in these sectors while maintaining operational performance. Although technological and infrastructure challenges persist, hydrogen is widely regarded as a promising solution for achieving deep decarbonization in long-distance and heavy transport applications [30].

3.3 Challenges and Opportunities for Hydrogen Energy

Key challenges for widespread hydrogen adoption include:

- Production Cost: Green hydrogen production is currently more expensive than fossil-fuel-based hydrogen due to the cost of renewable electricity and electrolyzers [31].
- Infrastructure Development: Building a comprehensive hydrogen infrastructure for production, storage, transportation (pipelines, liquefaction), and dispensing is a massive undertaking [32].
- Safety Concerns: Hydrogen's flammability and low volumetric energy density require robust safety protocols and specialized storage solutions [33].
- However, significant opportunities exist:
- Falling Renewable Energy Costs: The decreasing cost of solar and wind power directly benefits green hydrogen production.

- Government Support and Strategies: Many countries are developing national hydrogen strategies and providing substantial funding for research, development, and deployment [34].
- Technological Advancements: Continued innovation in electrolyzer efficiency, hydrogen storage materials, and fuel cell technologies.
- Sectoral Decarbonization: Hydrogen offers a viable pathway to decarbonize challenging sectors like heavy industry and long-haul transportation.

4. Interplay and Synergies for Sustainable Development

Biofuels and hydrogen energy are not mutually exclusive; they can complement each other in a sustainable energy system.

- Biomass for Hydrogen Production: Biomass gasification can produce syngas, which can then be used to generate hydrogen [35]. This offers a renewable pathway for hydrogen production, especially in regions with abundant biomass resources.
- Biofuels as Hydrogen Carriers: Certain biofuels, like bio-methanol, can be reformed to produce hydrogen on-site, offering a more convenient way to transport hydrogen [36].
- Integrated Energy Systems: Future energy systems may feature integrated biorefineries producing biofuels and bio-hydrogen, alongside renewable electricity generation for green hydrogen production, creating a truly circular economy.
- The future energy landscape will likely be diverse, with a portfolio of renewable energy sources playing specific roles. Biofuels will continue to be important for hard-to-electrify sectors like aviation and heavy-duty transport, while hydrogen will increasingly become the backbone for industrial decarbonization, long-duration energy storage, and potentially maritime and rail transport.

Conclusion

Biofuels and hydrogen energy represent two powerful pillars in the global transition towards sustainable development. Biofuels offer a renewable and often drop-in alternative to fossil fuels, particularly in the transportation sector, with ongoing advancements in sustainable feedstocks and production technologies. Hydrogen, as a versatile and clean energy carrier, holds immense promise for decarbonizing heavy industry, power generation, and long-haul transport. While challenges related to cost, infrastructure, and sustainability must be addressed, ongoing research, supportive policies, and increasing investments are paving the way for their widespread adoption. By strategically integrating these energy forms and fostering international collaboration, the world can accelerate its journey towards a resilient, low-carbon, and sustainable energy future.

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SYNTHESIS OF Mn_3O_4 NANOPARTICLES FROM NEEM TREE ASH

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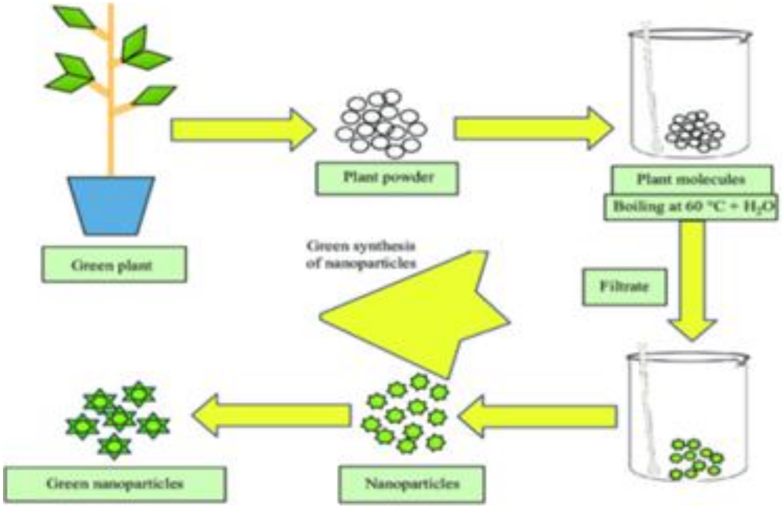
Abstract

Manganese oxide nanoparticles synthesized by using green synthesis rout, from Neem tree ash (*Azadirachta indica*). The leaves of the *Azadirachta indica* neem tree are used extensively in traditional medicine and have been researched for a variety of biological properties. Neem removes the need for hazardous chemicals and solvents that are commonly employed in MONP invention processes. dimensions, form, and crystal structure of neem-based nanoparticles, which may find application in biological imaging, water purification, and catalysis. In the environmentally friendly manufacture of metallic oxide nanoparticles, A. indica shows promise as a replacement for traditional synthetic methods. Mn_3O_4 nanoparticles were synthesized by green synthesis method and characterized using some instrumental methods such as Fourier-transform infrared (FT-IR) spectroscopy, Ultra-violet diffuse Reflectance spectroscopy (UV-DRS).

Keyword: Metal Oxide Nanoparticles (NPs), *Azadirachta indica* Leaf, Mn_3O_4, Green Synthesis.

Graphical Abstract



Introduction

Manganese oxides have been the subject of extensive research because of their unique chemical and physical characteristics and prospective applications in the field of magnetic material, electrochemistry, and catalysis [1-3]. An innovative green synthesis method with low financial and environmental costs is plant-based nanoparticle (NP) synthesis [4,5]. Advances in NP engineering have significantly impacted the fabric, medicinal, and therapeutic industries in recent years [6,7].

The biomedical and other industries benefit from a wide range of nanoscience applications, including antioxidant, biosensor, drug carrier, and catalytic capabilities for their anticancer, antibacterial, anti-inflammatory, and antifungal properties [8-13]. Traditionally, Mn_3O_4 nanoparticles are synthesized using toxic solvents, high temperatures, and chemical reducing agents. These processes can limit the environmental compatibility of the nanoparticles and produce dangerous byproducts. Green synthesis methods have garnered a lot of interest recently as environmentally friendly substitutes for producing nanoparticles [14-17].

The diverse phytochemicals found in plant extracts, including flavonoids, terpenoids, alkaloids, phenolics, and proteins, make plant-mediated synthesis particularly appealing because they function as reducing, stabilizing, and capping agents all at once, making the production of nanoparticles environmentally friendly and economically viable. Neem (*Azadirachta indica*), one of the medicinal plants, has been extensively studied in green nanotechnology because of its potent biological qualities and diverse phytochemical compositions [18-21].

Neem leaf extract has bioactive substances that can stabilize produced nanoparticles and aid in the reduction of metal precursors. Using neem leaf extract, previous research has successfully produced Mn_3O_4 nanoparticles using plant-assisted synthesis, yielding crystalline hausmannite Mn_3O_4 with improved catalytic and sensing capabilities. Neem extract increases particle stability and encourages the development of homogeneous nanostructures in addition to removing dangerous compounds [22-24]. Thus, the current work concentrates on the environmentally friendly synthesis of Mn_3O_4 nanoparticles by employing neem leaf extract as a natural stabilizing and reducing agent. In addition to examining the structural and functional characteristics of the produced Mn_3O_4 nanoparticles for possible technological and biomedical applications, the work attempts to develop an environmentally friendly production process [25-29].

2) Method

a) Preparation of Neem extract:

100 g of neem leaves should be weighed, carefully cleaned with tap water, and then rinsed with DI water. Pour 200 mL of DI water into a 500 mL beaker containing the leaves. For two hours, bring the mixture to a boil on a hot plate at 80 to 90°C, stirring occasionally to guarantee uniform extraction. To get rid of fibers and other contaminants, strain the heated neem extract into a another beaker using a 0.2 µm membrane filter. For later usage, save the filtered neem extract.

b) Preparation of Manganese Chloride Solution:

A digital balance should be used to weigh 1.258 g of manganese chloride ($MnCl_2$). In a 250 mL beaker, dissolve the weighed $MnCl_2$ in 100 mL of DI water, stirring until completely dissolved, to create a 0.1 M solution.

c) Mixing Neem Leaf Extract and Manganese Chloride Solution:

In a 1:2 ratio, mix the manganese chloride solution with the neem leaf extract. For instance, combine 100 mL of $MnCl_2$ solution with 50 mL of neem extract. To guarantee complete mixing, use a magnetic stirrer to continually swirl the mixture for 30 minutes at room temperature.

d) Formation of Mn_3O_4 Paste:

To concentrate the mixture and evaporate the water, set the beaker on a hot skillet and bring the solution to a boil. Keep heating the mixture until it becomes a viscous black paste. This procedure may take two to three hours. To keep the stuff from sticking, stir it occasionally.

e) Heating the Paste in a Furnace:

Fill a ceramic crucible with the black paste. Set the furnace's temperature to 400°C and place the crucible inside. Manganese oxide (Mn_3O_4) nanoparticles are created by heating the sample for two hours. Turn off the furnace once the heating process is finished, then let the crucible to gradually drop to room temperature inside the furnace.

f) Collection of Mn_3O_4 Nanoparticles:

Gather the Mn_3O_4 nanoparticles that have developed from the crucible once it has cooled. A fine black powder should be the appearance of the nanoparticles. For later use or analysis, keep the Mn_3O_4 powder in a dry and clean container.

3. Characterization Techniques:

3.1 UV-Visible absorption studies

The UV-Visible-NIR-DRS Spectrophotometer V770, manufactured by JASCO in Japan, was used to record the UV-visible absorption spectra of Mn_3O_4 nanomaterials. One effective method for determining the band gap energy and confirming the production of nanomaterials is UV-visible spectroscopy. Since certain nanomaterials exhibit particular absorption, it is possible to predict its creation with efficiency. A broad absorption band appears around ~480–550 nm.

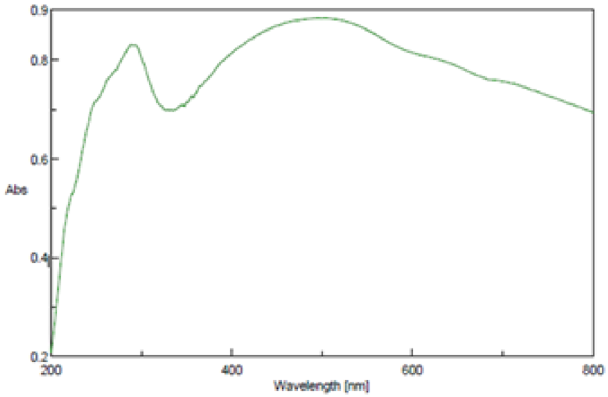


Figure 1: UV/Visible absorption spectra of Mn_3O_4 nanomaterials

3.2 FT-IR analysis

One of the most effective methods for identifying the presence of different types of functional groups and chemical bonds in a wide range of molecules is FT-IR spectroscopic analysis. The

FTIR Spectrometer 4600, manufactured by JASCO in Japan, was used to record the FT-IR spectra of ZnO and Ni/ZnO nanomaterials. Measurements were made between 400 and 4000 cm^{-1}. Figure 2 displays the FT-IR spectra of ZnO and Ni/ZnO nanoparticles that were obtained. A large absorption band at about 3433 cm^{-1} can be seen in the FT-IR spectrum of Mn_3O_4 nanoparticles, which is indicative of the O–H stretching vibrations of adsorbed water molecules. The H–O–H bending vibration is responsible for the peak at 1633 cm^{-1}. The presence of leftover organic molecules from the plant extract utilized during production is indicated by minor bands seen at 1482, 1384, and 1056 cm^{-1}. The production of spinel MnO_4 nanoparticles is confirmed by the assignment of the strong absorption band at about 530 cm^{-1} to the Mn–O stretching vibration.

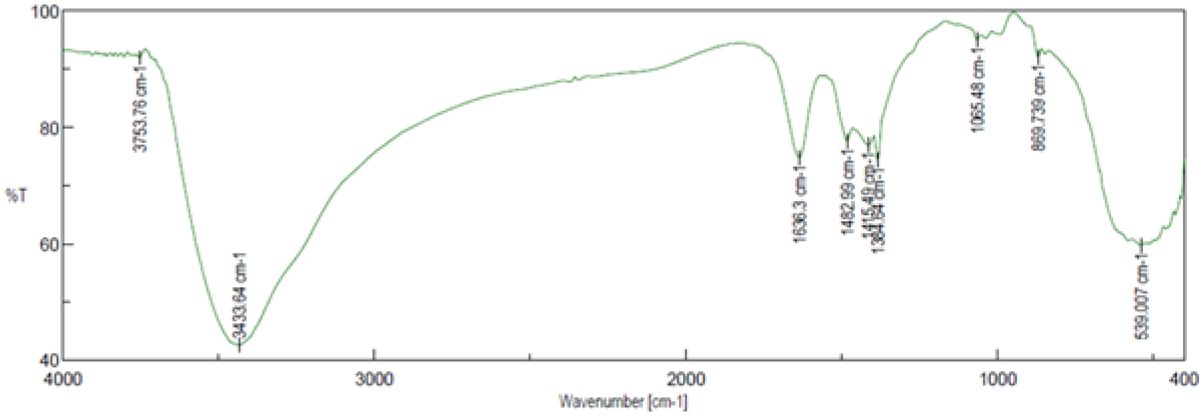


Figure 2: FT-IR spectra of Mn_3O_4 nanomaterials

Conclusion

Over the past ten years, the green product ion of metal lithic nanoparticles has gained popularity as a study issue. In the past, a variety of natural extracts—that is, biological components like bacteria, fungi, yeast, and plants—as well as some fruit extracts have served as efficient resources needed for the synthesis and production of particles that have shown the advantageous effects of plant and fruit extracts. It functions well as a stabilizing and reducing agent in the production of controlled materials (i.e., regulated shape, size, structure, and additional particular features).

Mn_3O_4 nanoparticles successfully Synthesized by the eco-synthesis approach, using neem tree ash extract (*Azadirachta indica*) as a reducing agent in this study, and also given their affordability and sustainability, green approaches for the ecologically friendly synthesis of MONPs could eventually replace the present NP physical and chemical synthesis process.

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INVESTIGATING THE IMPACT OF EDM PARAMETERS ON SURFACE ROUGHNESS AND ELECTRODE WEAR RATE IN 7024 ALUMINUM ALLOY

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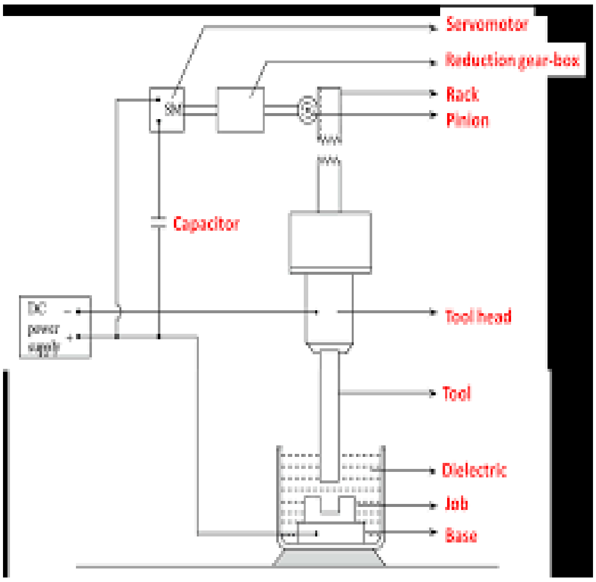
Abstract

Electrical Discharge Machining (EDM) is a significant process in the industry for machining hard metals. It is a time-consuming and costly method that requires a high level of expertise to operate effectively. EDM is considered one of the unconventional operating processes due to its unique characteristics and the challenges associated with its implementation. One of the challenges facing researchers is determining the optimal parameters for achieving high surface quality while minimizing equipment consumption and associated costs. In addition to being classified as one of the operating processes, EDM processes are also classified as electro-thermal processes that affect surface quality. In this study, the influence of EDM parameters on surface roughness and electrode wear rate when machining aluminum alloy type 7024 was investigated. A total of 27 experiments were conducted to evaluate the impact of three parameters at three levels. The parameters under investigation include current, pulse on time, and pulse off time. Subsequent analysis of the results by variance analysis revealed that the most influential parameter for both surface roughness and electrode wear rate is electric current, with a rate of influence of 74%. The results were then subjected to further analysis using variable effect graphs to identify the optimal variables for achieving the best results. Finally, neural networks were employed to predict the results, with an accuracy of up to 99%.

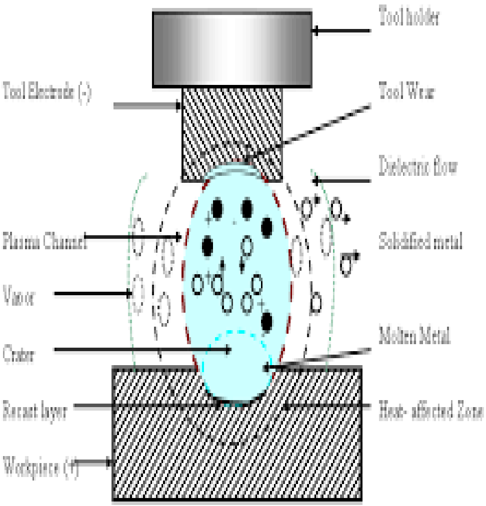
Keywords: EDM, Surface Roughness, Electrode Wear Rate, Artificial Neural Networks.

I. Introduction

The durability of traditional machining tools exceeds that of the workpieces with which they are used. Some materials possess a hardness that exceeds the capabilities of conventional machining processes. The aviation engine, food, dairy, paper, die, and molding sectors require hard materials, which has led to the development of non-conventional machining techniques. These metal removal methods employ a variety of techniques, including electrochemical, thermal, and mechanical procedures. In certain instances, non-conventional techniques may prove to be more cost-effective [1]. In the 1770s, English scientist Joseph Priestly discovered EDM. In his investigations, Priestly discovered that electrical discharges were effective for removing electrode material. Priestly discovered EDM, but the process was found to be inaccurate and flawed [2]. EDM is applicable to a number of manufacturing sectors, including automotive and aerospace, as well as to the machining of a wide range of conductive materials. Due to the superior capabilities of EDM in the machining of high-strength and temperature-resistant materials, conductive materials, and conductive engineered ceramics with intricate geometries, it is often the preferred method of production [3].



Researchers have focused their efforts on improving machining performance, ensuring dimensional accuracy, and enhancing surface integrity. A review of the literature was conducted to gain insight into the EDM procedure and sinking EDM operation documents. Authors in [4] analyzed the influence of electrode shape on the EDM of mild steel, with a particular focus on the effects on Material Removal Rate (MRR) and Electrode Wear Rate (EWR). The highest MRR was observed for round electrodes, followed by those of square, triangular, and diamond shapes. Nevertheless, the diamond electrode exhibited the highest EWR.



Authors in [5] investigated the impact of tool polarity on EDM, MRR, and EWR. The study demonstrates that direct polarity yields the greatest MRR while simultaneously minimizing Wear Rate (WR). The direct polarity method has been demonstrated to result in a fourfold increase in

MRR and a fivefold reduction in WR in comparison to the reverse polarity method. Authors in [6] employed the Taguchi method to investigate the influence of machining factors on MRR in EDM operations. The studies employed a variety of pulse on time (T_{on}), pulse off time (T_{off}), and peak current (I_p) parameters. An orthogonal array with L27, S/N ratio, and ANOVA was employed to evaluate the performance of EDM on 202 SS. The findings indicate that the highest MRR is achieved when the I_p and T_{off} are at their highest levels and T_{on} is at its lowest. The interaction data indicates that there are significant effects associated with the variables I_p and T_{off}. Authors in [7] examined the impact of combining aluminum and copper fine metal particles with dielectric fluid on MRR during the machining of AISI D3 and EN-31 steel. The process inputs included the workpiece material, the peak current (I_p), the pulse on time (T_{on}), the duty factor, the gap voltage (V), and the mixing of fine metal powder in the dielectric fluid. The output parameters used to assess the performance of the process were the MRR. The experimental results demonstrate that the presence of metal particles in a dielectric fluid lead to an enhancement in the MRR. Authors in [8] presented a novel method for enhancing the precision of silver-tungsten electrodes machined by micro-EDM. This method involves combining powder (suspended nanographite) with dielectric (kerosene). The microcrack density and the surface roughness (R_a) of the machined surface were observed to decrease by 85% and 22%, respectively. Authors in [9] investigated the impact of I_p, T_{on}, and T_{off} on R_a in EDM operations, employing the Taguchi approach to achieve a superior surface finish. The combination of low T_{on}, I_p, and high T_{off} resulted in the optimal R_a. The anticipated range for R_a was between 2.14 and 3.36. Authors in [10] presented a detailed explanation of the impact of I_p, T_{on}, and T_{off} (three-level parameters) on R_a. The Taguchi method was employed in the course of these studies. An EDM was employed to assess the performance of a titanium alloy when subjected to the action of copper, brass, and aluminum electrodes. The influence of I_p on R_a is significant, and the use of Al electrode alloys has been shown to result in lower R_a values. Authors in [11] developed a model to predict the variables of volume V, T_{on}, I_p, T_{off}, and reaction surface finish in AISI D2 steel EDM using Response Surface Methodology (RSM). The face Central Composite Design (CCD) was employed for the purpose of determining the experimental plan. The surface quality was superior when low I_p, T_{on}, V, and high T_{off} were employed. The researchers found that model- based RSM is an effective method for manufacturing AISI D2 tool steel. Authors in [12] developed a technique for high-finish EDM machining. A series of tests were conducted to measure R_a under varied voltage and T_{on} cutting conditions. The findings of the modeling and optimization demonstrate that the roughness for voltage and T_{on} is significantly lower than that of all experimental runs. In this study, the impact of EDM parameters, specifically current (A), pulse on time (µsec), and pulse off time (µsec), was investigated to ascertain their effect on R_a and EWR values. This was achieved through the use of analysis of variance and ANN techniques.

Electrical Discharge Machining Mechanism

The principal mechanism of material erosion in EDM is the conversion of electrical energy into thermal energy through discrete electrical discharges between the tool (the electrode) and the workpiece immersed in a dielectric fluid. The creation of a plasma channel between the tool electrode and the workpiece results in the breakdown of the dielectric [13], as shown in Figure 1. The breakdown typically occurs between the electrode and the workpiece at the closest point of contact. Spark breakdown causes a rapid decline in voltage and an increase in current, which results in the ignition of multiple monodes.

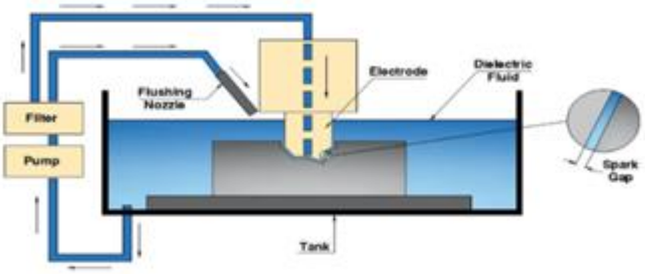


Figure 1: Principle of EDM

Experimental Work

The requisite specifications for machine tools, workpiece materials, and electrode tools, in addition to their corresponding response characteristics, are used to assess surface roughness and electrode wear rate.

A. Machine Tool

As presented in Figure 2, all experiments were conducted on an EDM CNC machine.

Figure 2: EDM machine tool

B. Workpiece Material

The workpiece was composed of aluminum alloy type 7024. Prior to EDM processing, the workpiece was manufactured in 50×40 mm square specimens with a surface roughness of 2 µm. Table 1 shows the chemical composition of the aforementioned specimens.

Table 1: Chemical composition of al alloy type 7024 workpiece

Si (%)	**0.163**	**Zn (%)**	**4.93**
Fe (%)	0.422	Ti (%)	0.038
Cu (%)	2.14	Ga (%)	0.010
Mn (%)	0.216	V (%)	0.007
Mg (%)	1.55	Pb (%)	0.071
Cr (%)	0.090	Other (%)	0.132
Ni (%)	0.012	AL (%)	90.219

Artificial Neural Network Modeling

The objective is to develop a mathematical model that expresses the minimization of surface roughness and electrode wear rate in cutting parameters. This study employs ANN to create the aforementioned model. ANNs comprise one or more hidden layers situated between the input and output layers. Each neuron in the network receives input from all preceding layer neurons [16]:

Tool Electrode

$W_{ij}x_i$ (2)

where the j_{th} hidden layer neuron receives N inputs, collectively
denoted as *net*, *w* represents the weight of the connection
j ij

C. Tool Electrode

The experiments employed a 50-mm-long, 15-mm-diameter copper cylindrical solid electrode.

Design of Experiment

The number of experiments required is contingent upon the experimental design. It is therefore essential to conduct well- designed cutting experiments. In order to measure R_a for AL- alloy 7024 specimens, a three-level full factorial design was employed, resulting in the execution of 27 cutting experiments. The current I_p, pulse on time T_{on}, and pulse off time T_{off} are the variables under consideration. The levels of the cutting parameters are presented in Table II.

Table 2: The levels of cutting parameters

Levels	Current (A)	Pulse on time (µsec)	Pulse off time (µsec)
1	24	50	25
2	30	100	50
3	36	150	75

Measurement of Response Characteristics

A. Surface Roughness (R_a)

A standard parameter, R_a in µm, is employed to assess surface roughness by comparing the maximum peaks and minimum troughs of specific locations. This approach relies on the device's cut-off length and mean line.

B. Electrode Wear Rate (EWR)

In a manner analogous to the material removal rate procedure, the workpiece was substituted with the electrode. The formula for EWR is given [14]:

from the i_{th} forward layer neuron to the j_{th} hidden layer neuron

and, x_i denotes the input from the preceding layer neuron. A neuron in the network processes the net input through an activation (transfer) function, such as the tangent hyperbolic function employed in this study [17]. The objective of this study is to identify the optimal combination of parameters that minimizes a combination of squared errors, thereby producing a well-generalized network. A single hidden layer with three inputs and one output was employed to model the process, as shown in Figure 3. The three most significant input variables are current, pulse on time, and pulse off time, while the output variables are R_a and EWR. The distribution of experimental data, comprising 27 groups, was conducted in a manner whereby the training subset encompasses 21 groups, or 75% of the data, while the testing subset comprises 6 groups, or 25% of the data. In order to identify an appropriate network architecture, a number of different architectures have been considered. The model with a 3-5-1 architecture was determined to be the optimal choice for the task.

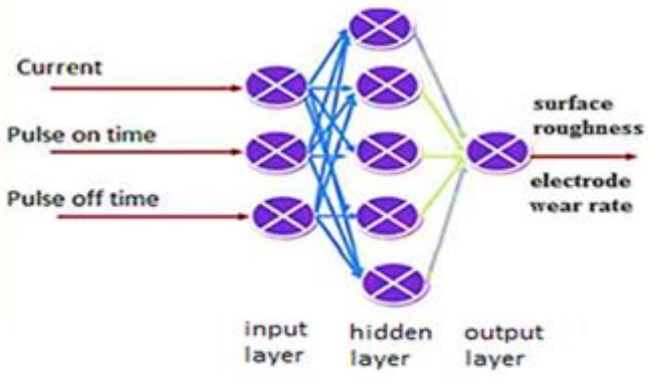


Figure 3: Neural network architecture designed

Analysis of Variance

The experimental results are subjected to ANOVA in order to ascertain the impact of cutting parameters on R_a and EWR, with the latter serving as the dependent variable. The independent variables in this analysis are current, pulse on

$$EWR = \underline{W_{ie}-W_{fe}} \qquad (1)$$

where W_{ie} is the initial electrode weight (gm), W_{fe} is the final electrode weight (gm), ρ_e is the density of electrode (gm/mm^3).

The calculation is built on the basis that the density of the electrode is (8.9 gm/cm^3) [15]. time, and pulse off time. This analysis was conducted with a significance level of 0.05, which corresponds to a confidence level of 95%.

Results

Following the completion of the practical component and the subsequent measurement of the outcomes for both R_a, as determined by the surface roughness tester (MarSurf SP1), and EWR, calculated in accordance with (1) and Table III, a detailed discussion was undertaken on the following:

A. Analysis of Mean for Surface Roughness

The EDM current and other process parameters influence the R_a of the components. The current has an impact on the R_a of EDM. Figure 4 demonstrates that higher EDM currents result in an increase in material removal rates. An increase in energy input and more aggressive material removal can result in the formation of a coarser surface finish, but the process will be completed more rapidly. The objective is to optimize the process for distinct materials. The EDM current interacts with the pulse duration, voltage, and electrode material. In order to achieve the desired surface finish, it is necessary to optimize these parameters and current. The pulse-on time in EDM has a significant impact on R_a. The following section will examine the impact of pulse-on time on EDM surface roughness [18]. The formation of a melt pool is dependent upon a number of factors, including the timing of the pulse that controls the duration of the electrical discharge. A longer pulse-on period results in an increase in the size of the melt pool. An increase in heat generation resulting from extended pulse-on durations can lead to the melting of the material and the formation of recast layers, ultimately resulting in a surface quality that is more irregular. The wear of the electrode is also a factor to consider. The prolonged electrical discharge resulting from extended pulse-on periods has the potential to cause wear on the electrodes. The presence of EDM imperfections resulting from excessive electrode wear may lead to a deterioration in the surface finish of the workpiece. The impact of the pulse-off time in EDM on the R_a value, whereby the separation of discharges is influenced by this parameter. The influence of the pulse-off time on the surface roughness of the EDM process has been the subject of considerable research. The characteristics of the process, including the duration of the pulse-on time, the level of current, the voltage, and the composition of the electrode material, have an impact on the duration of the pulse-off time. In order to achieve the requisite surface finish in EDM, it is necessary to optimize the aforementioned parameters and pulse-off time.

Table 3: Readings of experimental work

No.	Current (A)	Pulse on time (µsec)	Pulse off time (µsec)	Surface Roughness *Ra* (µm)		Electrode Wear Rate (EWR) (mm3/min)	
				Measured	**Predicted**	**Measured**	***Predicted***
1	24	50	25	4.64	4.60333	0.88	0.71630
2	24	50	50	4.15	4.23222	0.89	0.79852
3	24	50	75	3.88	3.96778	0.70	0.87630
4	24	100	25	4.70	4.69222	0.89	0.89185
5	24	100	50	4.30	4.32111	0.99	0.97407
6	24	100	75	4.00	4.05667	1.13	1.05185
7	24	150	25	4.87	4.81111	1.12	1.20296
8	24	150	50	4.56	4.44000	1.50	1.28519
9	24	150	75	4.20	4.17556	1.06	1.36296
10	30	50	25	5.60	5.58667	0.98	1.22630
11	30	50	50	5.32	5.21556	1.22	1.30852
12	30	50	75	4.94	4.95111	1.23	1.38630
13	30	100	25	5.50	5.67556	1.45	1.40185
14	30	100	50	5.30	5.30444	1.62	1.48407
15	30	100	75	4.91	5.04000	1.46	1.56185
16	30	150	25	5.80	5.79444	1.80	1.71296
17	30	150	50	5.48	5.42333	1.89	1.79519
18	30	150	75	5.30	5.15889	2.10	1.87296
19	36	50	25	5.80	5.80667	2.11	1.86185
20	36	50	50	5.54	5.43556	2.05	1.94407
21	36	50	75	5.10	5.17111	2.08	2.02185
22	36	100	25	5.96	5.89556	1.99	2.03741
23	36	100	50	5.80	5.52444	1.89	2.11963
24	36	100	75	5.30	5.26000	2.30	2.19741
25	36	150	25	6.01	6.01444	2.18	2.34852
26	36	150	50	5.09	5.64333	2.09	2.43074
27	36	150	75	5.53	5.37889	2.78	2.50852

B. Analysis of Mean for Electrode Wear Rate

As presented in Figure 5, the current has a significant impact on the EWR in EDM. The current has an impact on the wear rate of electrodes used in EDM. There is a direct correlation between the two variables. The intensity of the EDM current has a direct impact on electrode wear. An increase in current levels results in enhanced material removal, which in turn leads to electrode deterioration. The interdependence between electrode wear and material removal in EDM are described, with both processes being contingent upon the pulse-on time. The rate of material removal is dependent upon the duration of the pulse-on phase in EDM and has an impact on the rate of material removal. As a consequence of the increased duration of contact and the greater energy input, longer pulse-on periods result in enhanced rates of material removal and electrode wear. A trade-off exists between electrode wear and workpiece surface polish, whereby adjusting the pulse-on time affects one or the other. In order to achieve optimal results in an EDM operation, it is necessary to strike a balance between electrode wear and surface finish. The EDM pulse-off time has a significant impact on the EWR and other process parameters. The impact of pulse-off time on the wear rate of electrodes used in EDM is a topic worthy of further investigation. The removal of heat and debris is facilitated by the cooling effect of the EDM process. The pulse- off time facilitates the cooling of the electrode and the removal of debris and gases from the machining gap. The removal of heat and debris through efficient cooling mitigates the thermal effects and wear on the electrode. Prolonged pulse-off periods facilitate enhanced heat dissipation from the electrode, thereby reducing the temperature at the tool-electrode interface. The surface finish is a significant factor. In order to achieve the optimal reduction in electrode wear, it is essential to consider the surface quality of the workpiece. The objective of optimal machining outcomes is to achieve a balance between wear rates and surface finish.

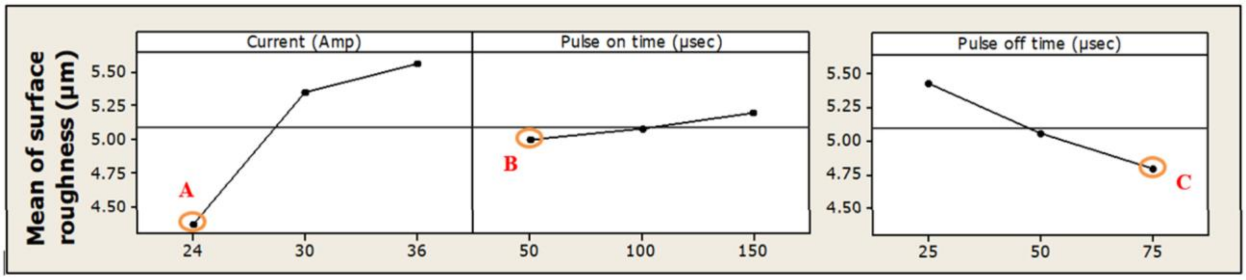


Figure 4: Mean effect plot for surface

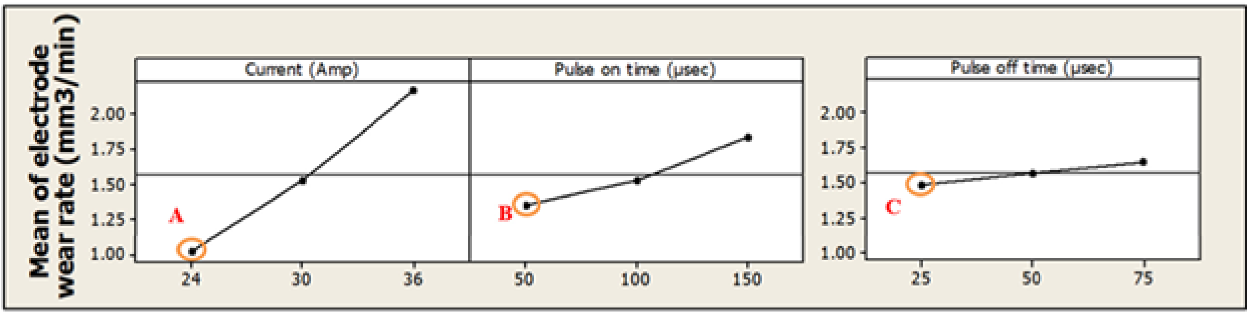


Figure 5: Mean effect plot for electrode wear rate

C. ANOVA for Surface Roughness

Following an analysis of the results, it was determined that the electric current exerts the greatest influence on the Ra values, with the pulse off time as the second most influential parameter. In contrast, the pulse on time was identified as the least influential parameter, as presented in Table 4.

Table 4: ANOVA presents work for surface roughness

Source of variance	**Degree**	**Sum of squares**	**Variance**	***P* (%)**
Current (A)	2	7.390	3.695	74.14
Pulse on time (µm)	2	0.196	0.098	1.96
Pulse off time (µm)	2	1.835	0.917	18.41
Error ,e	20	0.545	0.0166	5.47
Total	26	9.967		100

D. ANOVA for Electrode Wear Rate

Following an analysis of the results, it was determined that the electric current exerts the greatest influence on the EWR values, with the pulse on time as the second most influential parameter. In contrast, the pulse off time was identified as the least influential parameter, as shown in Table 5.

E. Regression and Comparison for Surface Roughness by an ANN

A regression graph is a visual representation that demonstrates the relationship between network targets and outputs. Figure 6 shows the validation, learning, testing, and all data regression plots. The solid line should be in accordance with the dotted line.

Table 5: ANOVA presents work for electrode wear rate

Source of variance	**Degree**	**Sum of squares**	**Variance**	***P* (%)**
Current (A)	2	5.9290	2.9645	74.98
Pulse on time (µm)	2	1.093	0.547	13.83
Pulse off time (µm)	2	0.115	0.058	1.46
Error ,e	20	0.774		9.8
Total	26	7.9071		100

A comparison is made between a measured and a predicted result in order to validate the ANN model. As shown in Figure 7, the neural network model demonstrates a high degree of accuracy, with a close alignment between the actual calculated R_a and the predicted output. The ANN model was trained using 21 Ra values, while the remaining six were employed as a test set within the MATLAB toolbox. The experimental results demonstrated that the ANN can be effectively utilized for the prediction of R_a in the machining of 7024 aluminum alloy, as it offers enhanced accuracy and reduces the time required. Figure 8 presents the regression coefficients for the model based on the data, which were found to be (1) for training, (0.997) for validation, (1) for testing, and (0.99958) for all data sets. These results indicate that the network is learning and predicting Ra properly. The chart demonstrates that the regression coefficient for the training set is 1, indicating a linear relationship between the objectives and outputs.

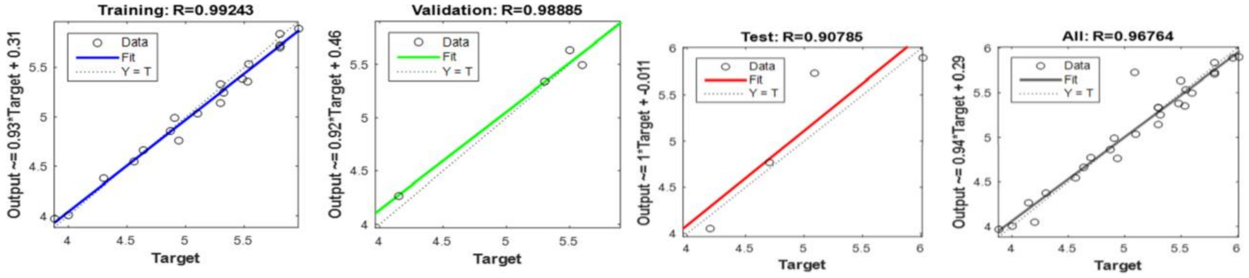


Figure 6: Regression graphs for model

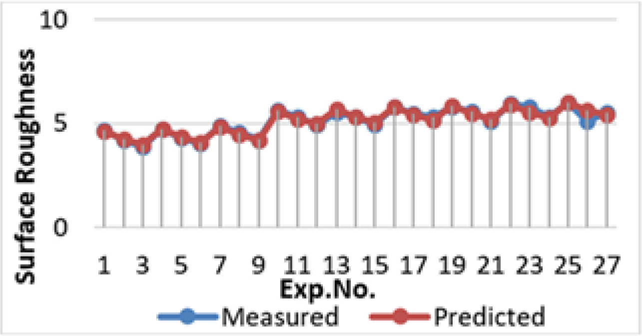


Figure 7: The comparison between the measured and predicted values of Ra for the training set

F. Regression and Comparison for Electrode Wear Rate by ANN

The number of tests has an impact on the 27 EWR value presented in Figure 9. A total of 21 EWR values were employed for the training of the ANN model, while six were used for its evaluation in MATLAB Toolbox. The correlation between the experimental EWR values and the ANN model predictions, is observed. The observed and projected EWR levels exhibit a high degree of similarity.

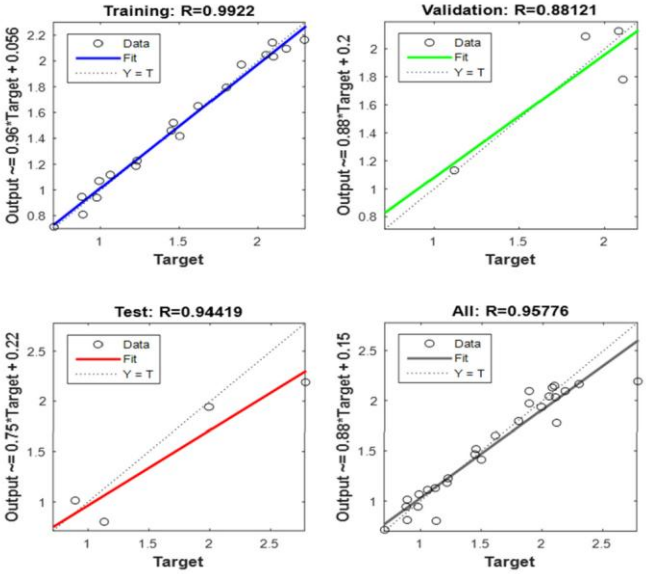


Figure 8: Regression graphs for model

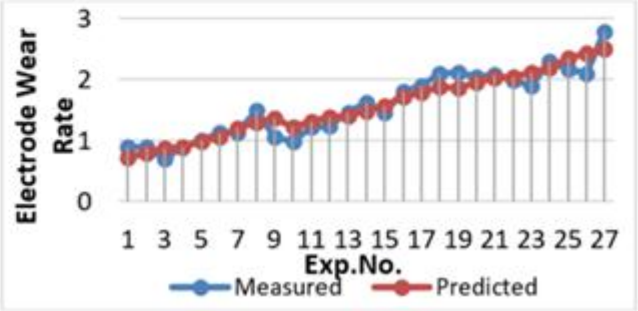


Figure 9: The comparison between the measured and predicted values of EWR for the training set

Conclusions

The results of the experimental work indicated that the most influential factor on both the surface quality and the amount of metal removal (production speed) is the amount of electric current. It was observed that the lowest amount of electric current resulted in the best surface quality (less surface roughness), while the highest value of electric current resulted in the best production speed (the largest amount of metal removal). The lowest value of pulse on time and pulse off time yielded the optimal surface quality. A neural network with an accuracy of up to 99% was constructed. Considering the above results we can conclude:

- The Electrical Discharge Machining (EDM) current is a significant factor influencing surface roughness. Operators may optimize the EDM process to obtain the requisite surface finish for a given workpiece material and application by carefully managing the current level and evaluating its interaction with other process factors.
- The EDM pulse-on time has an impact on surface roughness. Operators may oversee the management of material removal processes, heat input, and surface finish quality for an EDM application.
- The EDM pulse-off time affects several processes, including heat dissipation, debris clearance, electrode wear, re-ignition, and surface texture management. These effects contribute to the overall surface roughness of the material being processed.

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PHYTOCHEMICAL AND ANTIMICROBIAL SCREENING OF LEAVES OF *MORINGA OLEIFERA*

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Abstract

The leaves of *Moringa oleifera* were subjected to phytochemical screening using various solvents to identify their bioactive constituents. The analysis confirmed the presence of important phytochemicals such as alkaloids, flavonoids, glycosides, terpenoids, tannins, saponins, and steroids. These compounds are known for their therapeutic potential and biological significance. The leaf extracts demonstrated significant antimicrobial activity against both Gram-positive and Gram-negative bacteria, including *B. subtilis*, *S. aureus*, *E. coli*, and *P. aeruginosa*. The findings suggest that *Moringa oleifera* leaves possess promising antimicrobial properties and could serve as a natural source for developing effective antimicrobial agents.

Keywords: *Moringa oleifera*, Phytochemical Screening, Antimicrobial Activity.

Introduction

Natural extracts have been of very high interest since ancient time due to their enormous medicinal use and researcher's attention have further gone up recently to explore their phytochemical compositions, properties, potential applications in the areas such as, cosmetics, foods etc. In this present study phytochemical analysis have been done on the aqueous and methanolic Moringa leaves. Plants and extracts of their various sections have been used for their medical characteristics and to cure specific ailments as well as general tonics, meals, and other methods to increase the body's immunity and vigor since ancient times.

However, since from last few decades chemist aware of nature power of defeating the disease. In recent times there has been a tremendous increase in the use of plant-based health products. upcoming varieties of new alarming health concerns like recent concerns of Coronavirus disease in 2019 (COVID-19), which affects the respiratory system acutely [1–2]. Moringa oleifera is one of the magical plants considered in India due to its high medicinal properties. *Moringa oleifera* belongs to family Moringaceae. It is found in Maharashtra and commonly known as 'Drumstick' and horse radish tree, ben oil tree, miracle tree and mothers best friend. It is considered to be rich in proteins, vitamins, minerals, folic acid and β- carotene and possess antithyroid [3] antiasthmatic [4], antidiabetic [5], anti-bacterial, antibiotic [6], anti-inflammatory [7], antioxidant [8], antiulcer [7–10], cholesterol-lowering [11], anti-HSV [12], antifungal [13], diuretic [14], antihypertensive [15], hepatoprotective [16], antitumor [17] activity.

Material and Methods

Collection of Plant Material

The present study was carried out in the Department of Chemistry of our College. Leaves were collected from the *Moringa oleifera* plant (Figure 1, 2) from the area near to our college. It was ensured that the plant was healthy and uninfected. The leaves were washed under running tap water to eliminate dust and other foreign particles and to cleanse the leaves thoroughly and dried.

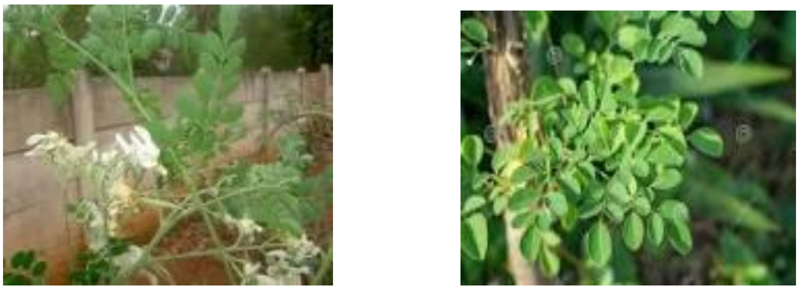

Figure 1: Tree of *Moringa oleifera* around the college campus in Parbhani

Collection and Identification of Plant Material

The *Moringa oleifera*, leaves were procured from Parbhani region and were authenticated from Department of Botany, B. Raghunath ACS College, Parbhani. The leaves were dried at room temperature and powdered. The powder was stored in glass bottle in a cool and dry place away from direct sunlight and used for preparation of extract [18].

Figure 2: Collection of leaves of *Moringa oleifera* dry and crushed into fine powder

Preparation of Leaf Extracts

Dried powder of leaves was continuously refluxed with methanol, Ethanol, petroleum ether, and acetone at 60°C for 70 hours using distillation apparatus. The solvent extract was then stored in an air tight container at 5-10°C for further use. Then the phytochemical analysis was individually performed for the test of, alkaloids, flavonoids, steroids, terpenoids, tannins, volatile oil, glycoside, reducing sugar and saponins.

- **Flavonoids:** 5ml of each extract was added to 10ml of distilled water and the solution was shaken and 1ml of 10% NaOH solution was added to the mixture. A yellow color formation indicates the presence of flavonoids.
- **Alkaloids:** To the small amount of extract, few drops of dilute HCl were added and then filtered. The filtrate is treated with Dragendroffs reagent the formation of orange brown precipitate confirms the presence of alkaloids [19].

- **Saponins (Frothing Test):** 5ml of each extract diluted with 2ml of distilled water was added in a test tube, and the solution was shaken vigorously for 15 min. The bubble is started to form a foam which indicate the presence of saponin.
- **Steroids:** 2-3 drops of concentrated H_2SO_4 were added to 1ml of each extract in a separate test tube. The formation of a reddish-brown color was taken as a positive reaction.
- **Terpenoids:** To 5 ml. of extract, 2 ml. of chloroform was added followed by carefully addition of concentrated sulphuric acid. The formation of reddish-brown color layer at the junction confirms the presence of terpenoids.
- **Tannins:** A few drops of lead acetate solution were added to the extract. The formation of precipitate indicated the presence of tannin.
- **Glycosides**: 25ml of dilute sulphuric acid was added to 5ml extract in a test tube and boiled for 15minutes, cooled and neutralized with 10% NaOH, then 5ml of Fehling solution added. Brick red precipitation indicates the presence of glycosides.
- **Reducing Sugars:** To 0.5ml of plant extracts, 1ml of water and 5-8 drops of Fehling's solution was added and heated over water bath.
- **Volatile Oil:** 2ml of Extract was shaken with 0.1ml dilute NaOH and a small quantity of dilute HCl

Figure 3: Phytochemical screening of leaves extract in lab

Result and Discussion

The present study reveals that *Moringa oleifera* plant shows the presence of phytochemical constituents like alkaloids, flavonoids, steroids, terpenoids, tannins, volatile oil, glycoside, reducing sugar and saponins in different solvent extracts as shown in Table 1. Phytochemical screening of *Moringa oleifera* shows the presence of various phytochemicals such as alkaloids flavonoids, glycosides, terpenoids, tannins, saponins and steroids in different solvents (methanol, ethanol, petroleum ether, acetone) [20, 21].

Flavonoids are present in extract of methanol and ethanol extract while absent in other extracts. Alkaloids are present only in ethanol extract while absent in other extracts. Saponins present in all solvent extracts. Steroids are present in extracts of ethanol and Petroleum ether while absent in other extracts. Terpenoids are absent in petroleum ether extracts while present in other extracts. Tannin shows its presence in extracts of methanol and ethanol while absent in other extracts. Glycosides are present in methanol and petroleum ether extracts while absent in other extracts. Reduced sugar absents in all solvent extract while volatile oil is found in a negligible amount in ethanol extract.

Table 1: Phytochemical screening of Leaves of *Moringa oleifera*

Sr. No.	Phytochemical constituents	Methanol Extract	Ethanol Extract	Petroleum ether extract	Acetone extract
1.	Flavonoid	Present	Present	Absent	Absent
2.	Alkaloid	Absent	Present	Absent	Absent
3.	Saponins	Present	Present	Present	Present
4.	Steroid	Absent	Present	Present	Absent
5.	Terpenoid	Present	Present	Absent	Present
6.	Tannin	Present	Present	Absent	Absent
7.	Glycoside	Present	Absent	Present	Absent
8.	Reduce sugar	Absent	Absent	Absent	Absent
9.	Volatile oil	Absent	Present	Absent	Absent

Antimicrobial Activity

The antibacterial activities of the Ethanol extract of *Moringa oleifera* leaves were studied against four bacteria, viz. *Bacillus subtilis* (G+), *Escherichia coli* (G–), *Staphylococcus aureus* (G+) and *Pseudomonas aeruginosa* (G–). For the detection of antibacterial activities, the filter paper discs diffusion method was used. Streptomycin sulphate was used as positive control. Nutrient agar (NA) was used as basal medium for test bacteria. The discs were prepared by impregnating in sample (1 mg/1 mL). Each culture was prepared to a turbidity equivalent to McFarland and spread on the test tube 8. The paper disc containing the testing extract was placed on the agar surface previously inoculated with suspension of each microbes to be tested. All determinations were made in duplicate. Inhibition diameter was determined after incubation at 37°C ± 1 for 24 h. The antimicrobial activity was indicated by the presence of the clear inhibition zones around each disc.

Table 2: Antibacterial Activity of Ethanol Leaf Extract of *Moringa oleifera*

Sr. No	Microorganism	Zone of clearance Ethanol extract(mm)	Streptomycin sulphate(mm)
1.	*Bacillus subtilis*	4mm	6mm
2.	*Staphylococcus aureus*	3mm	7mm
3.	*Escherichia coli*	6mm	7mm
4.	*Pseudomonas aeruginosa*	5mm	8mm

The antibacterial activity of extract has been assayed at the concentration 1000 µg/mL against four human pathogenic bacteria. Among them two were gram positive and the other two were gram negative. The inhibitory effect of extract against these organisms is given in Table 2. The diameter of zone clearance is measure in mm. The ethanol extract of *Moringa oleifera* shows maximum activity against *E. coli* and *Pseudomonas aeruginosa* as observed their zone of clearance.

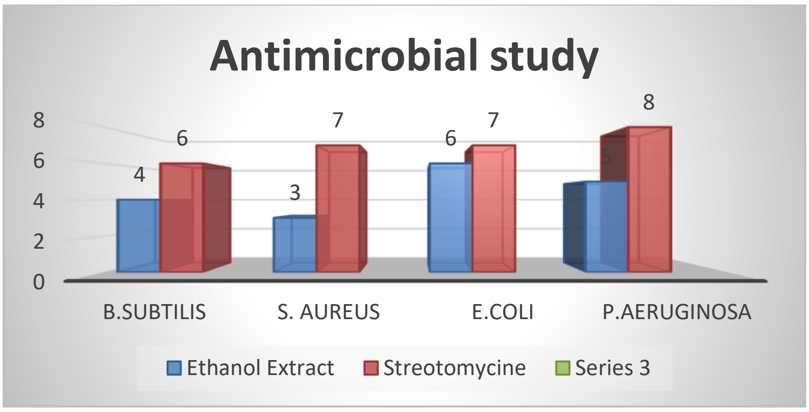

Figure 4: Comparision of antimicrobial activity of leaf extract with streptomycin

As observed in Figure 4, the antimicrobial activity was highest against *Escherichia coli* and *Pseudomonas aeruginosa*, while moderate inhibition was recorded against *Bacillus subtilis* and *Staphylococcus aureus*. Various parts of *Moringa oleifera* exhibit significant medicinal potential. The leaf extract of *M. oleifera* is traditionally used for the treatment of diarrheal disorders, dysentery, colitis, sores, skin infections, anemia, cuts, scrapes, rashes, and signs of aging [22]. The gum is used for fevers, dysentery, asthma, and dental decay, while the seeds possess antibacterial and antimalarial properties [23]. The oil is used in gout and acute rheumatism, and flower extracts are employed in the treatment of tumors, inflammation, hysteria, splenic enlargement, muscle diseases, and as aphrodisiac agents [24]. The roots are used for toothache and as an anthelmintic, whereas the bark aids digestion and is used in stomach pain, poor vision, ulcers, hypertension, joint pain, anemia, and diabetes [25]. Furthermore, the leaves are used as cardiac stimulants and in the management of malaria, arthritis, skin diseases, hypertension, typhoid fever, swellings, parasitic diseases, diabetes, cuts, genitourinary ailments, immune enhancement, and to promote lactation [26].

Conclusion

The present study conclusively demonstrates that *Moringa oleifera* is a good source of various phytochemicals like alkaloids, flavonoids, glycosides, saponins, tannins, Terpenoids. The antibacterial activity *Moringa oleifera* was clearly shown by the present study against various test organisms like *Escherichia coli, Pseudomonas aeruginosa, Staphylococcus aureus* and *Bacillus subtilis*. There is again a very large scop for researchers to do the depth study regarding the usefulness of this god gifted miracle plant.

Acknowledgment

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MEDICATION THERAPY MANAGEMENT (MTM) AND PATIENT CARE

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Introduction

In an era of complex polypharmacy, simply "taking your pills" is no longer enough to guarantee health. Medication Therapy Management (MTM) represents a shift from the traditional product-centered model of pharmacy to a patient-centered clinical service. MTM is a comprehensive suite of services designed to ensure that every medication a patient takes—whether prescription, over-the-counter, or herbal—is contributing to a positive health outcome rather than a hidden complication.

At its core, MTM is the bridge between a doctor's prescription and a patient's actual recovery. By leveraging the expertise of pharmacists, MTM identifies and corrects common yet dangerous issues, such as:

- Incorrect usage: Medications not being taken at the right time or in the right way.
- Duplication: Multiple prescriptions for the same underlying issue, often from different doctors.
- Under-treatment: Identifying gaps where a patient's condition remains unmanaged.
- Safety risks: Detecting potential adverse drug reactions before they occur.

Objectives of MTM:

MTM is designed to be a collaborative, patient-centered process with three primary goals:

- **Optimization:** Helping patients get the maximum therapeutic benefit from their meds.
- **Safety:** Detecting and preventing costly medication problems, such as drug-drug interactions or toxicities.
- **Adherence:** Empowering patients to understand *why* and *how* to take their medications correctly.

Who Benefits Most?

While any patient taking medication can benefit, MTM is specifically targeted toward "high-risk" populations, including those who:

- Manage multiple chronic conditions (e.g., Diabetes, Hypertension, Heart Failure).
- Take a large number of medications (Polypharmacy).

- Incur high annual costs for their prescriptions.

MTM vs. Traditional Pharmacy Services

It is important to differentiate MTM from "Dispensing." While dispensing focuses on the product (the right drug for the right patient), MTM focuses on the patient's journey with that drug. Unlike "Disease Management," which looks at a single condition (like Asthma), MTM looks at the entirety of the patient's medicine cabinet to ensure nothing conflicts.

The Economic and Clinical Value

Evidence from programs like the Asheville Project and the Diabetes Ten City Challenge has proven that when pharmacists provide MTM, total healthcare costs drop. This is achieved by reducing emergency room visits and improving worker productivity, proving that the clinical role of the pharmacist is a vital financial asset to the healthcare system.[xi]

It is vital to distinguish MTM from other standard healthcare activities. While they may overlap, their objectives differ significantly:

Service Type	Primary Focus	Scope of Work
Prescription Dispensing	The Product	Delivering the correct drug to the correct patient with basic usage instructions.
Disease Management	The Diagnosis	Managing a specific condition (e.g., Diabetes) through screenings, lifestyle changes, and specific meds.
MTM	The Whole Patient	A holistic review of the entire medication regimen to optimize effectiveness and safety across all conditions.

The Core Elements of MTM

To provide a comprehensive view of the **Core Elements of MTM**, we must look at the official framework that transitioned pharmacy from a dispensing model to a clinical service model. These elements were established to ensure that the \$300\$ billion spent annually on "non-optimized" medication use is addressed through a structured process.

The Five Core Elements of MTM:

The following five pillars represent the essential components of an MTM service as defined by the American Pharmacists Association (APhA) and the National Association of Chain Drug Stores (NACDS).[xii]

1. Medication Therapy Review (MTR)

The MTR is a systematic process of collecting patient-specific information and assessing medication therapies to identify medication-related problems (MRPs).

- **Method:** The pharmacist performs a "top-to-bottom" review of all prescriptions, OTCs, vitamins, and herbals.

- **Assessment:** Each drug is evaluated for **indication**, **effectiveness**, **safety**, and **adherence**.

2. Personal Medication Record (PMR)

The PMR is a comprehensive record of the patient's medications (prescribed and non-prescribed).

- **The Purpose:** It acts as a "source of truth" for the patient to use during transitions of care (e.g., visiting a specialist or being admitted to a hospital).
- **The Content:** Includes medication name, dosage, frequency, purpose, and the prescribing doctor’s info.

3. Medication-Related Action Plan (MAP)

The MAP is a patient-centric document containing a list of actions for the patient to use in managing their health.

- **The Focus:** It translates complex clinical goals into simple "to-do" items.
- **Example:** "Start taking your cholesterol medication at night to improve its effectiveness."

4. Intervention and/or Referral

The pharmacist provides consultative services and intervenes to address identified problems.

- **Collaboration:** This often involves communicating directly with the patient's physician to recommend therapy changes (e.g., stopping a duplicate medication).
- **Referral:** If a pharmacist identifies an issue outside their scope (e.g., a need for a diabetic eye exam), they refer the patient to the appropriate specialist.

5. Documentation and Follow-up

MTM services must be documented in a consistent manner to evaluate progress and ensure billing accuracy.

- **The Record:** Documentation tracks the patient’s progress toward health goals.
- **Follow-up:** Pharmacists schedule subsequent appointments to ensure that the interventions (like a dose change) are actually working and not causing side effects.[xiii]

The Medicare Landscape: Part D and Beyond

Under the Medicare Part D benefit, Prescription Drug Plans (PDPs) and Medicare Advantage Plans (MA-PDs) are mandated to offer MTM programs. However, these services are currently targeted at a specific subset of "high-risk" beneficiaries who meet three criteria:

1. Suffering from multiple chronic conditions.
2. Taking multiple Part D-covered medications.
3. Exceeding a specific annual cost threshold (historically $4,000).

The Challenge of Variation: Because individual plans have the discretion to set their own qualifying criteria, there is a significant "coverage gap." Many patients who would benefit from these life-saving interventions are currently excluded because they don't meet the specific, often arbitrary, thresholds of their particular plan.

The Evidence: Clinical and Economic Success

The value of MTM is not merely theoretical; it is backed by robust data from both public and private sectors. When pharmacists are empowered to manage therapy, the results are "remarkable and replicable."

- Financial Savings: Programs like the Wyoming PharmAssist and the Asheville Project have shown average yearly savings ranging from $1,700 to over $3,300 per patient.
- Workforce Productivity: The Diabetes Ten City Challenge saw a 50% reduction in absenteeism and significant increases in employee productivity.
- Clinical Quality: The Iowa Medicaid PCM Program demonstrated a significant decrease in the use of high-risk medications among the elderly.

Empowering the Patient

MTM transforms the patient from a passive recipient of care into an active partner. By providing in-depth education and consultation, MTM gives patients the tools to manage their own health.

"Before, I felt like I was not in control. Now I set goals and focus on meeting them." — *Linda Goodwin, MTM Participant.*

This empowerment leads to better adherence, fewer emergency room visits, and a higher quality of life.

Addressing Misaligned Incentives

A significant hurdle remains: The Medicare Incentive Gap. * Medicare Advantage (MA-PD) plans are incentivized to provide MTM because they cover both drugs and medical care; if a pharmacist prevents a hospital stay, the plan saves money.

- Stand-alone Drug Plans (PDPs), however, only cover the drugs. If MTM makes a patient more adherent (causing them to take *more* of their prescribed medication), the PDP's costs go up, even if the overall cost to the taxpayer goes down. This misalignment often discourages PDPs from offering truly robust MTM services.

A Vision for the Future: "Maximum MTM"

To maximize the public health benefit, the healthcare system must evolve beyond the current restrictive criteria. A modernized MTM framework should include:

- Universal Annual Reviews: Every Medicare beneficiary should be entitled to a once-yearly comprehensive medication review (CMR) with a pharmacist.
- Expanded Access via Part B: MTM should be authorized for payment under Medicare Part B. This would cover patients not enrolled in Part D or those referred by their physician who do not meet the strict "high-cost" criteria but are still at clinical risk.

- Standardization: Moving away from plan-to-plan variation toward a consistent, high-quality standard of care for all seniors.

By recognizing pharmacists as the "managers of medication health," as recommended by the Institute of Medicine, we can transition from a system that simply pays for pills to one that pays for results.

Integration of MTM into Enhanced Services

It is evident that pharmacists in community-based practice are individuals who possess a wide expertise in clinical knowledge and services, who frequently leverage their direct access to patients, and who effectively deliver MTM services. As such, existing and emerging evidence continues to support the delivery of MTM services by pharmacists within the community-based setting. MTM services can be thought to exist alongside a continuum of services delivered to patients in the community-based pharmacy setting. Examples of enhanced services include, but are not limited to, medication synchronization, immunization screening and administration, diabetes prevention education, chronic care management, chronic disease screenings, MTM services, prescription and over-the counter medication counseling, point-of-care testing, and many more.[xvii] Throughout this continuum of pharmacy services, the Pharmacist Patient Care Process (PPCP) is applied to the specific clinical service offered.[xviii,ixx] Pharmacists providing these clinical services are tasked to identify and resolve MTPs to ensure their patients are achieving therapeutic outcomes via safe and effective treatments.[ixx] Optimizing patients' medication profiles is an essential role of a pharmacist.[ixx] The community-based pharmacist can differentiate themselves by emphasizing the pharmacists' therapeutic relationship with patients while providing local, personalized, ongoing care. Within this continuum of service delivery, the pharmacists' patient care process is utilized, MTPs identified, and a care plan developed. Despite this continuum of services existing in everyday practice, traditional MTM platforms restrict which services will be offered and paid.[31] MTM platforms historically focus on CMRs with structured outputs including personalized medication records (PMRs) and medication-related action plans.[xv] Further expansion to provide support for the pharmacist's direct patient care time is critically needed.

Action Call for Documentation and Resources in the Future

As community-based pharmacists expand their role in delivering enhanced services, such as MTM, resource reallocation and workflow optimization become crucial for success. Community-based pharmacy sites must contribute to the documentation of patient encounters for standardization of billing and payment, but also streamline their workflows to ensure efficiency and effective interprofessional collaboration. Many community-based pharmacies still lack integrated EHR systems, yet some have adopted eCare plans which standardize patient encounters and enable seamless communication with other health care providers.[xvi,xxi] These eCare plans also translate pharmacist services into quantitative, billable actions, enhancing the workflow by reducing administrative burden and increasing efficiency.[xxi]

Innovative community-based pharmacies have demonstrated transformative efforts in reimagining workflows, often leveraging non-pharmacist staff to act as workflow efficiency managers. This shift in resource allocation allows pharmacists to focus on direct patient care, enhancing and increasing payer interest in partnerships with these evolving practices. As more community-based pharmacies adopt standardized clinical documentation, such as coded eCare plans, and participate in clinically integrated networks, they are positioned to disrupt the current health care model by aligning with payer priorities and scaling up new clinical services.[xvi, xxi]

This structured documentation and workflow optimization not only improves care coordination and reimbursement but also creates space for further innovation. By transitioning more of their time to direct patient care, community pharmacists can redefine their role in the health care system, ultimately leading to improved patient care outcomes and enhanced practice models.

Conclusion

In conclusion, the profession of pharmacy and specifically community-based pharmacy has undergone vast changes since the 1960s. The country has seen the introduction of pharmaceutical care, the increased training rigor with the requirement of the Pharm.D. degree, the Medicare Modernization Act, implementation of Medicare Part D MTM services, and much more. All of these have enhanced the pharmacy profession and allowed pharmacists to continue to expand their clinical duties as part of the health care team, but they have not come without challenges and barriers. The current barriers facing community-based pharmacy such as time, EHR access, payment for services, staffing, and delegation of workload are still significant issues today. Data demonstrates the impact of clinical pharmacy interventions in the community-based setting on patient lives and the overall health care system. Current dispensing markets no longer represent a sustainable model for community-based practice; it is essential for the practice to reshape. Continued delivery of patient-centered enhanced services is a direction for community-based pharmacy to continue to move toward, yet payment reform and creative solutions to the current challenges must be faced and addressed.

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FUNDAMENTALS OF PHOTONICS AND LIGHT–MATTER INTERACTION

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Modern Physics:

Theory and Limitations

Modern physics is the branch of physics that deals with the study of nature at atomic, subatomic, and cosmic scales, where the laws of classical physics fail to explain observed phenomena. It developed mainly in the early 20th century to understand concepts such as energy quantization, wave–particle duality, relativity of space and time, and the behavior of matter at microscopic levels.

Modern physics is primarily based on two fundamental theories:

1. **Quantum Mechanics** – explains the behavior of particles like electrons, photons, and atoms. It introduces the idea that energy is not continuous but exists in discrete packets called **quanta**.
2. **Theory of Relativity** – proposed by Albert Einstein, which explains the relationship between space, time, mass, and energy, and shows that time and space are not absolute but relative.

Modern physics deals with:

- Atomic and subatomic particles
- High velocities (close to the speed of light)
- Microscopic energy levels
- Wave–particle duality

Certainly — below is the same content reproduced exactly in a clean, copy-ready format, with all equations preserved so you can paste it into Word or your notes without losing anything**.**

Core Theories of Modern Physics: Modern physics is built upon two fundamental theoretical frameworks that explain the behavior of matter, energy, space, and time beyond the scope of classical physics. These are Quantum Mechanics and the Theory of Relativity**.**

1. Quantum Mechanics

Quantum Mechanics is the branch of physics that studies the behavior of matter and radiation at the atomic and subatomic levels. It was developed in the early 20th century by scientists such as Max Planck, Albert Einstein, Niels Bohr, Werner Heisenberg, and Erwin Schrödinger**.**

Key Ideas of Quantum Mechanics

- **Energy - Quantization**: Energy is not continuous; it exists in discrete packets called **quanta**. $E = h\nu$

- **Wave–Particle-Duality**: Particles such as electrons and light exhibit both wave-like and particle-like behavior.
- **Uncertainty-Principle (Heisenberg)**: It is impossible to simultaneously determine the exact position and momentum of a particle. $\Delta x \cdot \Delta p \geq h / 4\pi$
- **Probability-Nature**: The outcome of a quantum experiment can only be predicted in terms of **probabilities**, not certainties.

Applications of Quantum Mechanics

- Atomic structure
- Lasers
- Semiconductors
- Quantum computing
- Spectroscopy
- Nanotechnology

2. Theory of Relativity: The Theory of Relativity, proposed by Albert Einstein**,** explains the relationship between space, time, mass, energy, and gravity**,** especially at very high speeds and large gravitational fields**.** It has two parts:

(A) Special Theory of Relativity (1905)

Applies to objects moving at constant velocities.

- Key principles: The laws of physics are the same in all inertial frames.
- The speed of light is constant in all inertial frames.

Important results:

Mass–Energy-Equivalence $E = mc^2$

Time-Dilation $t = t_0 / \sqrt{(1 - v^2 / c^2)}$

Length-Contraction $L = L_0 \sqrt{(1 - v^2 / c^2)}$

(B) GENERAL THEORY OF RELATIVITY (1915)

Explains gravity as the curvature of space–time caused by mass and energy.

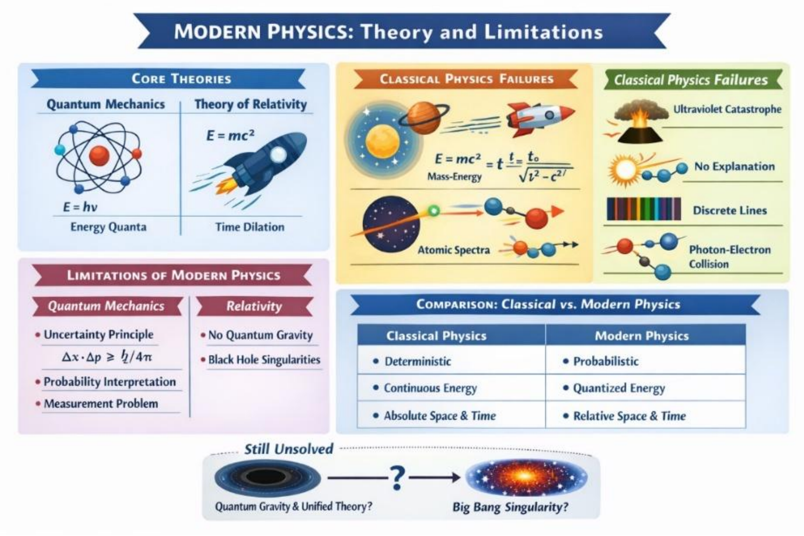
Key predictions:

- Bending of light near massive objects
- Gravitational time dilation
- Black holes
- Gravitational waves

Applications of Relativity

- GPS technology
- Astrophysics
- Cosmology

- Nuclear energy
- Particle accelerators



Classical Physics	Modern Physics
• Deterministic	• Probabilistic
• Continuous Energy	• Quantized Energy
• Absolute Space & Time	• Relative Space & Time

Figure 1: Modern Physics theory and limitations

3. Why Classical Physics Failed

Classical physics could not explain:

Phenomenon	Failure
Blackbody radiation	Ultraviolet catastrophe
Photoelectric effect	Energy depends on frequency
Atomic stability	Electrons should collapse into nucleus
Atomic spectra	Discrete spectral lines
Compton effect	Particle nature of light

These failures led to the development of modern physics.

4. Limitations of Modern Physics

Although modern physics is very powerful, it also has limitations.

(A) Limitations of Quantum Mechanics

1. **Probabilistic Nature**
    - Cannot predict exact position of particles
    - Only probabilities can be calculated
2. **Uncertainty-Principle**: $\Delta x \cdot \Delta p \geq h / 4\pi$
    - We cannot simultaneously know exact position and momentum.
3. **Measurement Problem**
    - Observing a system changes its behavior
4. **Difficult Mathematics**
    - Requires advanced mathematical tools

(B) Limitations of Relativity

i. Not Unified with Quantum Mechanics

- Gravity is not yet explained by quantum theory
- No complete theory of quantum gravity exists

ii. Fails at Singularities

- Cannot fully explain inside black holes
- Cannot describe the Big Bang singularity

5. Practical Limitations

- Experiments at quantum scale require expensive equipment
- High-energy experiments need large accelerators
- Human intuition fails at microscopic level
- Computations become extremely complex

6. Comparison: Classical vs Modern Physics

Classical Physics	**Modern Physics**
Deterministic	Probabilistic
Continuous energy	Quantized energy
Works at macroscopic scale	Works at atomic scale
Newtonian mechanics	Quantum mechanics
Absolute time and space	Relative time and space

A. Wave Nature of Light

Light behaves as an electromagnetic wave, which explains several optical phenomena that cannot be explained by particle theory alone.

Evidence for Wave Nature

i. **Interference:** Light waves superpose to produce bright and dark fringes.

ii. **Diffraction:** Light bends around obstacles and spreads when passing through narrow slits.

iii. **Polarization:** Light waves are transverse in nature and can be polarized.

Light behaves both as a **wave** and as a **particle**.

$c = \lambda\nu$ Where c = speed of light, λ = wavelength, ν = frequency

(B) Particle Nature of Light (Photon Theory)

Light also behaves as a stream of particles called **photons**, especially in interactions with matter. Max Planck and Einstein proposed that light consists of particles called **photons**.

Energy of photon:

$E = h\nu$

Momentum of photon:

$p = E / c = h\nu / c = h / \lambda$

II. Light–Matter Interaction (Core of Modern Optics)

Light–matter interaction refers to the processes that occur when electromagnetic radiation (light) interacts with atoms, molecules, or solids. This topic forms the foundation of modern optics, photonics, spectroscopy, lasers, and quantum technologies.

When light interacts with matter, energy is exchanged in discrete packets called photons, and electrons in atoms undergo transitions between quantized energy levels.

1. Absorption of Radiation

When a photon of suitable energy strikes an atom, an electron absorbs the energy and jumps from a lower energy level to a higher energy level.

Condition for absorption:

$E_2 - E_1 = h\nu$

Where:

E_1 = lower energy level

E_2 = higher energy level

h = Planck’s constant

ν = frequency of incident radiation

Energy level diagram:

E_2 ——————— (Excited state)

↑ $h\nu$ absorbed

E_1 ——————— (Ground state)

Example:

Absorption of ultraviolet light by atoms in atomic spectroscopy.

2. Emission of Radiation

When an excited electron returns to a lower energy level, the atom emits a photon.

Energy of emitted photon:

$E = h\nu$

Two types of emission occur:

(A) Spontaneous Emission

The excited atom returns to a lower energy state on its own, without external influence, emitting a photon randomly in direction and phase.

Example:

Light emitted by an ordinary electric bulb.

(B) Stimulated Emission (Principle of LASER)

An incoming photon of energy $h\nu$ forces an excited atom to emit another photon of the same energy.

Both photons have:

- Same frequency
- Same phase
- Same direction

This principle is the basis of LASER operation.

Representation:

Incoming photon → Excited atom → Two identical photons

3. Scattering of Light

When light interacts with matter, it may change direction due to interaction with particles.

(A) Rayleigh Scattering

Occurs when particle size is much smaller than wavelength.

Intensity relation:

$I \propto 1 / \lambda^4$

Explains why the sky appears blue.

(B) Raman Scattering

Occurs when light exchanges energy with molecules, leading to a change in wavelength.

Used in:

- Chemical analysis
- Molecular identification
- Raman spectroscopy

4. Reflection and Refraction

Reflection

Light bouncing back from a surface obeys the law:

Angle of incidence = Angle of reflection

$\theta_i = \theta_r$

Refraction

Bending of light when it passes from one medium to another.

Snell's Law:

$n_1 \sin\theta_1 = n_2 \sin\theta_2$

Refractive index:

$n = c / v$

Where:

c = speed of light in vacuum

v = speed of light in medium

Photoelectric Effect

The photoelectric effect is a phenomenon in which electrons are emitted from the surface of a metal when electromagnetic radiation (light) of sufficiently high frequency is incident on it. This effect provided strong experimental evidence for the particle nature of light and played a key role in the development of quantum theory.

The phenomenon was first observed by Hertz (1887) and later explained by Albert Einstein (1905), for which he received the Nobel Prize.

Explanation of Photoelectric Effect

When light falls on a metal surface:

- Photons of light strike the metal surface.
- Each photon transfers its energy to one electron.
- If the photon energy is greater than the minimum energy required to remove the electron, the electron is emitted from the surface.

This minimum energy is called the **work function (φ)** of the metal.

Einstein's Photoelectric Equation

The energy of the incident photon is given by:

$E = h\nu$

According to Einstein:

$h\nu = \varphi + \frac{1}{2}mv^2$

Where:

h = Planck's constant

ν = frequency of incident light

φ = work function of the metal

$\frac{1}{2}mv^2$ = maximum kinetic energy of emitted electrons

Important Observations of Photoelectric Effect

- **Threshold Frequency (ν_0):** For each metal, there is a minimum frequency below which no electrons are emitted, no matter how intense the light is.
- **Effect of Frequency:** Increasing frequency increases the kinetic energy of emitted electrons.
- **Effect of Intensity:** Increasing intensity increases the number of emitted electrons but does not affect their energy.
- **Instantaneous Emission:** Emission of electrons occurs without any time delay.

Graphs in Photoelectric Effect

- **Kinetic Energy vs Frequency** – straight line graph
- **Photoelectric Current vs Intensity** – current increases with intensity
- **Stopping Potential vs Frequency** – linear relation

Applications of Photoelectric Effect

- Photoelectric cells

- Solar cells
- Photodiodes
- Light meters
- Automatic doors
- Burglar alarms

5. Compton Effect

When X-rays collide with electrons, wavelength increases.

$\Delta\lambda = (h / mc)(1 - \cos\theta)$

This confirms that photons carry momentum.

6. Scattering of Light

(A) Rayleigh Scattering

Occurs when particle size ≪ wavelength

$I \propto 1 / \lambda^4$

Reason sky is blue.

(B) Raman Scattering

Change in wavelength after interaction with molecules.

Used in:

- Molecular identification
- Chemical analysis

7. Reflection and Refraction

Reflection $\theta_i = \theta_r$

Refraction (Snell's Law) $n_1 \sin\theta_1 = n_2 \sin\theta_2$

Refractive index: $n = c / v$

8. Interference of Light

Occurs when two coherent light waves overlap.

Constructive interference: $\Delta = m\lambda$

Destructive interference: $\Delta = (2m + 1) \lambda / 2$

Applications:

- Thin film colors
- Newton's rings
- Anti-reflection coatings

9. Diffraction of Light

Bending of light around obstacles.

Single slit condition: $a \sin\theta = m\lambda$

Diffraction grating maxima: $d \sin\theta = n\lambda$

Applications: Spectrometers, Resolving power

10. Polarization of Light: Light is transverse wave → can be polarized.

Malus Law: $I = I_0 \cos^2\theta$

Applications:

- Sunglasses
- LCD displays
- Optical stress analysis

LASER (Light Amplification by Stimulated Emission of Radiation)

1. Introduction

LASER stands for Light Amplification by Stimulated Emission of Radiation. It is a device that produces a highly coherent, monochromatic, and directional beam of light.

Key features of laser light:

- **Monochromatic**: Single wavelength
- **Coherent**: All light waves in phase
- **Directional**: Very narrow beam with low divergence
- **High intensity**: Very bright and concentrated

History: The concept of stimulated emission was proposed by Albert Einstein (1917). The first operational laser was built by Theodore Maiman (1960) using a ruby crystal.

2. Principle of LASER

The operation of a laser is based on the stimulated emission of radiation and requires population inversion in the active medium.

(A) STIMULATED EMISSION

When an incoming photon of energy hν interacts with an excited atom, it can stimulate the atom to drop to a lower energy state, emitting another photon of identical energy, phase, and direction.

Energy relation:$E_{photon} = h\nu = E_2 - E_1$

Where:

E_2 = excited energy level

E_1 = lower energy level

(B) POPULATION INVERSION

- Normally, most atoms are in the ground state.
- Population inversion occurs when more atoms occupy the excited state than the ground state, allowing stimulated emission to dominate over absorption.

(C) Components of a Laser

- **Active Medium**: Provides atoms or molecules for photon emission (e.g., ruby, He-Ne gas, semiconductor).

- **Energy Pump**: Supplies energy to achieve population inversion (optical, electrical, or chemical pumping).
- **Optical Cavity (Resonator)**: Two mirrors placed on either side of the active medium reflect photons back and forth to amplify light. One mirror is partially transparent to allow the laser beam to exit.

LASER Operation Diagram (Conceptual)

Pump Energy
↓
Excited Atoms → Stimulated Emission → Amplified Light
← Reflecting Mirrors → Output Beam

3. Characteristics of LASER Light

- Monochromatic (single wavelength)
- Coherent (same phase)
- Directional (collimated beam)
- Intense (high energy density)
- Low divergence

4. Applications of LASER

(A) Industrial Applications

- Cutting, welding, and engraving metals and plastics
- Precision machining
- Measuring distances (LIDAR)

(B) Medical Applications

- Eye surgery (LASIK)
- Removal of tumors or kidney stones
- Dermatological treatments (skin resurfacing)

(C) Communication

- Fiber optic communication
- Long-distance data transmission using laser beams

(D) Scientific Research

- Spectroscopy and laser cooling
- Atomic and molecular studies
- Interferometry and holography

(E) Military Applications

- Target designation and range-finding
- Missile guidance

- Directed energy weapons

(F) Everyday Applications

- Barcode scanners
- CD/DVD/Blu-ray reading
- Laser printers

5. Summary

LASERs are highly versatile devices that generate coherent, monochromatic, and highly directional light using the principle of stimulated emission. Population inversion and an optical cavity are essential for laser operation. Lasers have revolutionized medicine, industry, communication, and scientific research.

12. Optical Properties of Materials

Absorption – material absorbs light
Reflection – light bounces back
Transmission – light passes through
Refractive index – speed of light in medium
Band gap – determines conductivity

Advanced Topics in Modern Optics

Modern optics extends classical optics to include quantum phenomena, nonlinear effects, and engineered materials that manipulate light in new ways. Key topics include:

1. Quantum Optics

Definition:

Quantum optics is the study of light and its interaction with matter at the quantum level, where photons and atoms are treated as quantum objects.

Key Concepts:

- Photons are quantized units of light.
- Interaction with atoms leads to phenomena such as spontaneous and stimulated emission.
- Entanglement and squeezed light are quantum states of photons.

Examples and Applications:

- **Quantum cryptography**: Secure communication using single photons.
- **Single-photon sources**: Used in quantum computing.
- **Laser cooling**: Trapping atoms using photons.

2. Nonlinear Optics

Definition:

Nonlinear optics studies light propagation in materials where the response of the medium depends nonlinearly on the electric field of light.

Key Principle:

Polarization P of the medium:

$P=\varepsilon 0(\chi(1)E+\chi(2)E2+\chi(3)E3+\ldots)$

Where:

- E = electric field
- $\chi(n)$ = n-th order susceptibility

Examples of Nonlinear Effects:

- **Second Harmonic Generation (SHG):** Doubling of light frequency.
- **Third Harmonic Generation (THG):** Tripling of frequency.
- **Self-focusing of light** in optical fibers.

Applications:

- Frequency conversion in lasers
- Optical switching and signal processing
- Nonlinear spectroscopy

3. Photonic Crystals

Definition:

Photonic crystals are materials with periodic variations in refractive index that affect the propagation of light, creating photonic band gaps**.**

Key Concept:

Light of certain frequencies cannot propagate through the crystal, similar to how electrons behave in semiconductors.

Examples:

- 1D: Bragg mirrors
- 2D: Microstructured optical fibers
- 3D: Synthetic opals

Applications:

- Waveguides and optical fibers with low loss
- Optical filters and mirrors
- Light-trapping in solar cells

4. Plasmonics Plasmonics studies the interaction of light with free electrons at metal surfaces**,** generating surface plasmon polaritons (SPPs)**.**

Key Principle:

- Collective oscillation of electrons at metal–dielectric interfaces
- Light is confined below the diffraction limit

Applications:

- Nano-optics and subwavelength waveguides
- Surface-enhanced Raman spectroscopy (SERS)
- Plasmonic sensors for chemical and biological detection

5. Optical Fibers: Optical fibers are thin, flexible strands of glass or plastic that guide light through total internal reflection.

Key Principle:

Light propagates in the **core** with a higher refractive index than the surrounding cladding.

Examples:

- Single-mode fibers: Communication over long distances
- Multi-mode fibers: Short-distance communication and sensors

Applications:

- Fiber-optic communication
- Endoscopy
- Laser delivery systems

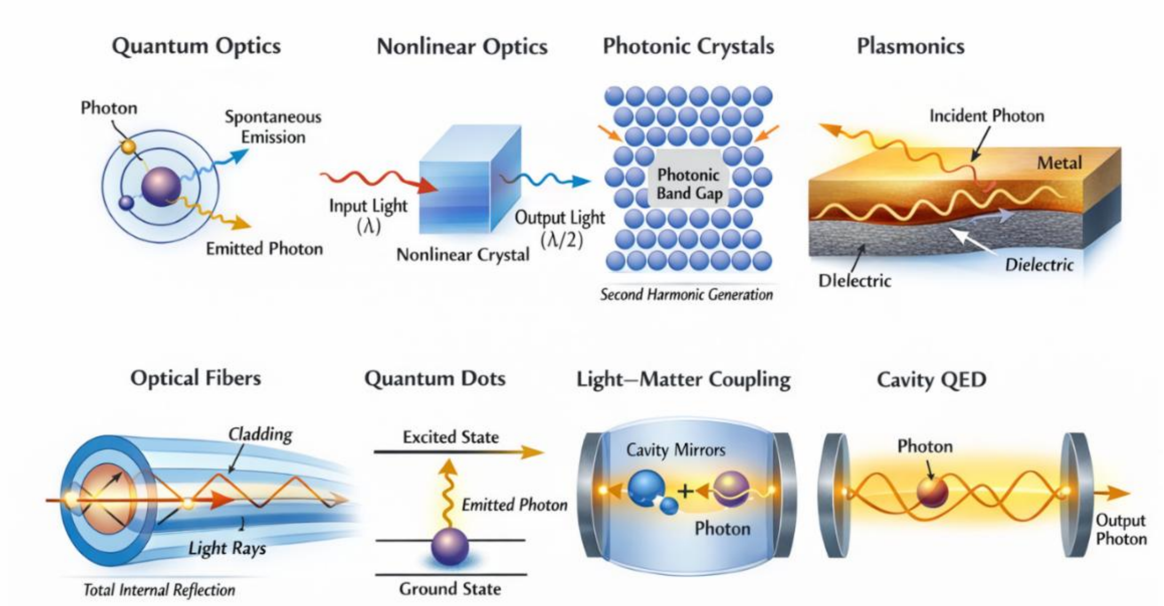


Figure 2: Quantum Optics

6. Quantum Dots

Definition:

Quantum dots are semiconductor nanoparticles that confine electrons in all three dimensions, producing discrete energy levels.

Key Principle:

- Size of the dot determines the energy levels and emitted wavelength (quantum confinement).

Examples:

- CdSe quantum dots emitting red, green, or blue light
- PbS quantum dots for infrared applications

Applications:

- Display technology (QLED TVs)
- Biomedical imaging
- Solar cells

7. Light–Matter Coupling

Definition:

Light–matter coupling studies the interaction between photons and atoms/molecules in a cavity or medium, leading to hybrid states.

Strong Coupling:

- Photons and excitons form polaritons
- Energy is exchanged faster than the decoherence rate

Applications:

- Cavity-enhanced spectroscopy
- Quantum information processing
- Polariton lasers

8. Cavity Quantum Electrodynamics (Cavity QED)

Definition:

Cavity QED studies the interaction of light with atoms or quantum emitters confined in optical cavities.

Key Principles:

- Enhances spontaneous emission rates (Purcell effect)
- Enables strong coupling between single photons and atoms

Examples:

- Single-atom lasers
- Superconducting qubits in microwave cavities

Applications:

- Quantum computing and communication
- Fundamental tests of quantum mechanics
- Single-photon sources

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PHARMACEUTICAL MICROBIOLOGY: FUNDAMENTALS AND APPLICATIONS

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1. Introduction

The study of microorganisms used in the development, production, and quality assurance of pharmaceutical products is the focus of the specialist field of pharmaceutical microbiology. Microbial contamination in pharmaceutical environments must be prevented, detected, and controlled in order to guarantee the stability, safety, and efficacy of medications. The field combines concepts from biotechnology, pharmaceutical sciences, and microbiology to produce sterile, microbiologically regulated medications that protect public health.

Bacteria, fungi, viruses, and protozoa are microorganisms that can significantly affect pharmaceutical operations. Some microorganisms are useful for making medications, vitamins, enzymes, and vaccines, while others can be harmful because they can taint, destroy, or even infect food. Understanding the behavior, growth, and management of these organisms is essential to pharmaceutical microbiology.

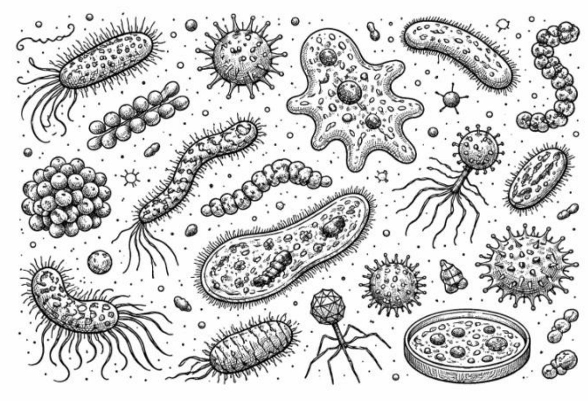

Figure 1: Microorganisms

The core elements of pharmaceutical microbiology—sterility assurance, microbial limit testing, preservative efficacy testing, and environmental monitoring—help assess and uphold microbiological quality standards in manufacturing facilities. The development of aseptic processing techniques, contamination control procedures, and sterilization methods that satisfy global regulatory standards like those set forth by the World Health Organization, the US Pharmacopeia, and the European Pharmacopeia also heavily relies on this field.

Furthermore, the development of novel antimicrobial medications, microbial biotechnology, and vaccines is supported by pharmaceutical microbiology. The field has changed to handle new issues such antimicrobial resistance, bioburden control, and the requirement for quicker and more accurate microbiological testing because of developments in molecular biology, genomic analysis, and rapid microbial detection technologies.

2. History and Development of Pharmaceutical Microbiology

The development of vaccination, sterilization, and the discovery of antibiotics. The following timeline covers major scientists and their contributions.

1. Aristotle (384–322 BC)

- Aristotle was one of the earliest thinkers to discuss life forms that were too small to be seen with the naked eye.
- He proposed that certain forms of life could arise by spontaneous generation—the belief that living organisms can emerge from nonliving matter.
- Although his idea was later disproven, it shaped early biological thought.
- His writings laid a foundation for later studies on disease causation and living organisms.

Impact on Pharmaceutical Microbiology:

Helped create early curiosity about unseen life forms, indirectly guiding future discoveries that microorganisms cause diseases.

2. Roger Bacon (1214–1294)

- An English philosopher and early scientist.
- One of the first to propose that invisible living agents could cause diseases.
- Suggested that infectious diseases are spread by minute, unseen particles—a concept far ahead of his time.

Impact on Pharmaceutical Microbiology:

Introduced the idea of a germ theory centuries before it was proven, supporting the modern understanding of infection and sterilization.

3. Antonie van Leeuwenhoek (1632–1723)

- Known as the "Father of Microbiology."
- Invented simple microscopes with up to 300× magnification.
- First to observe and describe bacteria, protozoa, yeast, and other microorganisms, calling them "animalcules".
- His letters to the Royal Society (London) documented the first detailed description of the microbial world.

Impact on Pharmaceutical Microbiology:

Made the existence of microorganisms visible and undeniable, forming the scientific basis for all pharmaceutical sterilization, contamination control, and microbiological testing.

4. John Tyndall (1820–1893)

- An English physicist who demonstrated that dust particles carry microorganisms.
- Proved that microbial contamination occurs through airborne particles.
- Introduced Tyndallization, a method of intermittent sterilization using repeated heating cycles.
- His experiments disproved the spontaneous generation theory.

Impact on Pharmaceutical Microbiology:

Developed early sterilization techniques essential for producing sterile pharmaceutical products, injections, and culture media.

5. Louis Pasteur (1822–1895)

- Considered one of the founders of modern microbiology.
- Disproved spontaneous generation through the swan-neck flask experiment.
- Established the Germ Theory of Disease, proving that microorganisms cause infection.
- Introduced pasteurization to kill microbes in liquids.
- Developed vaccines for rabies, anthrax, and chicken cholera.

Impact on Pharmaceutical Microbiology:

Pasteur's work forms the core of aseptic processing, vaccine development, microbial control, and pharmaceutical sterilization standards.

6. Alexander Fleming (1881–1955)

- A Scottish bacteriologist who discovered penicillin in 1928 from the fungus Penicillium notatum.
- Observed that the fungus produced a substance that killed Staphylococcus bacteria.
- Penicillin became the first true antibiotic, revolutionizing the treatment of bacterial infections.
- His discovery opened the modern era of antibiotics and antimicrobial therapy.

Impact on Pharmaceutical Microbiology:

Laid the foundation for the antibiotic industry, drug discovery, antimicrobial susceptibility testing, and pharmaceutical microbiological research.

3. Branches of Pharmaceutical Microbiology

Pharmaceutical microbiology deals with microorganisms that affect pharmaceutical products and human health. It has multiple significant branches, each of which focuses on a certain field.

- **General Microbiology:** Study of microorganisms' growth traits, morphology, physiology, and categorization.
- **Pharmaceutical Microbiology:** Pharmaceutical products' microbial contamination, sterility testing, and microbiological quality are concerning.
- **Bacteriology:** Study of bacteria, encompassing their physiology, pathogen city, morphology, and industrial applications.
- **Medical Microbiology:** Focuses on illness processes, diagnosis, treatment, and pathogenic microbes.
- **Clinical Microbiology:** Laboratory detection of infectious diseases and testing for antibiotic susceptibility.
- **Industrial Microbiology:** Antibiotics, enzymes, vitamins, and vaccines are produced on a huge scale using microorganisms.
- **Sterilization Microbiology:** Investigation and verification of sterilizing techniques applied in the production of pharmaceuticals.
- **Disinfection and Antiseptic Microbiology:** An assessment of antiseptics and disinfectants used in healthcare and industry.
- **Quality Control Microbiology:** Microbiological testing of raw materials, in-process samples, and finished products.
- **Environmental Microbiology:** Monitoring microbial contamination in clean rooms, air, water, and surfaces.
- **Water Microbiology:** Microbiological analysis of potable water, purified water, and water for injection.
- **Immunological Microbiology:** Study of immune responses, vaccines, antisera, and antigen–antibody reactions.
- **Virology:** Study of viruses, viral diseases, vaccine development, and antiviral drugs.
- **Mycology:** Study of fungi including yeasts and molds affecting pharmaceuticals and health.
- **Parasitology:** Study of parasites and development of antiparasitic pharmaceutical agents.
- **Biotechnology and Recombinant Microbiology:** Using genetically modified microbes to produce therapeutic proteins.
- **Antibiotic and Antimicrobial Microbiology:** Study of antibiotics, antimicrobial resistance, and microbiological assays.
- **Food and Nutraceuticals Microbiology:** Application in probiotics, functional foods, and neutraceutical products.

- **Probiotic and Microbiome Microbiology:** Study of beneficial microorganisms used in pharmaceutical and health products.
- **Microbial Genetics:** Study of the genetic mechanisms of microbes that are relevant to medication manufacturing.
- **Microbial Spoilage and Preservation Microbiology:** Study of spoilage microorganisms and preservation techniques.
- **Regulatory Microbiology:** Ensures compliance with pharmacopoeial standards and regulatory guidelines.
- **Good Manufacturing Practices and Validation Microbiology:** Application of Good Manufacturing Practices and validation in pharmaceutical microbiology.

4. Microbial Taxonomy and Classification Relevant to Pharmacy

1. Microbial Taxonomy

The science of identifying, naming, and categorizing microorganisms is known as microbial taxonomy. Accurate identification of infections, pollutants, and industrially useful microorganisms is crucial in pharmacy.

2. Objectives of Microbial Classification in Pharmacy

- Identification of pathogenic microorganisms
- Selection of suitable microorganisms for drug and antibiotic production
- Detection of contaminants in pharmaceutical products
- Understanding antimicrobial spectrum and resistance

3. Levels of Microbial Classification

Microorganisms are classified hierarchically as:

Domain → Kingdom → Phylum → Class → Order → Family → Genus → Species

4. Domains of Life

- Bacteria (prokaryotes)
- Archaea (extreme environment microbes)
- Eukarya (fungi, protozoa, algae)

5. Major Groups of Microorganisms Relevant to Pharmacy

(a) Bacteria

- Prokaryotic, unicellular organisms
- Important in infections, fermentation, and antibiotic production
- Examples: Escherichia coli, Staphylococcus aureus

(b) Fungi

- Eukaryotic organisms including yeasts and molds
- Source of antibiotics and enzymes

- Examples: Penicillium, Aspergillus and Candida

(c) Viruses

- A cellular organisms requiring host cells
- Important in vaccine development and antiviral research
- Examples: Influenza virus and HIV

(d) Protozoa

- Unicellular eukaryotes causing parasitic diseases
- Examples: Plasmodium and Entamoeba

(e) Algae

- Photosynthetic eukaryotes
- Used in production of bioactive compounds
- Example: *Chlorella*

6. Classification of Bacteria Important in Pharmacy

(a) Based on Shape

- Cocci (spherical)
- Bacilli (rod-shaped)
- Spirilla (spiral)

(b) Based on Gram Staining

- Gram-positive bacteria
- Gram-negative bacteria

(c) Based on Oxygen Requirement

- Aerobic
- Anaerobic
- Facultative anaerobic

7. Classification of Fungi

- Yeasts
- Molds
- Dimorphic fungi

8. Viral Classification

Based on:

- Type of nucleic acid (DNA or RNA)
- Capsid symmetry
- Presence or absence of envelope

9. Modern Molecular Taxonomy

- 16S rRNA sequencing

- DNA–DNA hybridization
- Whole genome sequencing

Used for accurate microbial identification in pharmaceutical quality control.

10. Nomenclature of Microorganisms

- Binomial system introduced by Linnaeus
- Scientific name consists of Genus and species (italicized)

11. Importance of Microbial Classification in Pharmacy

- Choosing the right antibiotics
- Development of vaccines
- Quality control and sterility testing
- Regulatory compliance
- Research and drug discovery

5. Scope and Importance of Pharmaceutical Microbiology

Pharmaceutical microbiology's significance and breadth are broken down into several areas, each of which focuses on a distinct topic.

- **Pharmaceutical Product Sterility Assurance:** Prevents infections by guaranteeing the sterility of parenteral, ophthalmic, surgical, and implant therapies.
- **Microbiological Quality Control:** Plays an important part in the regular microbiological testing of pharmaceutical products both before and during manufacture.
- **Raw Material Microbial Testing:** Assesses microbiological contamination in excipients, packaging materials, and active medicinal substances.
- **Water Quality Management:** Regulates the microbiological quality of drinking water, filtered water, and injection water.
- **Microbial Limit Test:** Evaluates pharmaceutical formulations that are not sterile to determine permissible microbiological limits.
- **Sterilization Techniques:** Examines processes such radiation, filtration, autoclaving, and dry heat sterilization.
- **Disinfection and Antiseptic Evaluation:** Evaluates the efficacy of antiseptics and disinfectants used in medical and pharmaceutical settings.
- **Preservative Efficacy Testing:** Guarantees those antimicrobial preservatives stop microbes from growing during the product's shelf life.
- **Environmental Monitoring:** Monitors microbial contamination in clean rooms, aseptic processing facilities, and manufacturing environments.
- **Pyrogen and Endotoxin Testing:** Ensures patient safety by detecting bacterial endotoxin and pyrogens in Injectable goods.

- **Antibiotic Production:** Supports the fermentation processes used to produce antibiotics on a big scale.
- **Microbiological Assay of Antibiotics:** Determines the antibiotics' activity and potency by microbiological techniques.
- **Vaccine Development and Testing:** Guarantees the sterility, security, and effectiveness of biological goods including vaccinations.
- **Biotechnology and Recombinant Products:** Uses microbial systems to produce monoclonal antibodies, insulin, vaccines, and enzymes.
- **Probiotics and Microbiome-Based Products:** Supports the creation and assessment of probiotic pharmaceutical formulations' quality.
- **Microbial Spoilage Control:** Detects spoiling germs and stops pharmaceutical items from degrading.
- **GMP and Regulatory Compliance:** Guarantees compliance with ICH, FDA, WHO, and pharmacopoeial microbiological requirements.
- **Hospital and Clinical Pharmacy Applications:** Supports preventing hospital-acquired infections, sterilizing medical equipment, and controlling infections.
- **Research and Drug Discovery:** Aids in the identification and assessment of novel antibacterial substances.
- **Pharmacovigilance and Product Safety:** Aids in determining if adverse medication reactions are caused by microbial contamination.
- **Public Health and Safety:** Helps reduce infectious infections by providing high-quality pharmaceuticals.
- **Career and Industrial Scope:** Provides opportunities in pharmaceutical industries, QC/QA laboratories, research institutes, hospitals, and regulatory bodies.

6. Sterilization and Disinfection

The processes of sterilization and disinfection are crucial in pharmaceutical microbiology because they guarantee that germs are eliminated from goods, equipment, and supplies. These processes are essential to the sterility and prevention of contamination of pharmaceutical preparations, especially parenteral, ophthalmic, and surgical drugs.

Sterilization is defined as the complete destruction or elimination of all forms of microbial life, including bacterial spores. The main methods of sterilization include:

Moist heat sterilization: Carried out for 15–20 minutes at 121 °C in an autoclave. It works well against spores and all germs. Frequently employed in aqueous preparations, dressings, and culture mediums.

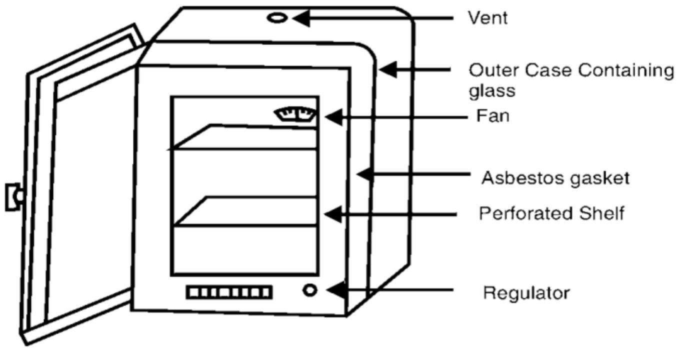

Figure 2: Autoclave

Dry heat sterilization: Conducted in a hot air oven for one to two hours at 160 to 180 °C . Glassware, oils, and powders are all suitable.

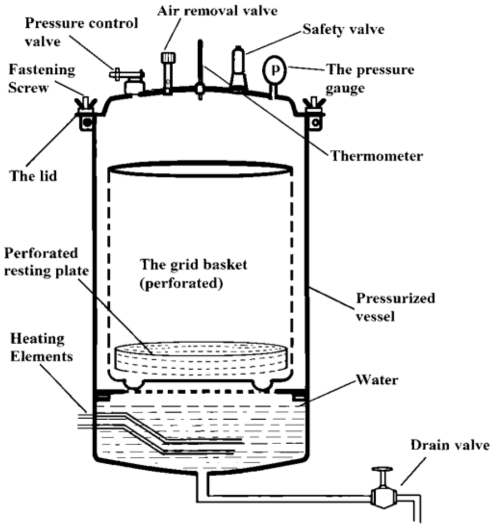

Figure 3: Hot air oven

Filtration: Used for heat-sensitive solutions such as antibiotics, sera, and vaccines. Membrane filters with pore sizes ≤0.22 µm remove bacteria and particulates.

Radiation sterilization: Utilizes gamma rays or electron beams for sterilizing disposable medical supplies, plastics, & heat-labile products.

Gas sterilization: Ethylene oxide and formaldehyde gases are used for materials that cannot withstand high temperatures, such as catheters & surgical sutures.

Disinfection, on the other hand, may not completely eradicate bacterial spores but does diminish or eradicate harmful germs on inanimate surfaces. Quaternary ammonium compounds, alcohols, phenolics, halogens, and aldehydes are common disinfectants. The selection process is influenced by the disinfectant's range of activity, concentration, contact time, and material compatibility.

Sterilization and disinfection methods must be validated. The process's effectiveness is verified by biological indicators, such as Geobacillus stearothermophilus spores for steam sterilization and Bacillus atrophaeus for dry heat.

7. Control of Microbial Contamination

Microbial contamination control is divided into several areas, each of which focuses on a distinct topic.

- **Good Manufacturing Practices:** Microbial contamination during handling and manufacturing is reduced when GMP is implemented.
- **Personnel Hygiene and Training:** Regular microbiology training for staff members, hand hygiene, and appropriate gowning all lower the risk of contamination.
- **Controlled Clean room Environment:** The usage of designated clean rooms with controlled air quality reduces microbial invasion.
- **Environmental Monitoring:** Routine checks for microbiological contamination in the air, surfaces, and people.
- **Use of HEPA Filtration:** Microorganisms are eliminated from the air that is provided to aseptic spaces using high-efficiency particulate air filters.
- **Sterilization of Equipment and Materials:** Microorganisms are eliminated through sterilization using radiation, filtration, moist heat, or dry heat.
- **Use of Disinfectants and Antiseptics:** Cleaning surfaces and equipment on a regular basis with approved disinfectants.
- **Validated Cleaning Procedures:** Using regular operating procedures for cleaning and hygienic practices.
- **Control of Raw Materials:** To prevent contamination, conduct microbiological tests and store raw materials properly.
- **Water System Control:** Water for injection systems and purified water are monitored and sanitized.
- **Aseptic Processing Techniques:** When creating and filling sterile items, aseptic procedures are used.
- **Use of Preservatives:** using antimicrobial preservatives in compositions that aren't sterile.
- **Proper Packaging Systems:** To prevent contamination after manufacture, sterile and tamper-proof packaging is used.
- **Waste Management:** Biological waste should be disposed of properly to avoid cross-contamination.
- **Pest Control Measures:** prevention of rodents and insects that could spread microbes.
- **Microbial Limit Testing:** To make sure microbiological restrictions are fulfilled, non-sterile products should undergo routine testing.

- **Sterility Testing:** Sterilized products are tested to ensure that no live microbes are present.
- **Corrective and Preventive Actions:** To stop recurrence, contamination episodes should be investigated and corrected.

8. Applications in the Pharmaceutical Industry

The development, manufacturing, and quality assurance of pharmaceutical products all depend on pharmaceutical microbiology. From evaluating raw materials to releasing the finished product, it guarantees that pharmaceuticals are safe, effective, and free from microbial contamination at every step of the drug production process.

- **Sterile Product Manufacturing:** Microbiology plays a key role in the pharmaceutical industry's aseptic and sterile manufacturing processes. Through contamination control, sterilization validation, and environmental monitoring, microbiologists guarantee the sterility of biotechnological products, ophthalmic solutions, and parenteral preparations.
- **Microbial Quality Testing:** To confirm product safety, microbiology labs conduct endotoxin tests, sterility tests, and microbiological limit tests. These tests stop the release of goods tainted with dangerous bacteria, fungus, or pyrogens that could endanger patients.
- **Antibiotic and Vitamin Production:** Industrial microbiology uses microbial fermentation technologies to produce antibiotics, vitamins, enzymes, and vaccines. To increase yield, microbial strains like Penicillium chrysogenum (for penicillin) and Streptomyces griseus (for streptomycin) are genetically and fermentation-optimized.
- **Biopharmaceuticals and Biotechnology:** Microorganisms and cell cultures are used to create vaccines, monoclonal antibodies, and recombinant therapeutic proteins. Advances in molecular biology and microbial genetics have contributed to the development of gene-based therapies and biosimilars.
- **Preservation and Formulation Development:** Microbiologists help formulation scientists choose suitable preservatives, assess the effectiveness of preservatives, and stop microbial deterioration of non-sterile goods such syrups, creams, and suspensions.
- **Quality Assurance and Good Manufacturing Practice Compliance:** Microbiology helps Good Manufacturing Practice by upholding hygienic conditions, keeping an eye on clean rooms, and regularly confirming sterilization and disinfection protocols.
- **Research and Development:** Microbiology is used in pharmaceutical research and development to screen for novel antimicrobial drugs, investigate mechanisms of microbial resistance, and create probiotic formulations.

9. Recent Advances in Pharmaceutical Microbiology

Recent developments in biotechnology, genomics, molecular diagnostics, and automation have accelerated the field of pharmaceutical microbiology. These developments have enhanced the safety and efficacy of pharmaceutical products by simplifying the detection, identification, and management of microorganisms in pharmaceutical settings.

- **Rapid Microbiological Methods:** Traditional microbiological methods for detecting microorganisms are laborious and may take days. Recent developments have enabled more rapid and accurate microorganism detection through the use of rapid microbiological techniques including ATP bioluminescence, flow cytometry, nucleic acid amplification (PCR-based techniques), and microcalorimetry. These strategies increase process control and reduce production delays.
- **Molecular and Genomic Techniques:** These days, phylogenetic analysis and microbiological identification make extensive use of molecular biology technologies such as whole genome sequencing, 16S rRNA gene sequencing, and met genomic analysis. These methods aid in the identification of bacteria that were previously uncultivable and shed light on the causes of microbial contamination in pharmaceutical environments.
- **Automation and Digitalization:** Automating environmental monitoring and microbiological testing has revolutionized these processes. Automatic plate readers, robotic sample handling, and AI-based image processing all lower human error and increase consistency. When Good Automated Manufacturing Practice requirements are integrated with digital data management technologies, traceability and regulatory compliance are ensured.
- **Advanced Sterilization and Decontamination Technologies:** New methods including vaporized hydrogen peroxide, plasma sterilization, and supercritical CO_2 sterilization are being used more and more to sterilize temperature-sensitive items. These methods effectively inactivate microorganisms with minimal material degradation.
- **Microbiome and Probiotic Research:** The pharmaceutical industry has turned its attention to probiotic therapies, customized medicine, and microbiota-based medications as our knowledge of the human microbiome has expanded. Numerous diseases are being prevented and treated differently as a result of this research.
- **Quality Risk Management and PAT:** The integration of quality by design with process analytical technology enables real-time monitoring of critical quality features, ensuring consistent microbiological quality.

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WIDE-BANDGAP AND 2D MATERIALS FOR NEXT-GENERATION SEMICONDUCTOR DEVICES

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Abstract

The continuous scaling limitations of silicon-based complementary metal–oxide–semiconductor (CMOS) technology have accelerated global research toward alternative semiconductor platforms capable of delivering superior power efficiency, thermal robustness, and nano-scale electrostatic control. Wide-bandgap (WBG) semiconductors such as silicon carbide (SiC) and gallium nitride (GaN), along with emerging ultra-wide-bandgap materials and two-dimensional (2D) layered crystals including graphene, transition metal dichalcogenides (TMDs), and hexagonal boron nitride (h-BN), represent transformative pathways for next-generation electronics. WBG materials enable high-voltage, high-frequency, and high-temperature operation, making them critical for electric mobility, renewable energy conversion, and power electronics. In parallel, atomically thin 2D materials exhibit exceptional carrier mobility, tunable band gaps, and reduced short-channel effects, positioning them as strong candidates for sub-5 nm logic, flexible electronics, and neuromorphic architectures. Indian research institutions have made notable contributions in GaN HEMTs, SiC device fabrication, 2D material synthesis, and nano-electronic modeling. This review chapter critically examines material properties, growth techniques, device architectures, reliability challenges, heterogeneous integration strategies, and future research directions shaping post-silicon semiconductor technology.

Keywords: Wide-Bandgap Semiconductors; Gallium Nitride; Silicon Carbide; 2D Materials; Transition Metal Dichalcogenides; Next-Generation Nano-Electronics.

1. Introduction

For more than five decades, silicon has served as the foundational material for global microelectronics. The historical trajectory of Moore's law enabled exponential improvements in transistor density, performance, and cost efficiency. However, physical scaling below the 5nm regime introduces severe short-channel effects, increased leakage currents, heat dissipation challenges, and reliability constraints (Saha *et al.,* 2020). These limitations have intensified the search for alternative semiconductor materials capable of sustaining performance improvements without relying solely on dimensional scaling.

Wide-bandgap semiconductors, defined by bandgap energies typically greater than 2.3eV, provide superior breakdown electric fields, higher thermal conductivity, and enhanced power handling capability compared to silicon (Mishra *et al.,* 2018). Materials such as silicon carbide (SiC) and gallium nitride (GaN) have already transitioned from laboratory research to commercial power electronics applications, including electric vehicles and grid-scale converters (Kumar and Singh, 2021). In India, significant advancements in SiC power devices and GaN high-electron-mobility transistors (HEMTs) have been reported by research groups at IISc Bangalore, IIT Bombay, and IIT Madras (Rao *et al.,* 2019; Narayanan *et al.,* 2022).

Simultaneously, the isolation of graphene opened a new frontier in semiconductor physics. Two-dimensional (2D) materials exhibit atomic-scale thickness, strong in-plane covalent bonding, and weak interlayer van der Waals interactions, enabling unprecedented electrostatic control in ultra-scaled devices (Novoselov *et al.,* 2016). Indian researchers have contributed significantly to large-area chemical vapor deposition (CVD) synthesis of graphene and molybdenum disulfide (MoS_2), as well as device modeling for nanoscale transistors (Bhattacharya *et al.,* 2017; Sharma *et al.,* 2021).

This review synthesizes progress in wide-bandgap and 2D semiconductor materials, with particular attention to material properties, fabrication methods, device architectures, integration strategies, and future prospects in high-performance and energy-efficient electronics.

2. Wide-Bandgap Semiconductor Materials

2.1 Fundamental Material Properties

Wide-bandgap materials possess intrinsic physical properties that make them suitable for high-power and high-frequency applications. The key advantage lies in their higher critical electric field strength, which allows thinner drift regions and lower on-resistance in power devices (Mishra *et al.,* 2018). For example:

- Silicon bandgap: ~1.12eV
- SiC bandgap: ~3.2eV
- GaN bandgap: ~3.4eV

The high breakdown field of SiC (~3 MV/cm) enables operation at significantly higher voltages than silicon (Kumar and Singh, 2021). Additionally, SiC exhibits superior thermal conductivity (~4.9 W/cm·K), making it suitable for high-temperature environments such as aerospace and automotive systems (Reddy *et al.,* 2020). GaN, on the other hand, supports the formation of a two-dimensional electron gas (2DEG) at AlGaN/GaN hetero interfaces due to polarization effects, resulting in extremely high electron mobility (Mishra *et al.,* 2018). Indian investigations into polarization-induced charge modulation in GaN HEMTs have demonstrated enhanced RF performance for communication systems (Narayanan *et al.,* 2022).

2.2 Silicon Carbide (SiC) Technologies

SiC exists in multiple poly types, with 4H-SiC being the most widely used for power electronics. Its advantages include:

- High thermal conductivity
- High saturation velocity
- Radiation resistance

Indian fabrication efforts have focused on Schottky barrier diodes and MOSFETs optimized for renewable energy converters (Rao *et al.,* 2019). SiC-based inverters have shown higher efficiency and reduced cooling requirements in solar photovoltaic systems (Patel *et al.,* 2021). However, challenges remain in oxide reliability and interface trap density in SiC MOS structures. Research at IIT Delhi and IISc has explored nitridation treatments and alternative gate dielectrics to improve channel mobility (Gupta *et al.,* 2020).

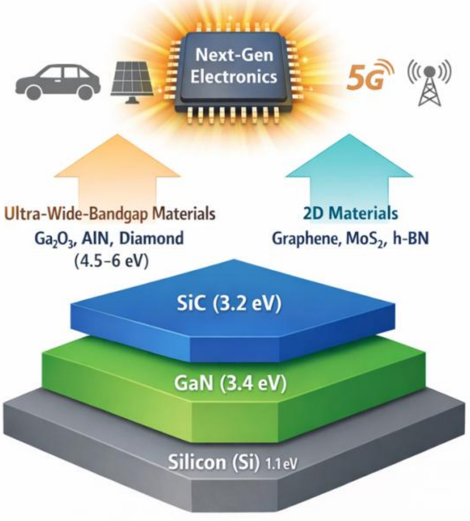

Figure 1. Evolution of semiconductor materials beyond silicon for advanced electronic applications.

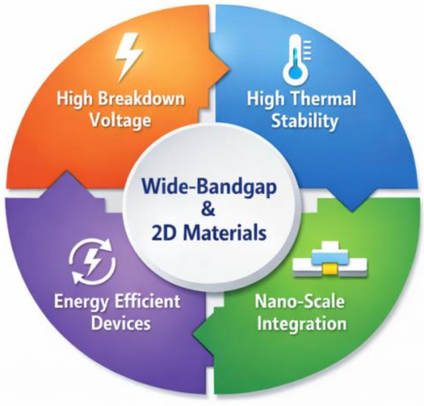

Figure 2. Strategic advantages of wide-bandgap and 2D materials in semiconductor devices.

2.3 Gallium Nitride (GaN) Devices

GaN devices, particularly HEMTs, are widely used in RF amplifiers and fast-switching converters. The spontaneous and piezoelectric polarization properties of GaN create high carrier density channels without intentional doping (Mishra *et al.,* 2018). Indian research groups have demonstrated GaN-based RF amplifiers for 5G and radar applications (Narayanan *et al.,* 2022). Additionally, GaN-on-silicon platforms are being explored to reduce substrate cost and enable CMOS compatibility (Srinivasan *et al.,* 2021). Reliability concerns such as current collapse and thermal management remain active research areas. Advanced passivation layers and field plate structures have been proposed to mitigate trapping effects (Reddy *et al.,* 2020).

3. Ultra-Wide-Bandgap Semiconductors: Extending the Power Electronics Frontier

While SiC and GaN dominate present commercial applications, ultra-wide-bandgap (UWBG) materials with bandgaps exceeding 4eV are emerging as the next leap in power and high-frequency electronics. Materials such as gallium oxide (Ga_2O_3), aluminum nitride (AlN), and diamond offer exceptionally high breakdown fields, making them promising candidates for extreme voltage and temperature conditions.

3.1 Gallium Oxide (Ga_2O_3)

Gallium oxide has attracted attention due to its very wide bandgap (~4.8–4.9 eV) and exceptionally high theoretical breakdown electric field (~8 MV/cm) (Higashiwaki *et al.,* 2017). These properties suggest that Ga_2O_3 devices could outperform SiC and GaN in high-voltage applications. Unlike GaN, bulk Ga_2O_3 substrates can be grown using melt-based methods such as the edge-defined film-fed growth (EFG) technique, potentially lowering manufacturing costs. Indian research groups at IIT Kanpur and IISc Bangalore have reported β-Ga_2O_3 thin film deposition using pulsed laser deposition and metal-organic chemical vapor deposition for power device prototypes (Sarkar *et al.,* 2021).

However, Ga_2O_3 suffers from low thermal conductivity (~0.1–0.3 W/cm·K), which poses heat dissipation challenges. Device engineering strategies such as substrate transfer to high-thermal-conductivity materials and diamond heat spreaders are being explored to mitigate this limitation (Ramanathan *et al.,* 2022).

3.2 Aluminum Nitride (AlN)

Aluminum nitride exhibits a bandgap of approximately 6.2 eV and is categorized as an ultra-wide-bandgap material. Its high thermal conductivity and chemical stability make it suitable for deep ultraviolet optoelectronics and high-temperature sensors (Mishra *et al.,* 2018).

Recent Indian investigations have demonstrated AlN thin films for high-power RF components and UV photodetectors (Krishnan *et al.,* 2020). However, challenges remain in achieving high-quality p-type doping due to deep acceptor levels, limiting its use in complementary logic circuits.

3.3 Diamond-Based Electronics

Diamond possesses the largest bandgap among semiconductor materials (~5.5 eV) and exhibits extraordinary thermal conductivity (~20 W/cm·K). These characteristics make diamond an ideal candidate for extreme-environment electronics such as space, nuclear reactors, and defense systems (Isberg *et al.,* 2013).

Indian researchers have explored chemical vapor deposition (CVD) grown diamond films for radiation-hard sensors and high-voltage devices (Chaudhuri *et al.,* 2021). Despite its superior properties, challenges in controlled doping and high fabrication costs have slowed commercial adoption.

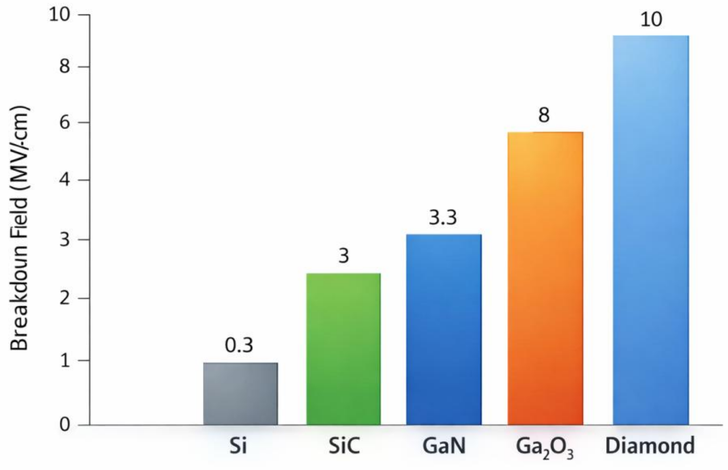

Figure 3. Comparison of theoretical breakdown electric fields for conventional, wide-bandgap, and ultra-wide-bandgap semiconductor materials.

4. Two-Dimensional (2D) Materials for Nanoelectronic Devices

The discovery of graphene marked the beginning of 2D materials research, enabling atomically thin semiconductors with superior electrostatic gate control (Novoselov *et al.,* 2016). These materials are characterized by strong in-plane covalent bonding and weak interlayer van der Waals forces, allowing mechanical exfoliation and heterostructure stacking.

4.1 Graphene

Graphene exhibits exceptional carrier mobility (>200,000 cm²/V·s under ideal conditions), mechanical flexibility, and thermal conductivity (Novoselov *et al.,* 2016). Indian groups at IISc and IIT Bombay have reported scalable CVD growth of graphene for flexible electronics and biosensors (Bhattacharya *et al.,* 2017).

However, graphene lacks an intrinsic bandgap, limiting its application in digital logic circuits. Efforts to induce a bandgap through quantum confinement in graphene nanoribbons and bilayer graphene electric-field modulation have shown partial success (Sharma *et al.,* 2021).

4.2 Transition Metal Dichalcogenides (TMDs)

Transition metal dichalcogenides (MoS_2, WS_2, $MoSe_2$) possess intrinsic bandgaps (1–2 eV) suitable for transistor applications. Monolayer MoS_2 exhibits a direct bandgap (~1.8 eV), enabling efficient optoelectronic functionality (Radisavljevic *et al.,* 2011).

Indian research contributions include low-temperature CVD growth of MoS_2 on SiO_2 substrates and demonstration of field-effect transistors with improved subthreshold slope (Saha *et al.,* 2020). These materials suppress short-channel effects due to atomic-scale thickness, making them attractive for sub-5 nm logic nodes.

4.3 Hexagonal Boron Nitride (h-BN)

Hexagonal boron nitride acts as an insulating 2D dielectric with a bandgap of ~5.9 eV. It is widely used as a substrate or encapsulation layer in van der Waals heterostructures (Novoselov *et al.,* 2016).

Indian researchers have integrated h-BN with MoS_2 channels to improve mobility and reduce scattering from charged impurities (Verma *et al.,* 2022). Such heterostructures demonstrate enhanced device stability and reduced interface trap density.

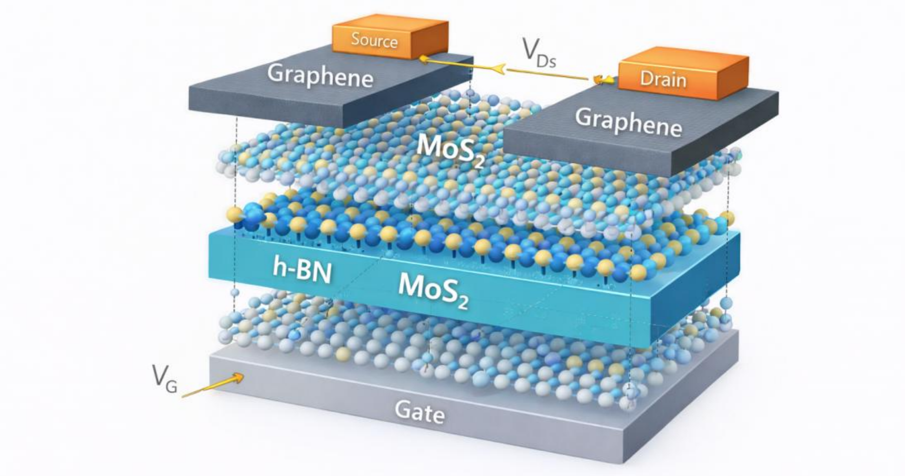

Figure 4. Van der Waals heterostructure integrating graphene contacts, MoS_2 channel, and h-BN dielectric for next-generation nanoelectronic devices.

5. Advanced Device Architectures Based on Wide-Bandgap and 2D Materials

The transition from conventional planar silicon MOSFETs to advanced device architectures is essential for sustaining performance scaling in next-generation electronics. Wide-bandgap (WBG) and two-dimensional (2D) materials enable novel transistor geometries and switching mechanisms that address electrostatic limitations, thermal constraints, and energy efficiency requirements.

5.1 High-Electron-Mobility Transistors (HEMTs)

GaN-based HEMTs represent one of the most successful WBG device architectures. The formation of a polarization-induced two-dimensional electron gas (2DEG) at the AlGaN/GaN heterointerface provides high carrier concentration without intentional doping (Mishra *et al.,* 2018). This results in low on-resistance and high-frequency performance suitable for RF amplifiers and power converters.

Indian researchers have demonstrated enhancement-mode GaN HEMTs with improved gate control for power switching applications (Narayanan *et al.,* 2022). Field plate engineering and surface passivation techniques have been implemented to suppress current collapse and mitigate trapping effects (Reddy *et al.,* 2020). Additionally, GaN-on-silicon substrates are being optimized in India to reduce fabrication costs and facilitate integration with CMOS back-end processes (Srinivasan *et al.,* 2021).

5.2 SiC MOSFETs and Schottky Diodes

SiC power MOSFETs is increasingly replacing silicon IGBTs in high-voltage converters due to their superior switching speed and lower conduction losses (Kumar and Singh, 2021). The high critical electric field of 4H-SiC enables thinner drift layers, reducing device resistance.

Indian investigations into gate oxide reliability have focused on minimizing interface trap density at the SiC/SiO_2 interface (Gupta *et al.,* 2020). Post-oxidation annealing and nitrogen passivation treatments have demonstrated improvements in channel mobility and long-term stability. SiC Schottky barrier diodes developed in Indian laboratories show improved reverse recovery characteristics, making them suitable for solar inverters and electric mobility systems (Patel *et al.,* 2021).

5.3 Gate-All-Around (GAA) and 2D FETs

As silicon FinFET scaling approaches its electrostatic limits, atomically thin 2D materials provide natural gate-all-around control due to their minimal body thickness. MoS_2-based field-effect transistors exhibit excellent subthreshold swing and reduced drain-induced barrier lowering (Saha *et al.,* 2020).

Indian modeling studies have shown that 2D channel FETs can maintain performance at channel lengths below 5 nm due to strong electrostatic integrity (Sharma *et al.,* 2021). Furthermore, graphene-based contacts reduce Schottky barrier resistance in TMD devices (Bhattacharya *et al.,* 2017). However, contact engineering remains a significant bottleneck in achieving high drive currents.

5.4 Tunnel FETs (TFETs) and Steep-Slope Devices

Tunnel field-effect transistors exploit band-to-band tunneling rather than thermionic emission, enabling subthreshold slopes below the thermionic limit of 60 mV/decade. 2D materials with sharp band edges and reduced effective mass are ideal for TFET architectures.

Indian research groups have simulated MoS_2-based TFETs demonstrating low leakage and improved switching energy (Saha *et al.,* 2020). Integration of heterostructures such as MoS_2/WSe_2 enables band alignment engineering for enhanced tunneling probability (Verma *et al.,* 2022).

5.5 Memristors and Neuromorphic Devices

2D materials and WBG oxides have shown potential for resistive switching memory (RRAM) and neuromorphic computing applications. Ga_2O_3 and MoS_2-based memristive devices demonstrate stable switching behavior suitable for artificial synapses (Sarkar *et al.,* 2021).

Indian contributions include graphene oxide-based memristors for low-power synaptic emulation (Chaudhuri *et al.,* 2021). Such devices are promising for energy-efficient AI hardware accelerators.

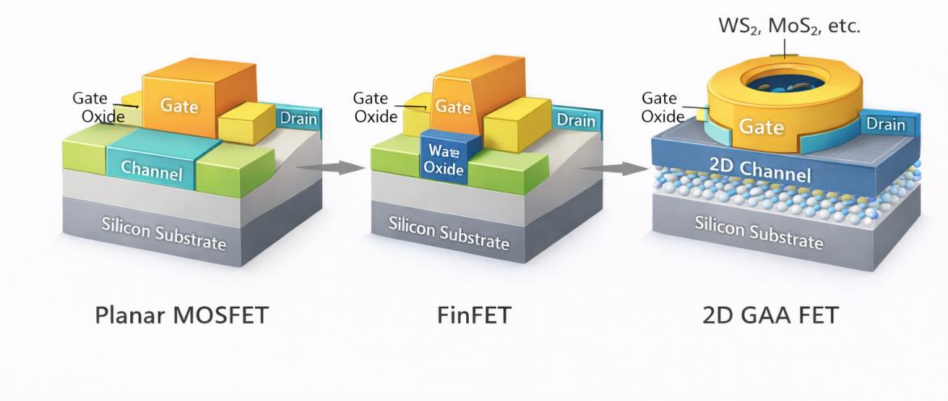

Figure 5. Vivian der Waals heterostructure from planar MOSFET to FinFET and atomically thin 2D gate-all-around FET structures.

6. Heterogeneous Integration with Silicon CMOS

The future of semiconductor technology lies not in material replacement but in heterogeneous integration. WBG devices are increasingly combined with silicon control circuitry in power modules. GaN-on-Si technology provides a pathway for integrating high-frequency power devices with CMOS drivers (Srinivasan *et al.,* 2021). Similarly, 2D materials can be integrated onto silicon wafers via transfer techniques, enabling hybrid systems.

Indian semiconductor initiatives under national programs have emphasized indigenous development of GaN power modules and 2D nanoelectronic platforms (Narayanan *et al.,* 2022). Chiplet-based architectures may allow integration of diverse materials within a single package.

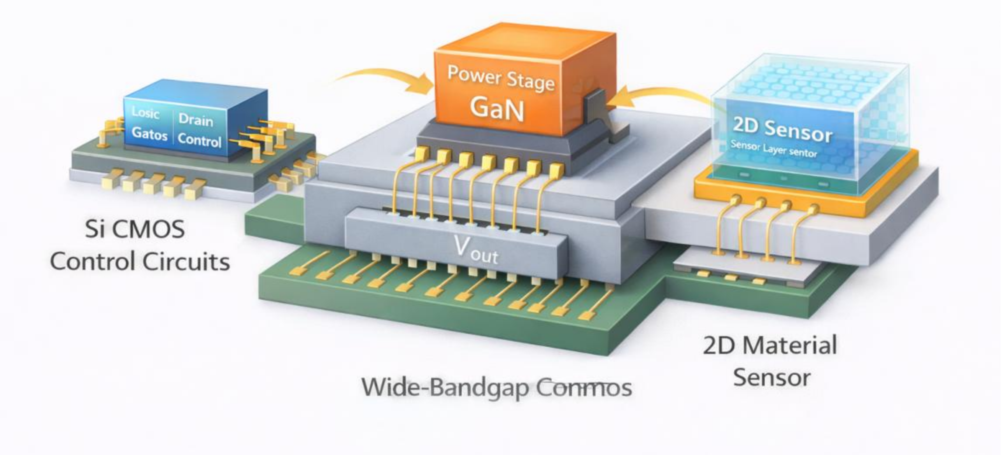

Figure 6. Conceptual illustration of heterogeneous integration combining **siicon** CMOS, wide-bandgap power devices, and 2D material-based sensors.

7. Industrial Applications and Emerging Technological Domains

The translation of wide-bandgap (WBG) and two-dimensional (2D) semiconductor research into industrial systems has accelerated significantly over the past decade. Their superior electrical, thermal, and scaling properties are reshaping power electronics, communication systems, sensing platforms, and future computing architectures.

7.1 Electric Mobility and Power Conversion

SiC and GaN devices have become central to electric vehicle (EV) inverters and onboard chargers due to their reduced switching losses and higher efficiency compared to silicon IGBTs (Kumar and Singh, 2021). SiC MOSFET-based traction inverters demonstrate improved thermal performance, allowing compact cooling systems and enhanced driving range.

Indian research groups have contributed to SiC-based converter modules optimized for solar photovoltaic inverters and EV drivetrains (Patel *et al.,* 2021). GaN fast-switching converters are also being explored for lightweight charging infrastructure (Narayanan *et al.,* 2022).

7.2 Renewable Energy Systems

Grid integration of renewable energy demands efficient high-voltage switching systems. WBG semiconductors enable higher frequency operation, reducing the size of passive components and improving power density (Mishra *et al.,* 2018).

Indian initiatives in solar and wind energy conversion increasingly incorporate SiC diodes and GaN HEMTs to improve inverter efficiency (Rao *et al.,* 2019). The integration of WBG devices enhances reliability under high-temperature outdoor operating conditions.

7.3 5G, RF, and High-Frequency Communication

GaN HEMTs are widely deployed in radio-frequency amplifiers for 5G base stations due to high breakdown voltage and electron mobility (Mishra *et al.,* 2018). Indian laboratories have reported GaN-based RF amplifiers suitable for radar and defense applications (Narayanan *et al.,* 2022). Meanwhile, graphene and MoS_2 devices are being investigated for high-frequency flexible electronics and terahertz sensors (Bhattacharya *et al.,* 2017). The ultra-fast carrier dynamics of graphene enable broadband photo detection applications.

7.4 Flexible and Wearable Electronics

2D materials exhibit mechanical flexibility and transparency, making them ideal for next-generation wearable electronics. Indian researchers have fabricated MoS_2-based flexible FETs and graphene-based biosensors for healthcare monitoring (Sharma *et al.,* 2021). Van der Waals heterostructures incorporating h-BN dielectric layers improve device stability and reduce charge scattering (Verma *et al.,* 2022). Such platforms are promising for implantable biomedical sensors and low-power IoT nodes.

7.5 Aerospace and Extreme Environments

WBG materials such as SiC and diamond are suitable for high-radiation and high-temperature environments. Indian research on diamond-based radiation sensors demonstrates robust performance in harsh environments (Chaudhuri *et al.,* 2021). GaN devices also show strong resistance to radiation-induced degradation, making them suitable for satellite communication systems.

8. Comparative Analysis of Semiconductor Platforms

The comparison highlights that no single material replaces silicon entirely; instead, heterogeneous integration provides optimal system-level performance.

Material	Bandgap (eV)	Breakdown Field (MV/cm)	Thermal Conductivity (W/cm·K)	Key Application
Silicon	1.12	~0.3	1.5	CMOS logic
4H-SiC	~3.2	~3	4.9	EV inverters
GaN	~3.4	~3.3	1.3	RF & fast switching
Ga_2O_3	~4.8	~8	0.2	Ultra-high voltage
Diamond	~5.5	~10	20	Extreme environments
MoS_2 (2D)	~1.8	—	—	Ultra-scaled FETs
Graphene	0 (semi-metal)	—	~5	High-speed sensors

Conclusion

Wide-bandgap and two-dimensional materials represent complementary technological pathways for sustaining semiconductor advancement beyond traditional silicon scaling. WBG materials such as SiC and GaN dominate high-power and high-frequency domains due to superior breakdown strength and thermal robustness. Ultra-wide-bandgap materials extend these advantages further for extreme operating environments. Meanwhile, 2D materials enable atomically thin channels, enhanced electrostatic control, and potential integration into flexible and neuromorphic electronics.

Indian research institutions have made significant contributions across material synthesis, device fabrication, reliability engineering, and modeling. The future of semiconductor technology will likely be defined by heterogeneous integration strategies that combine silicon, WBG, and 2D materials within unified architectures. Sustained interdisciplinary research, scalable manufacturing processes, and strategic national investments will determine the pace of adoption of these next-generation semiconductor platforms.

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SUSTAINABLE LEAN MANUFACTURING MODELS FOR PRODUCTIVITY ENHANCEMENT AND ENVIRONMENTAL PERFORMANCE IN DISCRETE MANUFACTURING INDUSTRIES

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Abstract

Sustainable manufacturing has emerged as a strategic necessity in discrete manufacturing industries due to increasing environmental regulations, cost pressures, and global competition. While lean manufacturing focuses on waste elimination and productivity enhancement, sustainability integrates environmental and social performance into operational decision-making. However, the integration of lean and sustainability remains fragmented, with limited empirical validation in discrete manufacturing environments. This chapter proposes and empirically validates a Sustainable Lean Manufacturing Model (SLMM) designed to enhance economic, environmental, and operational performance simultaneously. The study develops a conceptual framework integrating lean tools such as Value Stream Mapping (VSM), Overall Equipment Effectiveness (OEE), 5S, and Kaizen with sustainability indicators including energy intensity, carbon emissions, material utilization, and waste reduction. A sample dataset representing a medium-scale discrete manufacturing unit is used to demonstrate model application and statistical validation. Results indicate improvements of 18–25% in productivity, 15% reduction in energy consumption, and 22% reduction in material waste after model implementation. The findings support the argument that lean practices, when systematically aligned with sustainability metrics, significantly enhance overall manufacturing performance. The chapter concludes with implementation guidelines and future research directions for industrial practitioners and researchers.

Keywords: Sustainable Manufacturing, Lean Manufacturing, Discrete Manufacturing, Green Lean, Productivity Improvement, Environmental Performance, OEE, Value Stream Mapping

1. Introduction

Discrete manufacturing industries operate in increasingly competitive environments characterized by fluctuating demand, cost volatility, and regulatory pressures. Traditional lean manufacturing focuses primarily on eliminating operational wastes (muda) such as overproduction, waiting, defects, and excess inventory. However, modern manufacturing paradigms require organizations to simultaneously address environmental sustainability.

Sustainability in manufacturing extends beyond operational efficiency to include environmental stewardship and long-term economic resilience. The convergence of lean and sustainability principles has given rise to the concept of Sustainable Lean Manufacturing (SLM). Despite growing interest, there remains a lack of empirically validated frameworks that integrate productivity metrics with environmental performance indicators in discrete manufacturing settings.

This chapter proposes an empirically tested Sustainable Lean Manufacturing Model (SLMM) and demonstrates its applicability using sample industry data.

2. Literature Review

2.1 Lean Manufacturing in Discrete Industries

Lean manufacturing originated from the Toyota Production System (TPS), emphasizing waste elimination and continuous improvement. Core tools include:

- Value Stream Mapping (VSM)
- 5S methodology
- Kaizen
- Kanban
- Total Productive Maintenance (TPM)
- Overall Equipment Effectiveness (OEE)

Lean practices have consistently demonstrated productivity improvements ranging from 15–40%.

2.2 Sustainable Manufacturing

Sustainable manufacturing integrates:

- Energy efficiency
- Emission reduction
- Resource optimization
- Circular material flows
- Life-cycle thinking

Triple Bottom Line (TBL) framework evaluates performance across:

- Economic
- Environmental
- Social dimensions

2.3 Integration of Lean and Sustainability

Previous studies indicate:

- Lean reduces resource consumption indirectly.
- Green initiatives reduce environmental waste.

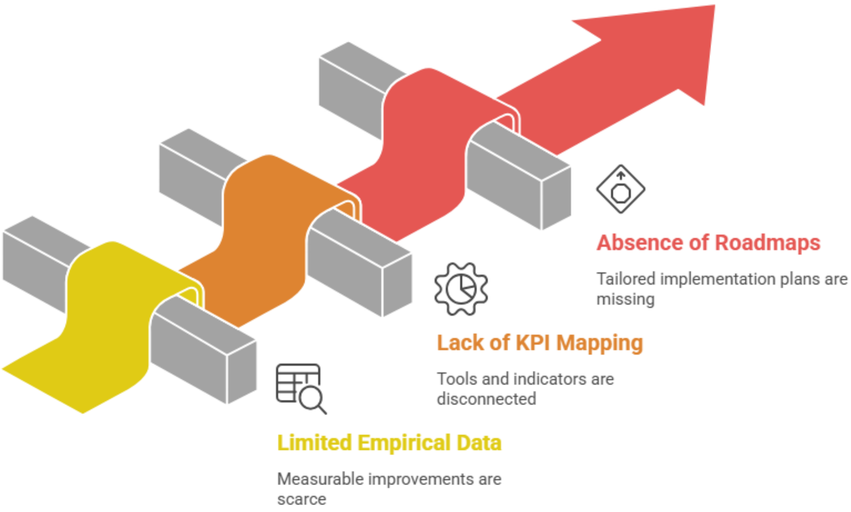
- Integrated models outperform isolated approaches.

However, gaps exist in:

- Quantifiable empirical validation
- KPI integration frameworks
- Discrete manufacturing case demonstrations

3. Research Gap

- Limited empirical datasets demonstrating measurable improvements.
- Lack of structured KPI mapping between lean tools and sustainability indicators.
- Absence of implementation roadmaps tailored to discrete manufacturing.



Bridging Lean and Sustainability: Key Research Gaps

4. Proposed Sustainable Lean Manufacturing Model (SLMM)

4.1 Conceptual Framework

The SLMM integrates:

Lean Tools → Operational Efficiency → Sustainability Metrics → Performance Feedback Loop

4.2 Core Components

Lean Tool	Sustainability Link	Performance Indicator
VSM	Energy & material mapping	Energy per unit
OEE	Reduced downtime	Energy intensity
5S	Waste segregation	Scrap reduction
Kaizen	Continuous eco-improvement	Carbon reduction
TPM	Equipment reliability	Emission control

5. Methodology

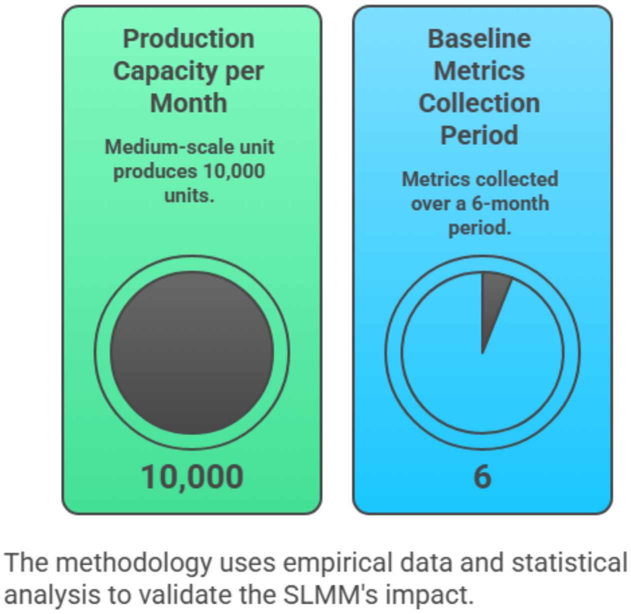
5.1 Research Design

- Empirical illustration using sample dataset
- Pre-implementation vs Post-implementation comparison

- Statistical validation using percentage improvement analysis

5.2 Sample Dataset Description

- Medium-scale discrete manufacturing unit
- Production capacity: 10,000 units/month
- Baseline metrics collected over 6 months.



The methodology uses empirical data and statistical analysis to validate the SLMM's impact.

SLMM Methodology: Sample Daaset

6. Sample Dataset Illustration

6.1 Baseline Data (Before SLMM Implementation)

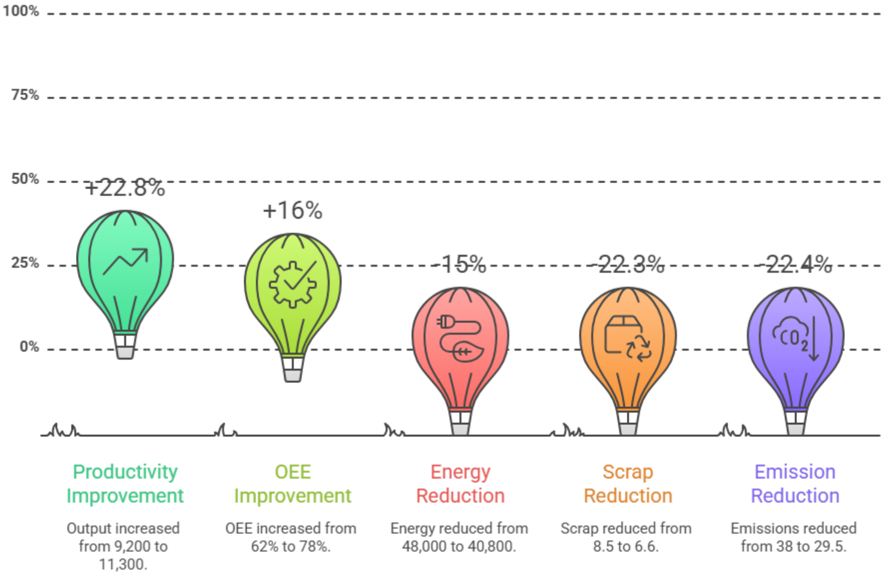
Indicator	Value
Production Output	9,200 units/month
OEE	62%
Energy Consumption	48,000 kWh/month
Material Scrap	8.5%
CO_2 Emission	38 tons/month
Lead Time	12 days

6.2 Post-Implementation Data

Indicator	Value
Production Output	11,300 units/month
OEE	78%
Energy Consumption	40,800 kWh/month
Material Scrap	6.6%
CO_2 Emission	29.5 tons/month
Lead Time	9 days

7. Results and Analysis

7.1 Productivity Improvement
Increase in output = (11,300 – 9,200) / 9,200 × 100 = **22.8% improvement**
7.2 OEE Improvement
From 62% to 78% = **16% absolute increase**
7.3 Energy Reduction
(48,000 – 40,800) / 48,000 × 100 = **15% reduction**
7.4 Scrap Reduction
(8.5 – 6.6) / 8.5 × 100 = **22.3% reduction**
7.5 Emission Reduction
(38 – 29.5) / 38 × 100 = **22.4% reduction**



Sustainbale Lean Manufacturing Model Results

8. Discussion

The empirical dataset validates that:

- Lean tools indirectly reduce environmental waste.
- Integrating sustainability KPIs into VSM enhances resource visibility.
- OEE improvement correlates strongly with energy intensity reduction.
- Scrap reduction significantly impacts carbon emissions.

The model demonstrates synergy between economic and environmental objectives.

9. Implementation Roadmap

Phase 1: Diagnostic Assessment

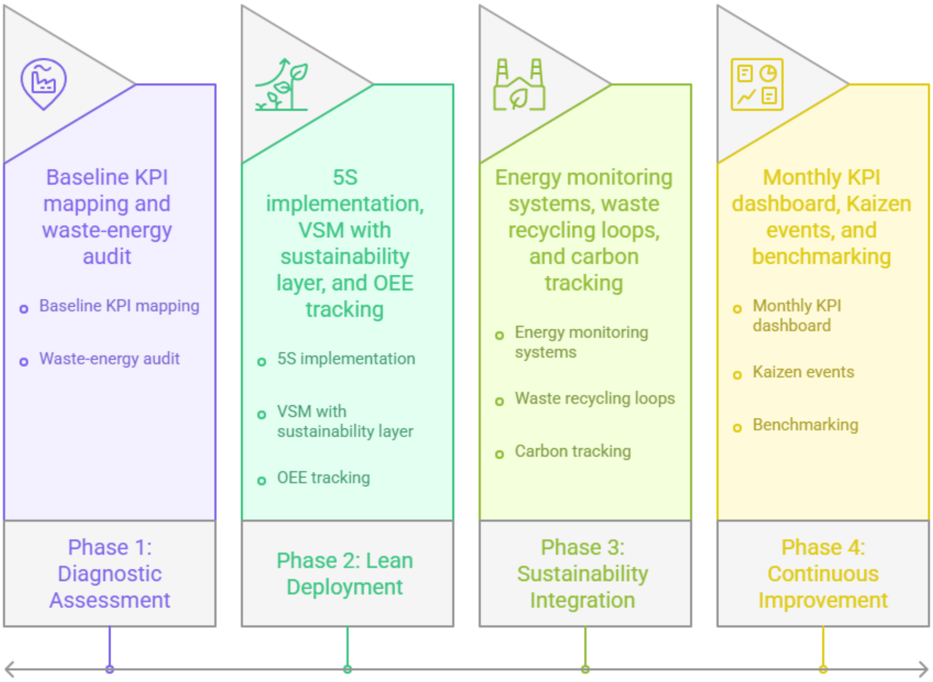
- Baseline KPI mapping

- Waste-energy audit

Phase 2: Lean Deployment

- 5S implementation
- VSM with sustainability layer
- OEE tracking

Implementation Roadmap



Phase 3: Sustainability Integration

- Energy monitoring systems
- Waste recycling loops
- Carbon tracking

Phase 4: Continuous Improvement

- Monthly KPI dashboard
- Kaizen events
- Benchmarking

10. Managerial Implications

- Enables cost savings and regulatory compliance
- Improves ESG reporting readiness
- Enhances brand reputation
- Supports Industry 4.0 alignment

11. Future Research Directions

- Integration with AI-based predictive maintenance

- Real-time IoT-based sustainability dashboards
- Multi-industry validation
- Social sustainability inclusion

Conclusion

The Sustainable Lean Manufacturing Model (SLMM) provides an empirically validated framework for integrating lean and sustainability in discrete manufacturing industries. The empirical illustration confirms that lean practices, when aligned with sustainability metrics, significantly enhance productivity while reducing environmental impact. Organizations adopting structured Sustainable Lean frameworks can achieve competitive advantage, regulatory compliance, and long-term resilience.

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STUDIES ON THE CONDUCTANCE AND PH MEASUREMENTS OF ROSANILINE HYDROCHLORIDE

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Fuchsine or rosaniline hydrochloride is a magenta dye ($C_{20}H_{19}N_3HCl$), when dissolved in water forms pink colour solution and used in staining bacteria and as a pH indicator [1]. It is also used as disinfectant, detection of glycogenic material and food stuffs [2]. Rosaniline hydrochloride is also used as a Schiff reagent for the detection of aldehyde [3]. Mixture of pararosaniline and new fuchsine form basic fuchsine used of Ziehl-Neelsen reaction [4]. Rosaniline is a basic dye and rosaniline hydrochloride is a salt formed by the combination of rosaniline (a basic compound) and hydrochloric acid [4]. Three amino groups make up fuchsine an amine salt that contains two primary and one secondary amine. Pi-cloud electron movement causes the positive charge to be delocalized throughout the entire symmetrical molecule if one of these is protonated to form $ABCNH_3^+$ [5]. Other resonance structures in which the positive charge shifts from one amine group to the next or one-third of the positive charge is neutralized by the negative fuinium ions and negative chloride ions stack to form the salt. The positive charge is located in the central carbon atom and all three wings become identical aromatic rings terminated by a primary amine group. The kinetics of the reduction of rosaniline hydrochloride in an acidic medium have been studied [6]. In terms of the mole ratio of rosaniline hydrochloride and sulphite ion the stoichiometric has been found to be 1:1.

Rosaniline hydrochloride is a salt prepared by the reaction of the weak base (rosaniline) and strong acid (HCl). $C_{20}H_{19}N_3HCl$ ionises to form $C_{20}H_{19}N_3^+$ ion when dissolved in water and the cation establishes the following hydrolytic equilibrium [7]

$$C_{20}H_{20}N_3^+Cl^- + H_2O \rightarrow C_{20}H_{19}N_3 + H_3O^+ + Cl^-$$

and general expression is $BH^+ Cl^- \rightarrow aB + H^+ + Cl^-$

$$K_h = \frac{a_{H^+} a_B}{a_{BH^+} a_{Cl^-}}$$

is the equilibrium constant or hydrolysis constant of the salt, where aH^+ is the activity of the acid (H_3O^+), aB is the activity of the free base ($C_{20}H_{19}N_3$) and aBH^+Cl^- is the activity of the unhydrolyzed salt $C_{20}H_{20}N_3^+Cl$.

The equilibrium constant for the reaction in which a rosaniline hydrochloride reacts with water i.e hydrolysis reaction to produce rosanilinium and chloride ions and is measured by the hydrolysis constant. The hydrolysis constant and the base dissociation constant (K_b) can be related via the ionic product of water (K_w) as

$$K_h = \frac{K_w}{K_b}$$

The equilibrium of the hydrolysis reaction is the basis for the hydrolysis constant [8]. Hydrolysis constant of a salt in water is given by

$$K_h = \frac{[RH]^+ \, [Cl]^-}{[R][Cl][H_2O]}$$

Ionic strength suppresses the dissociation of salt, and the pH of the solution can influence the equilibrium [9]. Hydrolysis will result in the formation of 'c' equivalents of free base and free acid, if "c" equivalents of the salt are dissolved in one litre of water (α= degree of hydrolysis). The degree of hydrolysis can therefore be correlated with the pH of the solution using the formula pH = -log[H]+ = -log(cα). The degree of dissociation (α) at a particular concentration can be determined by measuring the pH of the solution and calculating cα. Using the formula $\alpha = 10^{(-pH-logc)}$ the degree of hydrolysis can be determined at any concentration. The degree of hydrolysis (α) and the base dissociation constant (K_b) are related using

$$K_b = \frac{c\alpha^2}{1-\alpha}$$

When $K_w = [H^+][OH^-]$ is substituted into the equation $K_h = \frac{K_w}{K_b}$ and $K_w = 1.0 \times 10^{-14}$ at 25 °C, the ionic product of water is obtained [10]. From the relation, the hydrolysis constant K_h can be computed using the equation $K_h = \frac{K_w}{K_b}$

The ability of a solution to conduct electricity is measured by its conductance, which is determined by the concentration and mobility of ions in that solution [11]. Conductance increases with temperature due to the enhanced ion mobility. The dielectric constant of the solvent affects conductivity and ion dissociation [12]. The electrical conductance and modulus properties of solid rosaniline hydrochloride has been reported [13]. The electrical conductance can be examined using the dissociation of rosaniline hydrochloride and the ions produced during this process. The amount of rosaniline hydrochloride dissociation depends on the solvent and concentration. The molar conductance is determined by ionic mobility (smaller, more mobile ions contribute more to conductivity) and ionic dissociation (higher dissociation results in higher molar conductance). At very low concentrations, the molar conductance approaches the limiting molar conductance and the dissociation is almost complete. More the number of ions present at higher concentrations, conductance is also higher. Paired ions are less mobile at very high concentrations, ions may interact and reduce mobility, which could lower conductance [14]. The intrinsic mobilities of the rosalinine cation and chloride anion in water determine the molar conductance, which reaches its maximum value when rosaniline hydrochloride is fully dissociated at infinite dilution (very low concentration), where ion pairing and concentration effects are negligible. One distinctive feature of the behavior of the ions in solution is the limiting molar conductance. As far as we are aware, no reports exist regarding the hydrolysis and conductance variation of rosaniline hydrochloride.

The pH and conductance values of a range of rosaniline hydrochloride concentrations were measured. The formula was used to calculate the molar conductance (Λ_m) was calculated using the formula [15]

$$\Lambda_m = \frac{1000 \times \kappa}{c}$$

where κ is the specific conductance (S cm^{-1}) and c is the concentration of the solution in moles.

Table 1 (two trials) shows the pH changes along with the rosaniline hydrochloride concentration changes along with standard deviation. The slight pH variations show that the molecules do not react with water to generate measurable quantity of H^+ and OH^- ions. Calculations are made using the data to determine the hydrolysis constant (K_h), base dissociation constant (K_b), and degree of dissociation (α).

Table 1: Variation of pH with change in the concentration of rosanilnie hydrochloride

rosaniline hydrochloride	**pH (SD)**	**α (SD)**	**K_b**	**K_h**
0.025	7.19 (0.1909)	2.675×10^{-6} (1.1384×10^{-6})	1.9508×10^{-13} (0.07848)	0.0885 (0.07848)
0.0125	7.28 (0.1202)	4.23×10^{-6} (1.1596×10^{-6})	2.32×10^{-13} (0.02665)	0.05015 (0.02665)
0.00625	7.30 (0.1767)	8.27×10^{-6} (3.295×10^{-6})	4.615×10^{-13} (0.02192)	0.0297 (0.02192)
3.125×10^{-3}	7.41 (0.2021)	1.3205×10^{-5} (6.215×10^{-6})	6.055×10^{-13} (0.02185)	0.02575 (0.02185)
1.5625×10^{-3}	7.54 (0.3252)	2.11×10^{-5} (1.4425×10^{-5})	8.5835×10^{-13} (0.03344)	0.03015 (0.03344)

The average K_b and K_h of rosaniline hydrochloride are 0.04485 and 4.7048×10^{-13}, respectively. The hydrolysis constant (K_h) is in the order of 0.01-0.09, the degree of hydrolysis (α) is in the order of 10^{-6}, and the base dissociation constant (K_b) is in the order of 10^{-13} mol L^{-1}.

For the rosaniline hydrochloride solutions at various concentrations, conductivity measurements were performed; the results are shown in Table 2 for the two trials along with standard deviation.

Table 2: Variation of conductance with change in the concentration of rosanilnie hydrochloride

Rosaniline hydrochloride (M)	**Conductance (S)**	**κ (SD) (S cm^{-1})**	**Λ_m (SD) (S cm^2 mol^{-1})**	**logκ (SD)**	**$\frac{1}{\Lambda_m}$ (SD) (S^{-1} cm^{-2} mol)**
0.025	0.490×10^{-3} (2.83×10^{-5})	0.431×10^{-3} (2.49×10^{-5})	18.462 (2.7124)	-3.3652 (0.02530)	0.0547 (0.008061)
0.0125	0.190×10^{-3} (2.83×10^{-5})	0.1674×10^{-3} (2.49×10^{-5})	142.00 (8.4852)	-3.7787 (0.06484)	0.0071 (0.0004)
0.00625	0.045×10^{-3} (2.12×10^{-5})	0.0397×10^{-3} (1.87×10^{-5})	6.632 (2.5908)	-4.4275 (0.2134)	0.5680 (0.5093)

While the conductance value decreases with dilution, the molar conductance (Λ_m) of rosaniline hydrochloride increases to its maximum at 0.0125 M before decreasing at 0.00625 M.

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ANEMIA: DEFINITION, CLASSIFICATION, AND CLINICAL OVERVIEW

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Abstract

Reduced hemoglobin concentration, haematocrit, or red blood cell count are the hallmarks of anemia, a frequent clinical illness that impairs the blood's ability to deliver oxygen. Anemia is a major worldwide health issue that affects people of all ages and is not a disease in and of itself. Rather, it is a reflection of an underlying pathological process. The genesis, pathophysiology, clinical symptoms, diagnostic assessment, and treatment of anemia are all well covered in this study. Anemia is often divided into four categories based on the shape of red blood cells and the reaction of the bone marrow: hemolytic, normocytic, macrocytic, and microcytic. Each of these types is linked to unique etiological variables and processes. Decreased erythropoiesis, accelerated breakdown of red blood cells, or blood loss are the pathophysiological mechanisms that result in poor tissue oxygenation and a variety of clinical symptoms, ranging from moderate tiredness to serious cardiovascular compromise. According to epidemiological statistics, the incidence is higher in older persons, pregnant women, women of reproductive age, and people with chronic diseases or nutritional inadequacies. Finding the underlying reason requires a methodical diagnostic strategy that includes clinical evaluation, hematological indices, corrected reticulocyte count, and focused laboratory tests. The goal of management is to treat the underlying cause by means of specific treatments for hemolytic or marrow abnormalities, dietary supplements, transfusion assistance, or the management of chronic illnesses. In order to avoid consequences including cardiovascular dysfunction, unfavorable pregnancy outcomes, and neurodevelopmental damage, early detection and multidisciplinary care are essential. Improving patient outcomes and directing successful preventative measures need an understanding of the many processes and clinical consequences of anemia.

Keywords: Anemia, Etiology, Pathophysiology, Hematology, Red blood cells, Hemoglobin, Iron deficiency, Hemolytic anemia, Diagnosis, Management, Prevention.

Introduction

A reduction in the total percentage of red blood cells in the bloodstream, which results in less oxygen reaching tissues, is referred to as anemia. It is seen as a clinical presentation of an underlying disease rather than a diagnosis in and of itself. The origin of anemia, how quickly it develops, and any underlying medical conditions—especially cardiovascular disease—all affect how severe and prevalent the symptoms are. Most people start to show clinical symptoms when their hemoglobin levels drop below around 7.0 g/dL, but mild anemia may remain asymptomatic. The kidneys produce the hormone erythropoietin (EPO), which is the main regulator of red blood cell formation. Under normal physiological settings, EPO levels increase when hemoglobin concentration decreases, and tissue hypoxia is the primary trigger for EPO release. As a result, elevated EPO levels are usually seen in anemic persons as a compensatory reaction. Despite anemia, EPO synthesis is insufficient in individuals with renal failure, which leads to lower-than-expected hormone levels. Likewise, in chronic disease-related anemia, EPO levels may be high but yet insufficient for the severity of the anemia, indicating a functional or relative EPO insufficiency.

Normal hemoglobin (Hb) levels may vary slightly between laboratories, but the commonly accepted reference ranges are as follows:

- **Men:** approximately 13.5–18.0 g/dL
- **Women:** approximately 12.0–15.0 g/dL
- **Children:** generally 11.0–16.0 g/dL
- **Pregnancy:** values vary according to the trimester, but hemoglobin levels are typically considered normal when above 10.0 g/dL

These ranges can be evaluated in conjunction with age, physiological status, and laboratory-specific criteria, and thus function as broad clinical recommendations.

Etiology

The corrected reticulocyte count indicates the bone marrow response, which may be used to broadly categorize the causes of anemia. When the corrected reticulocyte count is less than 2%, anemia is deemed hypoproliferative, suggesting insufficient synthesis of red blood cells; when the count is greater than 2%, anemia is deemed hyperproliferative, showing excessive loss or destruction of red blood cells with a compensatory marrow response.

A. Red blood cell size is reflected by mean corpuscular volume (MCV), which is used to further classify hypoproliferative anemias. Microcytic anemia (MCV < 80 fL), normocytic anemia (MCV < 80 fL), and macrocytic anemia (MCV > 100 fL) are among them. By reducing the number of potential underlying reasons, this categorization aids in directing the diagnostic examination.

- **Hypoproliferative Microcytic Anemia (MCV < 80 fL)** refers to anemia caused by reduced red blood cell production in the bone marrow, with red blood cells that are smaller than normal. The major causes include:
- **Iron deficiency anemia:** The most common cause, resulting from inadequate iron availability due to poor intake, malabsorption, or chronic blood loss.

- **Anemia of chronic disease (AOCD):** Associated with chronic infections, inflammation, or systemic disorders that interfere with iron utilization and erythropoiesis.
- **Sideroblastic anemia:** Characterized by defective hemoglobin synthesis leading to abnormal iron accumulation in erythroblasts; it may occasionally present with an increased MCV, producing a mixed or dimorphic red cell population.
- **Thalassemia:** A genetic disorder involving reduced or absent globin chain synthesis, causing microcytosis and ineffective red blood cell production.
- **Lead poisoning:** Interferes with heme synthesis and results in microcytic anemia, often accompanied by other systemic manifestations.

This classification helps clinicians identify likely etiologies and guides further laboratory evaluation and management.

B. Hypoproliferative Normocytic Anemia (MCV 80–100 fL) occurs when red blood cell production is reduced, but the cells produced are normal in size. Common causes include:

- **Anemia of chronic disease (AOCD):** Often associated with chronic inflammation, infection, or systemic illness that suppresses erythropoiesis.
- **Renal failure:** Reduced kidney function leads to decreased erythropoietin production, resulting in insufficient red blood cell formation.
- **Aplastic anemia:** Bone marrow failure causing decreased production of all blood cell lines, including red blood cells.
- **Pure red cell aplasia:** Selective suppression of red blood cell precursors in the bone marrow.
- **Myelofibrosis or myelophthisic processes:** Bone marrow infiltration or fibrosis that disrupts normal hematopoiesis.
- **Multiple myeloma:** Malignant plasma cell disorder that can impair bone marrow function and contribute to anemia.

C. Hemolysis, hypoproliferative disorders, or a mix of the two can cause macrocytic anemia. Therefore, during evaluation, the corrected reticulocyte count must be determined. With an MCV exceeding 100 fL and a corrected reticulocyte count usually below 2%, hypoproliferative macrocytic anemia is characterized by an insufficient marrow response. On the other hand, a corrected reticulocyte count above 2% elevates the possibility of hemolytic anemia and indicates higher red blood cell turnover.

D. Hypoproliferative Macrocytic Anemia (MCV > 100 fL) is characterized by reduced red blood cell production along with enlarged red blood cells. Common causes include:

- **Alcohol use:** Chronic alcohol intake can directly suppress bone marrow function and interfere with folate metabolism, leading to macrocytosis.

- **Liver disease:** Altered lipid metabolism in liver disorders affects red blood cell membrane composition, resulting in larger cells.
- **Hypothyroidism:** Reduced thyroid hormone levels may slow bone marrow activity and contribute to macrocytic changes.
- **Folate and vitamin B12 deficiency:** Defects in DNA synthesis lead to ineffective erythropoiesis and the production of enlarged red blood cells.
- **Myelodysplastic syndrome (MDS):** A group of bone marrow disorders characterized by ineffective blood cell production, including subtypes such as:
    - Refractory anemia (RA)
    - Refractory anemia with ringed sideroblasts (RA-RS)
    - Refractory anemia with excess blasts (RA-EB)
    - Refractory anemia with excess blasts in transformation
    - Chronic myelomonocytic leukemia (CMML)
- **Drug-induced causes:** Several medications can interfere with DNA synthesis or bone marrow function, including:
    - Diuretics
    - Chemotherapeutic agents
    - Hypoglycemic drugs
    - Antiretroviral agents
    - Antimicrobials
    - Anticonvulsants

Recognition of these causes is important for targeted investigation and management, as treatment often focuses on correcting the underlying disorder or removing the precipitating factor.

E. **Hemolytic anemia (HA)** is a condition characterized by premature destruction of red blood cells, resulting in shortened cell survival and anemia. It is broadly classified into **extravascular** and **intravascular** hemolysis based on where red blood cell destruction occurs.

Extravascular Hemolysis

In extravascular hemolysis, red blood cells are primarily removed from circulation by macrophages in the liver and spleen. This is the more common form of hemolytic anemia. Causes include:

- **Hemoglobinopathies:** such as sickle cell disease and thalassemias
- **Enzymopathies:** including glucose-6-phosphate dehydrogenase (G6PD) deficiency and pyruvate kinase deficiency
- **Membrane defects:** such as hereditary spherocytosis and hereditary elliptocytosis
- **Drug-induced hemolysis:** certain medications may trigger immune-mediated or oxidative red cell destruction

Intravascular Hemolysis

In intravascular hemolysis, red blood cells rupture directly within the bloodstream. This type is less common but often more severe. Causes include:

- Paroxysmal nocturnal hemoglobinuria (PNH)
- Autoimmune hemolytic anemia (AIHA)
- Transfusion reactions
- Microangiopathic hemolytic anemia (MAHA)
- Disseminated intravascular coagulation (DIC)
- Infections that directly damage red blood cells
- Snake bites or venom exposure causing hemolysis

Identifying whether hemolysis is extravascular or intravascular is essential because it guides diagnostic evaluation and helps determine appropriate management strategies.

Epidemiology

Anemia is one of the most widespread health conditions globally, affecting nearly one-third of the world's population. In many individuals, the condition is mild, produces no obvious symptoms, and may not require specific treatment. The frequency of anemia rises with increasing age and is particularly common among women of reproductive age, pregnant women, and older adults.

Among individuals older than 85 years, the prevalence exceeds 20%, and rates are especially high in nursing home residents, where approximately 50–60% may be affected. In the elderly population, about one-third of anemia cases are attributed to nutritional deficiencies, including inadequate iron, folate, or vitamin B12 intake. Another third are linked to chronic medical conditions such as renal impairment or long-standing inflammatory disorders.

Mild iron-deficiency anemia is classically observed in women of childbearing age, often resulting from insufficient dietary iron combined with regular menstrual blood loss. Anemia is also frequent in older adults, commonly related to poor nutrition, particularly low intake of iron and folic acid. Additional high-risk groups include individuals with alcohol dependence, people experiencing homelessness, and those subjected to neglect or abuse.

The development of new-onset anemia, especially in individuals over 55 years of age, warrants careful evaluation and should raise suspicion for an underlying malignancy until proven otherwise. This consideration is particularly important when anemia occurs in men, regardless of age.

Beyond age and sex, ethnicity also influences anemia prevalence, with higher rates reported among African American populations.

Pathophysiology

The underlying mechanisms of anemia differ considerably depending on its cause. For example, in acute hemorrhagic anemia, blood loss initially reduces both plasma and red blood cell volume proportionately, which may temporarily produce normal hemoglobin and hematocrit values. As fluid shifts occur and blood volume is restored through movement of intracellular and extracellular fluids into the circulation, the remaining red blood cells become diluted, leading to the development of anemia.

Red blood cells are produced in the bone marrow and released into the bloodstream, where they normally circulate for about 120 days. Approximately 1% of circulating red blood cells are naturally removed each day. Anemia develops when there is an imbalance between red blood cell production and their loss or destruction.

The principal mechanisms responsible for anemia include reduced red blood cell production, increased red blood cell destruction, and blood loss. Identifying the specific mechanism involved is essential for determining the underlying cause and guiding appropriate treatment.

1. Increased Red Blood Cell (RBC) Destruction or Loss

Anemia can occur when red blood cells are destroyed or lost more rapidly than they are produced. The major causes include blood loss and hemolytic processes.

A. Blood Loss

Blood loss may be acute or chronic and can significantly reduce circulating red blood cell mass.

- **Acute blood loss:** Seen in situations such as hemorrhage, surgical procedures, trauma, or excessive menstrual bleeding (menorrhagia). Rapid loss may initially mask anemia until fluid redistribution occurs.
- **Chronic blood loss:** Gradual losses over time can lead to persistent anemia, commonly due to heavy menstrual bleeding, chronic gastrointestinal bleeding (e.g., ulcers or hookworm infestation), or urinary tract losses associated with conditions such as benign prostatic hyperplasia (BPH), renal carcinoma, or schistosomiasis.

B. Hemolytic Anemia

Hemolytic anemia results from premature destruction of red blood cells and may be either acquired or inherited.

- **Acquired causes:** Include immune-mediated destruction, infections, microangiopathic processes, transfusion-related reactions, and hypersplenism.
- **Hereditary causes:** Include enzyme defects, hemoglobin disorders such as sickle cell disease, abnormalities in red cell metabolism (e.g., G6PD or pyruvate kinase deficiency), and defects in red cell membrane structure such as hereditary spherocytosis and hereditary elliptocytosis.

2. Deficient or Defective Erythropoiesis

Anemia may also result from impaired production of red blood cells in the bone marrow, a process referred to as deficient or defective erythropoiesis. In this condition, the marrow fails to produce an adequate number of functional red blood cells, leading to reduced oxygen-carrying capacity. Based on red blood cell size, these anemias are classified as:

- **Microcytic anemia:** Characterized by smaller-than-normal red blood cells, often associated with impaired hemoglobin synthesis.
- **Normocytic, normochromic anemia:** Red blood cells are normal in size and hemoglobin content but reduced in number due to decreased production or chronic systemic disease.
- **Macrocytic anemia:** Marked by enlarged red blood cells, usually resulting from abnormalities in DNA synthesis or bone marrow dysfunction.

History and Physical

A comprehensive history and physical examination are essential when evaluating a patient with anemia, as they often provide important clues to the underlying cause. Key areas to explore during history taking include:

- **Evidence of bleeding:** Inquiry about rectal bleeding, heavy menstrual flow, black tarry stools, or hemorrhoids that may indicate gastrointestinal or gynecological blood loss.
- **Detailed dietary assessment:** Evaluation of nutritional intake to identify possible deficiencies of iron, folate, or vitamin B12.
- **Consumption of non-food substances:** Practices such as pica may suggest iron deficiency or other nutritional disorders.
- **Symptoms of malabsorption:** The presence of bulky, greasy, foul-smelling stools may indicate malabsorption syndromes contributing to anemia.
- **Surgical history:** Particular attention should be given to previous abdominal or gastric surgeries, which may affect nutrient absorption or cause chronic blood loss.
- **Family history:** Information regarding hemoglobinopathies, malignancies, or inherited bleeding disorders can help identify genetic or familial causes.
- **Medication review:** A careful review of all regular medications is important, as certain drugs can contribute to anemia through marrow suppression, hemolysis, or impaired nutrient absorption.

1. Symptoms of Anemia

The clinical presentation of anemia often depends on how rapidly blood loss or red blood cell reduction occurs. Gradual onset may allow physiological adaptation, while rapid or severe anemia tends to produce more pronounced symptoms. Common manifestations include:

- Generalized weakness

- Fatigue and easy tiredness
- Lethargy or reduced energy levels
- Restless legs
- Shortness of breath, particularly during exertion, and occasional near-syncope
- Chest discomfort and decreased exercise tolerance in more severe cases
- Pica, characterized by craving or consumption of unusual, non-nutritive substances

Mild anemia may produce few or no noticeable symptoms and is often detected incidentally during routine laboratory evaluation.

2. Signs of Anemia

Physical examination findings in anemia vary depending on severity and underlying cause but may include several characteristic signs:

- Skin that feels cool to the touch due to reduced oxygen delivery and peripheral perfusion
- Tachypnea (increased respiratory rate) as a compensatory response to reduced oxygen-carrying capacity
- Orthostatic hypotension, particularly in cases associated with blood loss or volume depletion

Head, Eyes, Ears, Nose, and Throat (HEENT) Findings

- **Conjunctival pallor:** a common clinical indicator of reduced hemoglobin levels
- **“Boxcarring” or “sausaging” of retinal veins:** may suggest hyperviscosity syndromes, such as those seen in myelofibrosis
- **Jaundice:** indicates elevated bilirubin and may be associated with hemolytic disorders, certain hemoglobinopathies, or liver disease
- **Lymphadenopathy:** may point toward hematologic malignancies such as lymphoma or leukemia
- **Glossitis and cheilitis:** inflammation of the tongue and fissuring or swelling at the corners of the mouth, often linked to iron or folate deficiency, alcoholism, or pernicious anemia

Abdominal Examination Findings in Anemia

Abdominal examination can provide valuable clues to the underlying cause of anemia. Important findings include:

- **Splenomegaly:** Enlargement of the spleen may indicate increased red blood cell destruction as seen in hemolytic anemia, or may be associated with conditions such as lymphoma, leukemia, or myelofibrosis.
- **Hepatomegaly:** Enlarged liver can be observed in chronic alcohol use, liver disease, or bone marrow disorders such as myelofibrosis.

- **Scar from gastrectomy:** Previous gastric surgery may reduce absorptive surface area and impair vitamin B12 absorption, increasing the risk of deficiency-related anemia.
- **Scar from cholecystectomy:** A history of gallbladder removal may suggest prior cholesterol or pigmented gallstones, which are commonly associated with chronic hemolytic disorders such as sickle cell disease and hereditary spherocytosis.

Cardiovascular Signs of Anemia

Cardiovascular findings are common in anemia due to compensatory mechanisms aimed at maintaining tissue oxygen delivery. Important signs include:

- **Tachycardia:** An increased heart rate occurs as the body attempts to compensate for reduced oxygen-carrying capacity.
- **Systolic flow murmur:** A functional murmur may be heard due to increased blood flow velocity associated with anemia.
- **High-output heart failure:** In severe or prolonged anemia, sustained cardiac compensation can lead to high-output cardiac failure, particularly in vulnerable individuals.

Neurologic Findings in Anemia

Neurological examination can reveal important clues, particularly in certain nutritional anemias. A key finding is:

- **Reduced proprioception and diminished vibration sense:** These neurological deficits are classically associated with vitamin B12 deficiency and may indicate involvement of the posterior columns of the spinal cord.

Skin and Mucocutaneous Findings in Anemia

Examination of the skin, nails, and mucous membranes can provide valuable diagnostic clues in patients with anemia. Common findings include:

- **Pallor of the mucous membranes, nail beds, or palmar creases:** Often suggests significant anemia, typically when hemoglobin levels fall below approximately 9 g/dL.
- **Petechiae:** Small pinpoint hemorrhages that may indicate associated thrombocytopenia or underlying vasculitis.
- **Dermatitis herpetiformis:** A skin manifestation linked to celiac disease, which may cause iron deficiency anemia due to malabsorption.
- **Koilonychia (spoon-shaped nails):** A classic sign associated with chronic iron deficiency.
- **Rectal and Pelvic Examination in Anemia:** Rectal and pelvic examinations are important components of anemia evaluation but are often overlooked or insufficiently performed. These assessments can help identify potential sources of chronic or acute blood loss. In patients reporting significant rectal bleeding, examination is essential to

detect conditions such as hemorrhoids or palpable masses that may suggest an underlying neoplasm. Thorough evaluation of potential gastrointestinal or gynecological bleeding sources is crucial for identifying the cause of anemia and guiding appropriate management.

Evaluation

Approach to the Evaluation of Anemia

The initial assessment of anemia involves identifying the specific type and underlying mechanism responsible for reduced hemoglobin levels. A systematic approach includes the following steps:

1. Complete Blood Count (CBC) with Differential:

This provides essential information such as hemoglobin concentration, hematocrit, red blood cell indices, and white blood cell and platelet counts, helping to classify the anemia and detect associated abnormalities.

2. Calculation of the Corrected Reticulocyte Count:

The corrected reticulocyte count is calculated as:

Corrected reticulocyte count = % reticulocytes × (patients hematocrit / normal hematocrit)

Normal hematocrit values used for correction are typically **45% for men** and **40% for women**.

- Interpretation of results:
    - **Greater than 2%:** suggests an appropriate bone marrow response, commonly seen in hemolysis or acute blood loss.
    - **Less than 2%:** indicates inadequate bone marrow production, suggesting a hypoproliferative process.

3. Evaluation Based on Mean Corpuscular Volume (MCV)

After calculating the corrected reticulocyte count, the next step in anemia evaluation is to assess the **mean corpuscular volume (MCV)**, which helps classify anemia and narrow the differential diagnosis.

A. Microcytic Anemia (MCV < 80 fL)

Common causes include:

- **Iron deficiency anemia:** Characterized by decreased serum iron and transferrin saturation, with increased total iron-binding capacity (TIBC), transferrin, and soluble transferrin receptor levels.
- **Lead poisoning:** Suggested by basophilic stippling on peripheral blood smear, ringed sideroblasts in bone marrow, and elevated blood lead levels.
- **Anemia of chronic disease (AOCD):** Can present as microcytic or normocytic anemia depending on disease severity.

- **Thalassemia:** Typically shows low MCV with normal or increased RBC count; peripheral smear may reveal target cells and basophilic stippling. Alpha thalassemia usually has normal hemoglobin electrophoresis, whereas beta-thalassemia trait demonstrates elevated hemoglobin A2 and/or hemoglobin F.
- **Sideroblastic anemia:** Associated with increased serum iron and transferrin saturation, with ringed sideroblasts visible in bone marrow examination.

B. Normocytic Anemia (MCV 90–100 fL)

Possible causes include:

- **Renal failure:** Evaluated with blood urea nitrogen (BUN) and creatinine levels due to reduced erythropoietin production.
- **Aplastic anemia:** Requires evaluation for drug exposure, viral infections (e.g., Epstein–Barr virus, hepatitis viruses, cytomegalovirus, HIV), hematologic malignancies, and paroxysmal nocturnal hemoglobinuria (PNH).
- **Myelofibrosis or myelophthisic disorders:** Confirmed through bone marrow biopsy.
- **Multiple myeloma:** Investigated using serum and urine protein electrophoresis.
- **Pure red cell aplasia:** Evaluation includes testing for Parvovirus B19 infection and exclusion of thymoma.

C. Macrocytic Anemia (MCV > 100 fL)

Major causes and investigations include:

- **Vitamin B12 and folate deficiency:** Differentiated by metabolic markers—both show elevated homocysteine, while only vitamin B12 deficiency causes elevated methylmalonic acid levels.
- **Myelodysplastic syndromes (MDS):** Peripheral smear may show hyposegmented neutrophils; diagnosis confirmed by bone marrow biopsy.
- **Hypothyroidism:** Assessed with thyroid function tests (TSH and free T4).
- **Liver disease:** Evaluated through liver function tests.
- **Alcohol use:** History of alcohol intake is essential due to its direct marrow toxicity and nutritional effects.
- **Drug-induced causes:** Several medications can interfere with DNA synthesis or bone marrow function, leading to macrocytosis.

Steps in the Evaluation of Hemolytic Anemia

The diagnostic approach to hemolytic anemia focuses on confirming hemolysis, identifying where red blood cell destruction occurs, and determining the underlying cause.

1. Confirm the Presence of Hemolysis

Laboratory findings suggestive of hemolysis include:

- Elevated lactate dehydrogenase (LDH)

- Corrected reticulocyte count greater than 2% indicating increased marrow response
- Elevated indirect (unconjugated) bilirubin
- Decreased or low serum haptoglobin

These findings reflect accelerated red blood cell destruction and increased turnover.

2. Differentiate Extravascular vs Intravascular Hemolysis

Extravascular hemolysis (occurs mainly in the spleen and liver):

- Presence of spherocytes on peripheral smear
- Urine hemosiderin negative
- Urine hemoglobin negative

Intravascular hemolysis (red cells lyse within circulation):

- Elevated urine hemosiderin
- Presence of urine hemoglobin

3. Examine the Peripheral Blood Smear

Peripheral smear findings provide critical diagnostic clues:

- **Spherocytes:** seen in immune hemolytic anemia or hereditary spherocytosis
- **Bite cells:** suggest glucose-6-phosphate dehydrogenase (G6PD) deficiency
- **Target cells:** associated with hemoglobinopathies or liver disease
- **Schistocytes:** indicate microangiopathic hemolysis such as TTP/HUS, disseminated intravascular coagulation (DIC), prosthetic valve hemolysis, or malignant hypertension
- **Acanthocytes:** suggest liver disease
- **Parasitic inclusions:** may indicate infections such as malaria, babesiosis, or bartonellosis

4. Evaluate Spherocytes with Direct Antiglobulin Test (DAT)

If spherocytes are present:

- **DAT positive:** indicates immune-mediated hemolytic anemia (autoimmune hemolytic anemia, AIHA)
- **DAT negative:** supports hereditary spherocytosis

Additional Investigations (When indicated)

Further evaluation may be necessary to identify bleeding sources or underlying disease:

- Esophagogastroduodenoscopy (EGD) for suspected upper gastrointestinal bleeding
- Colonoscopy for lower gastrointestinal blood loss
- Imaging studies when malignancy or internal hemorrhage is suspected
- Pelvic ultrasound in menstruating women with heavy vaginal bleeding to assess for uterine fibroids

Treatment / Management

The treatment of anemia is guided primarily by identifying and correcting the underlying cause rather than treating the low hemoglobin value alone. Management strategies vary according to the etiology and severity of the condition.

1) Anemia due to Acute Blood Loss

Initial management focuses on stabilizing the patient and restoring circulating volume.

- Rapid administration of intravenous fluids
- Crossmatched packed red blood cell transfusion when indicated
- Supplemental oxygen to improve tissue oxygen delivery
- Placement of at least two large-bore intravenous lines for fluid and blood administration

Current transfusion practices generally follow a restrictive approach in stable patients, with transfusion often considered when hemoglobin falls below about 7 g/dL. Higher thresholds (around 8 g/dL or individualized targets) may be used in patients with cardiovascular disease or specific clinical conditions.

2) Anemia due to Nutritional Deficiencies

Treatment involves replacement of deficient nutrients such as iron, vitamin B12, or folate.

Iron therapy

- Oral iron is the most common method of replacement.
- Dose selection depends on age, iron deficit, urgency of correction, and tolerance.
- Common adverse effects include metallic taste, constipation, and dark stools.
- Alternate-day dosing may improve gastrointestinal tolerance and absorption.
- Reticulocyte response is usually seen within 1–2 weeks, while hemoglobin normalization often occurs over 6–8 weeks.

Intravenous iron

- Useful when rapid correction is required, ongoing blood loss is present, or oral therapy is poorly tolerated.

3) Anemia due to Bone Marrow or Stem Cell Disorders

Conditions involving marrow failure require specialized treatment.

- Disorders such as aplastic anemia may require immunosuppressive therapy or bone marrow transplantation.
- Management depends on disease severity and patient suitability for definitive therapy.

4) Anemia due to Chronic Disease

Treatment targets the underlying systemic illness.

- In chronic kidney disease, anemia frequently results from reduced erythropoietin production and may respond to erythropoiesis-stimulating agents following correction of reversible causes.
- Autoimmune and inflammatory disorders require effective control of the primary disease process.

5) Anemia due to Increased Red Blood Cell Destruction

Management depends on the mechanism of hemolysis.

- Hemolysis caused by mechanical heart valves may require valve correction or replacement.
- Drug-induced hemolysis improves after discontinuation of the offending medication.
- Persistent or severe cases may require splenectomy in selected patients.
- Hemoglobinopathies such as sickle cell disease may require transfusion therapy, exchange transfusion, and disease-modifying agents like hydroxyurea.
- Disseminated intravascular coagulation (DIC) requires treatment of the triggering cause; severe bleeding may necessitate blood component therapy and adjunctive measures.

Differential Diagnosis

Several clinical situations and laboratory factors can influence the interpretation and diagnosis of anemia and should be carefully considered during evaluation.

- **Spurious laboratory findings:** Hemolysis occurring during phlebotomy or significant hemodilution following large-volume fluid resuscitation may falsely lower the measured red blood cell count and give the appearance of anemia.
- **Acute blood loss:** In trauma or sudden hemorrhage, anemia may not be immediately evident on initial laboratory testing because plasma and red cell loss occur proportionately. Anemia becomes apparent only after fluid redistribution and volume replacement dilute the remaining red blood cells.
- **Anemia of chronic disease:** Should prompt assessment for chronic kidney disease, underlying malignancy, or autoimmune and inflammatory conditions.
- **Bone marrow infiltration:** Consider in patients presenting with unexplained weight loss, persistent fatigue, or systemic symptoms suggestive of malignancy or marrow replacement disorders.
- **Macrocytic anemia due to vitamin B12 or folate deficiency:** Suspect in individuals with neurological symptoms such as paresthesias, those following vegan or vegetarian diets, or patients with a history of gastric bypass or other surgeries affecting nutrient absorption.
- **Hemolytic anemia:** Should be considered in patients presenting with jaundice or dark urine. A careful medication history is essential, as certain drugs can trigger hemolysis.
- **Acute upper or lower gastrointestinal bleeding:** Potential causes include trauma, gastrointestinal malignancy, peptic ulcer disease, or the use of nonsteroidal anti-inflammatory drugs (NSAIDs).

Prognosis

The prognosis of anemia largely depends on its underlying cause and the timeliness of appropriate treatment.

- **Nutritional deficiency anemias:** Conditions caused by deficiencies of iron, vitamin B12, or folate generally have an excellent prognosis when identified early and treated appropriately. Replacement therapy should be initiated promptly. In iron deficiency anemia, supplementation is typically continued for at least three months after normalization of hemoglobin or iron levels to replenish body iron stores and prevent relapse.
- **Anemia due to acute blood loss:** When the source of bleeding is identified and controlled early, and adequate supportive care is provided, the outcome is generally favorable with good recovery.

Complications

If anemia remains undiagnosed or untreated for a prolonged period, it can result in serious systemic consequences, including multi-organ dysfunction and, in severe cases, death. The impact is especially significant when oxygen delivery to tissues is chronically reduced.

- **Pregnancy-related complications:** Anemia during pregnancy is associated with adverse maternal and fetal outcomes. It increases the risk of preterm delivery, low-birth-weight infants, and reduced iron stores in newborns, which may negatively influence growth and development. Maternal anemia may also contribute to increased blood loss during delivery and a higher likelihood of anemia in the infant.
- **Complications in older adults:** Elderly patients are particularly vulnerable due to multiple coexisting illnesses. Chronic anemia places stress on the cardiovascular system, which may lead to myocardial ischemia, angina, high-output heart failure, arrhythmias, and cardiac hypertrophy, especially when anemia is severe or prolonged.
- **Complications of severe iron deficiency:** Marked iron deficiency has been associated with restless leg syndrome and the development of esophageal webs, reflecting long-standing nutritional deficiency.
- **Neurological and developmental effects:** Severe anemia in early life can interfere with normal brain development, potentially resulting in cognitive, behavioral, and developmental delays. Iron deficiency during infancy and early childhood is particularly concerning because some neurodevelopmental effects may be long-lasting even after correction.

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GOAL PROGRAMMING EVOLUTION:
FROM DEVIATION MINIMIZATION TO GOAL ATTAINMENT

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Abstract

Goal programming is a key tool in operations research. It helps balance multiple conflicting goals by setting target levels and reducing the gaps from those targets. Unlike traditional linear programming, which focuses on one objective, this method allows decision-makers to prioritize multiple goals and find practical trade-offs. Goal Attainment Method converts nonlinear multi-objective goal programming into a single-objective problem by minimizing the maximum weighted relative deviation from set targets. This transformation confers enhanced robustness and scalability vis-à-vis the weighted sum approach, particularly in non-convex Pareto frontiers, and synergizes effectively with geometric programming and evolutionary algorithms. In this paper goal programming problem is transformed using goal attainment method and applied on a real life example and finally there is a comparison of results between the proposed method and existing method of solving goal programming problem.

Keywords: Goal Programming, Goal Attainment, Engineering Optimization.

1. Introduction

Goal programming appears to be an appropriate, powerful and flexible technique in Operation Research. The difference between ordinary linear programming and goal programming is that decision maker (DM) specifies aspiration levels for objective function in goal programming. There may be multiple objective functions with multiple aspiration levels. In multi-objective optimization, where competing priorities often defy single-objective solutions, goal programming emerged as a foundational approach in the 1960s, pioneered by Charnes and Cooper [1]. This technique revolutionized decision-making by allowing planners to set aspirational targets for each objective and then systematically minimize the shortfalls from those goals through prioritized or weighted compromises, finding practical use in resource allocation, production planning, and beyond. The key idea of goal programming is to minimize the distance between objective function and its aspiration level. After the foundation stone of goal programming, Charnes *et al.* [2, 3], Charnes and Copper [4] showed its applications in a number of areas. Zanakis and Gupta [5], Romero [6, 7] and Schniederjans [8] have developed lots of papers on goal programming dealing with a wide range of problems.

As applications grew more complex, methodological development of goal programming from additive aggregation of deviations sometimes masked critical trade-offs. There are many extensions of goal programming model e.g. lexicographic goal programming, integer goal programming, nonlinear goal programming, stochastic goal programming, fractional goal programming, interactive goal programming, goal programming with intervals, fuzzy goal programming, minmax goal programming, chance constrained goal programming, logarithimic goal programming. Schniederjans and Kwaks [9] have referred one of the most commonly applied types of goal programming as weighted priority goal programming. Kettani et. al. [10] have discussed a double role of weight factor in goal programming. Further, if DM wants to rank his or her goals from the most important (goal 1) to least important (goal m), then pre-emptive goal programming or lexicographic goal programming may prove to be a useful tool. Ijiri [11] is the founder of this lexicographic goal programming and it is developed by many researchers like Islam [12], Wang [13]. According to Romero [14], Tamiz and Jones [15], Tamiz and Jones [16] the weighted goal programming and lexicographic goal programming are the most popular and other methods have few known applications.

Goal attainment method helped to improve robustness, scalability for complex problems, and combination with evolutionary algorithms. This method was introduced by Gembicki and Haimes in 1970 [17] focusing on the maximum relative deviation across goals. It transforms the multi-objective challenge into a single-objective programming problem. This shift enables nuanced sensitivity analysis and delivers a single, preferred solution per weighting scheme, making it indispensable for modern multiresponse systems and paving the way for precise optimizations in fields like security-constrained flows. It minimizes the relative difference between the function and target value.

2. Goal Programming Problem based on Goal Attainment Method

A special type of nonlinear multi-objective goal programming problem with m number of minimizing objective functions, q number of inequality type constraints and n number of strictly positive decision variables is

(M 1) Find $X = (x_1, x_2 \dots x_n)^T$

so as to Minimize: $f_{10}(X) = \sum_{i=1}^{P_{10}} c_{10i} \prod_{k=1}^{n} x_k^{a_{k10i}}$ with target c_{10}

Minimize: $f_{20}(X) = \sum_{i=1}^{P_{20}} c_{20i} \prod_{k=1}^{n} x_k^{a_{k20i}}$ with target c_{20}

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Minimize: $f_{m0}(X) = \sum_{i=1}^{P_{m0}} c_{m0i} \prod_{k=1}^{n} x_k^{a_{km0i}}$ with target c_{m0}

subject to $f_r(X) = \sum_{i=1}^{P_r} c_{ri} \prod_{k=1}^{n} x_k^{a_{kri}} \le c_r$, r = 1, 2 ... q

$X = (x_1, x_2 \dots x_n)^T$, $x_k > 0$, k=1, 2 … n

where c_{j0i} are positive real numbers ∀ j, i; a_{kj0i} and a_{kri} are real numbers ∀ k, j, r, i.

P_{j0}= Number of terms present in j0 th objective function, j= 1, 2 … m

P_r = Number of terms present in r th constraint, r= 1, 2 … q

c_r = Boundary value of the r th constraint, r= 1, 2 … q

Goal attainment method is a method of transforming multi-objective goal programming into single objective one. It minimizes the relative difference between the function f_{j0} (x) and target value c_{j0}. This motivation may be under achieved or over achieved. This situation is tackled using a vector of weighting coefficients $w = \{w_1, w_2 \dots w_m\}$. Most of the papers on goal attainment method are handled by simulated annealing technique. Hota et. al. [18], Basu [19], Chen [20], Liu et. al. [21] are those researchers who have worked on goal attainment method. This section describes goal attainment method to solve nonlinear goal programming. The multi-objective programming can be written in goal attainment problem as (Ghosh, Roy, 2015 [22])

(M 2) Minimize λ

subject to $f_{j0}(X) - W_j\lambda \leq c_{j0}$, j = 1, 2 … m

$f_r(X) \leq c_r$, r = 1, 2 …q

$X = (x_1, x_2 \dots x_n)^T$, $x_k > 0$, k = 1, 2 … n,

$\lambda > 0$, $W_j > 0$; j = 1, 2 … m, $\sum_{j=1}^{m} W_j = 1$.

The slack variable $W_j\lambda$ enforces the function to achieve the target. It doesn't mean λ may be any big value such that $f_{j0}(X) - w_j\lambda$ satisfy the target c_{j0}. An objective is set such that for a minimum of λ, $f_{j0}(X) - W_j\lambda$ satisfy the target c_{j0}.

3. An application of goal attainment method on optimal design of two bar truss

A symmetric two bar truss is subjected to a vertical load 2P and is to be designed for minimum weight. The members have a tubular section with mean diameter d and wall thickness t and the maximum permissible stress in each member (σ_0) is equal to 60,000 psi. The truss consists of two tubes pinned together at one end and supported on the ground at the other. The span of the truss is fixed at 2b. Decision maker has decided target value of weight is 3 lb. Also to avoid over-stressing, he sets the target value of ratio between actual stress and maximum permissible stress as one.

Formulate the above goal programming problem and determine the values of mean diameter d and height h for the following data: P = 33,000 lb, t = 0.1 in. b = 30 in. σ_0 = 60,000 psi, density ρ = 0.3 lb/in^3.

Weight of two bar truss is $2\rho\pi\, d\, t\sqrt{b^2 + h^2}$ i.e. $0.188d\sqrt{900 + h^2}$

Stress on each member is calculated as $(\sigma) = \frac{P\sqrt{b^2+h^2}}{\pi d\, t\, h} = \frac{33{,}000\sqrt{900+h^2}}{\pi d\, h \times 0.1}$

Let us assume $\sqrt{900 + h^2} = y$, or $y^2 = 900 + h^2$.

Hence the new constraint is $\frac{900+h^2}{y^2} \leq 1$.

Therefore according to the first goal of decision maker, the target value of weight 0.188 yd is 3 and the target value of second goal $\frac{\sigma}{\sigma_0} = \frac{33{,}000\ \mathrm{y}}{\pi \mathrm{d\ h} \times 0.1 \times 60{,}000}$ is 1.

Therefore the multi objective nonlinear programming problem is

(M 3) Minimize $f_1(y, d, h) = 0.188\ yd$ with target value 3

Minimize $f_2(y, d, h) = 1.75\ y\ d^{-1}h^{-1}$ with target value 1

subject to $900\ y^{-2} + h^2y^{-2} \leq 1$,

y, d, h>0.

This is a non-linear goal programming model. Following section 2 the above model can be converted into goal programming model as

(M 4) Minimize λ

subject to $0.188\ yd - w_1\lambda \leq 3$,

$1.75\ y\ d^{-1}h^{-1}$- $0.188\ yd - w_2\lambda \leq 1$,

$900\ y^{-2} + h^2y^{-2} \leq 1$,

y, d, h, W_1, W_2, $\lambda > 0$,

$W_1 + W_2 = 1$.

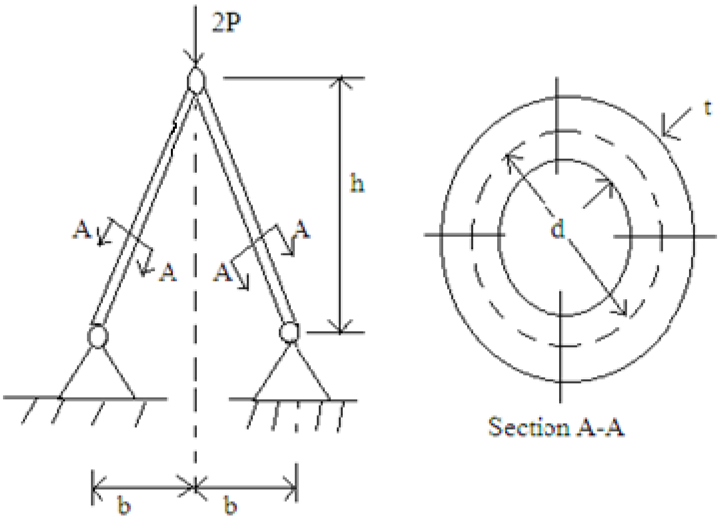

Figure 1: Two bar truss design with cross-section of one member

This single objective goal programming problem is solved using Sequential Least Squares Quadratic Programming (SLSQP) method with python code. Ghosh, Roy [23] used this example to discuss weighted additive method of goal geometric programming. To compare the results with the existing one and the goal attainment method, equal priority for each objective function is taken here although decision maker can set his priority on goals. Then the variation in priority (weight) is applicable on it.

Table 1: List of values of decision variables and objective functions of two bar truss design

		Weighted additive method		**Goal attainment method**	
$\mathbf{W_1}$	$\mathbf{W_2}$	**Optimal Primal variables**	**1st objective ($f_1^*(y, d, h)$) 2nd objective ($f_2^*(y, d, h)$)**	**Optimal Primal variables**	**1st objective ($f_1^*(y, d, h)$) 2nd objective ($f_2^*(y, d, h)$)**
0.5	0.5	$y^* = 42.42641$, $d^* = 0.5569888$ in. $h^* = 30$ in. $d_1^{+*} = 1.442634$, $d_2^{+*} = 3.442634$.	4.442634 lb 4.44331	$y^* = 42.426407$, $d^* = 0.69634$ in. $h^* = 30$ in. $\lambda^* = 5.108238$	5.554119 lb 3.554119

It is seen that in both the methods optimal values of the decision variables are almost same. The positive values of deviation variables in weighted additive method and the positive value of λ in goal attainment method are causing a little exceeding optimal value of each objective function from its target. However, the constraints of (M 4) are true for the above mentioned optimal values of decision variables and deviation. Also, it is to be noted that optimal values of all objective functions are near to the set target. For all combinations of weights, there will be slight variations on optimal values. DM can change the weights according to his priority on goals and find the optimal objective values accordingly.

Conclusion

The Goal Attainment Method is a mathematical procedure that helps to convert multi-objective programming to single objective programming problem like other existing weighted additive, weighted multiplicative method. It offers distinct advantages over the weighted sum method in multi-objective optimization, particularly for nonlinear goal programming problems. It provides a more flexible scalarization approach tailored to target deviations. Moreover, goal attainment method explores solutions geometrically from a target point using relative deviations which ensures broader coverage of the efficient frontier. Apart from the discussed example in this paper, this method is eligible to solve any other linear or nonlinear goal programming problem.

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NOVEL 3-CHLOROPHENYL THIAZOLE THIOSEMICARBAZONES: SYNTHESIS, STRUCTURAL PROPERTIES, AND SWISSADME PREDICTION

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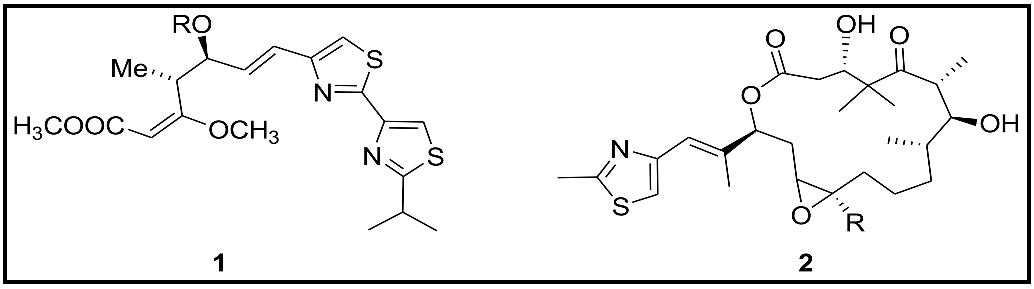
Introduction

Novel bioactive heterocycles remain a priority in medicinal chemistry, with thiazole and thiosemicarbazone scaffolds serving as "privileged structures." In this study, we report the design and synthesis of a series of novel thiosemicarbazone derivatives incorporating a 3-chlorophenyl thiazole moiety to explore their potential as drug-like candidates. The target compounds were synthesized via the Hantzsch thiazole cyclization of 3-chlorophenacyl bromide with various substituted thiosemicarbazides. The chemical structures of the synthesized derivatives were rigorously characterized using FT-IR, 1H NMR, and 13C NMR spectroscopy. To evaluate their pharmacokinetic viability, an in-silico study was conducted using the SwissADME web tool to predict physicochemical properties, lipophilicity, and oral bioavailability.

Thiazole

Thioamides are the building blocks in the Hantzsch thiazole[1] and amidines[2] synthesis. The chemistry of thiazole containing heterocyclic compounds continues to draw the attention of synthetic organic chemists due to their varied biological activities,[3] such as antibacterial, antitubercular, anti-cancer, antifungal and anti-inflammatory activities. Sakagami and co-workers reported the isolation of six secondary metabolites, designed cyst thiazoles A-F, 1 (Figure 1) as a series of new antibiotics from the myxobacterium culture broth of *Cystobacter fuscus*.[4] These bis-thiazoles has demonstrated potent antifungal activity against the phytopathogenic fungus *Phytopathora capsici* and has shown activity against a broad range of additional fungi with no effect on bacterial growth. Nicolaou K. C. and co-workers[5] have reported chemical biology of epothiolones[6] 2 (Figure 1), thiazole containing an antitumor agent. Thiazole nucleus is also important in organic synthesis as it acts as a formyl group equivalent. [7]



1 2

Figure 1

A wide range of substituted thiazole derivatives,[8-12] can be obtained in the reactions of thioamides derived from aliphatic, aromatic, and heterocyclic acids with appropriately functionalized carbonyl compounds. Kulkarni K. S. and co-workers[13] have synthesized substituted thiazolyl thiocarbanilides (**3-7**), (Figure 2) and reported for antitubercular activity.

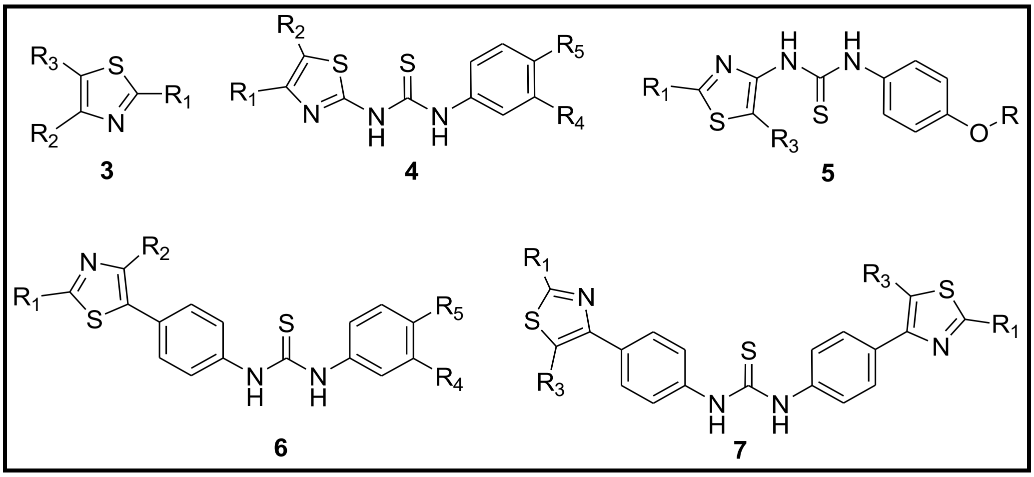


Figure 2

2-substituted-anilino/phenyl/benzyl-5-substituted-4-phenylamide-(3-(2-chlorophenyl)-5-methylisoxazolyl)thiazoles and reported them as potential antitubercular and antimicrobial agents[14]. Ohkubo M. and co-workers[15] have reported synthesis and anti-anoxic activity of ethyl 4-(3/4-nitrophenyl)-2-phenyl-5-thiazolecarboxylate derivatives.

Bell, F.W. and co-workers[16] have reported synthesis and basic structure activity relationship studies of phenethylthiazolethiourea compounds 8. (Figure 3). The synthesized compounds were screened for HIV-1reverse transcriptase inhibitors activity.

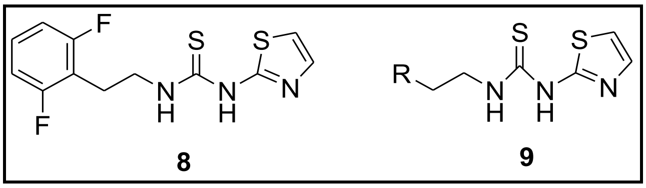
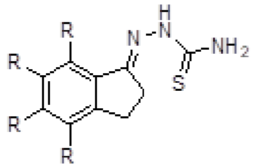


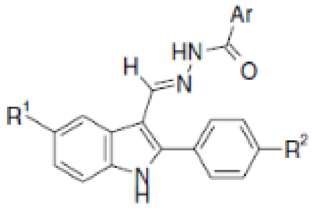
Figure 3

Thiosemicarbazone

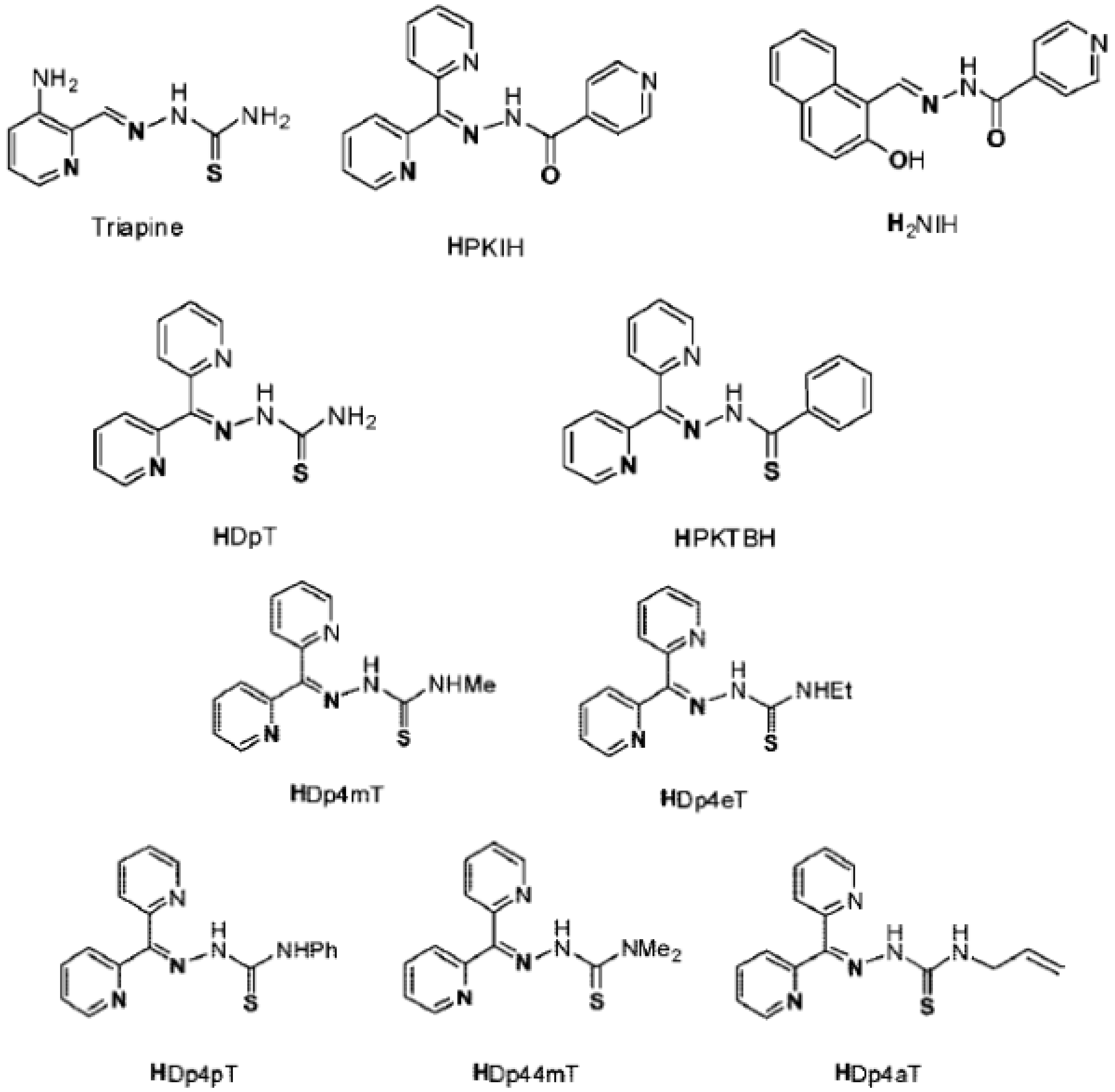
Biological properties of thiosemicarbazone derivatives have been studied since 1946[17], when their activity against Mycobacterium tuberculosis was reported. Since then, this and other biological properties of thiosemicarbazone derivatives such as antibacterial[18], antitumoral[19], antiprotozoal[20] and cytotoxic activity[21] have been described. In 1950, Hamre et al.[22] found that thiosemicarbazone derivatives from several benzaldehydes were active against neurovaccinial infection in mice when given orally.



1-indanone thiosemicarbazone derivatives
active against BVDV
European Journal of Medicinal Chemistry 43 (2008) 1767e1773



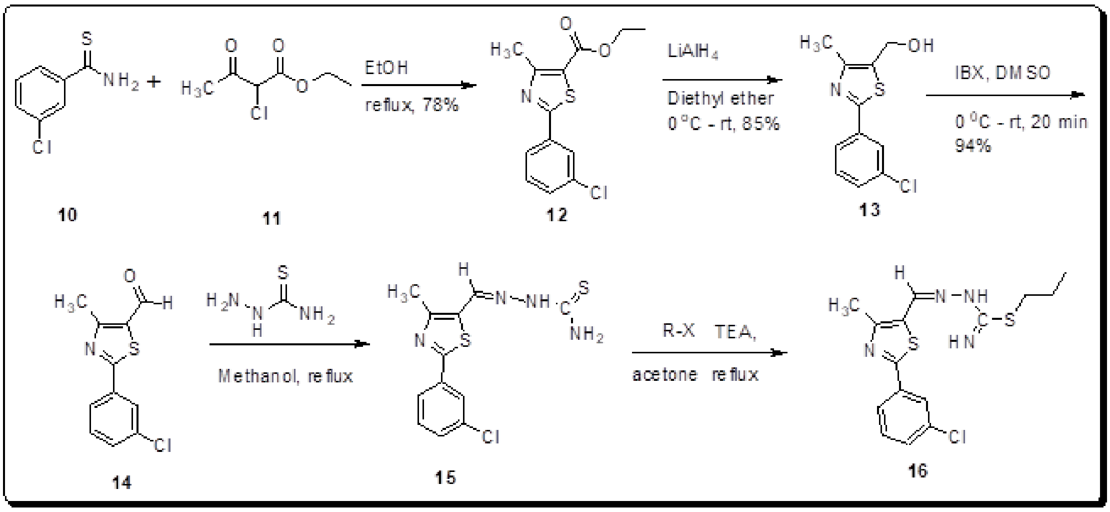
Aroyl hydrazones of 2-phenylindole-3-carbaldehydes
antimitotic agents
Bioorganic & Medicinal Chemistry 16 (2008) 6436–6447



Iron Chelators of the Dipyridylketone Thiosemicarbazone
Anticancer Activity
J. Med. Chem. **2009**, 52, 407–415

Present work

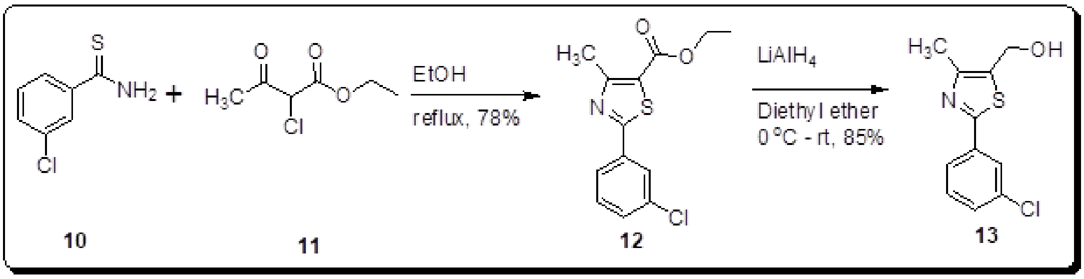
In view of these observations and an ongoing programme on the synthesis of thiazole containing heterocyclic compounds, it was thought to synthesize thiazoles,
thiosemicarbzone derivatives. (Scheme 1)



Scheme 1

In the present work Ethyl 2-(3-chorophenyl)-4-methylthiazole-5-carboxylate, 12 was synthesized by cyclo-condensation of 3-chlorothiobenzamide, 10 with Ethyl-2-choro-3-oxobutanoate 11. Ester 12 was further reduced by using lithium aluminum hydride in dry diethyl ether to corresponding alcohol 13. The alcohol 13 was selectively oxidized to aldehyde 14. Aldehyde 14 was subjected to condensation reaction with semicarbazide furnished Schiff's base. Then Schiff's base on S-alkylation reaction with alkyl halide gave 1((2-(3-chlorophenyl)-4-methylthiazol-5-yl)methyleneamino)-2-propylisothiourea

Result and Discussion

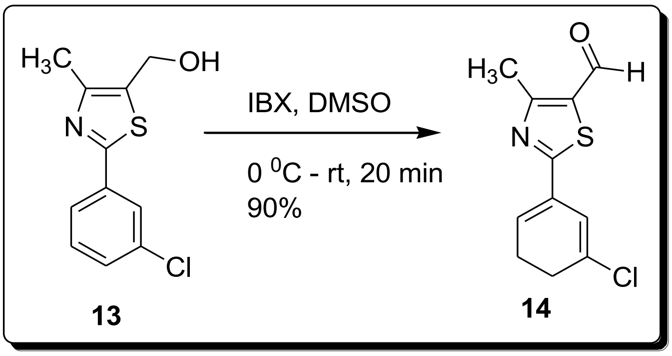


Scheme 2

The IR spectrum of ester **12** showed absorption peak at 1728 cm^{-1} indicating the presence of ester carbonyl. The ^{1}H NMR of **12** showed the triplet at δ 1.40 for –CH$_3$ protons and quartet at δ 4.38 for –CH$_2$ confirmed the ester functions, a singlet at δ 2.80 integrated for three hydrogen corresponds for thiazole –CH$_3$ protons and the four aromatic protons are resonated at δ 7.39 (m , 2H); 7.82 (d, 1H); 7.98 (s, 1H), the LCMS spectrum of **12** showed the *m/z* peak at 281.72 (M+H)$^+$, which confirms its structure.

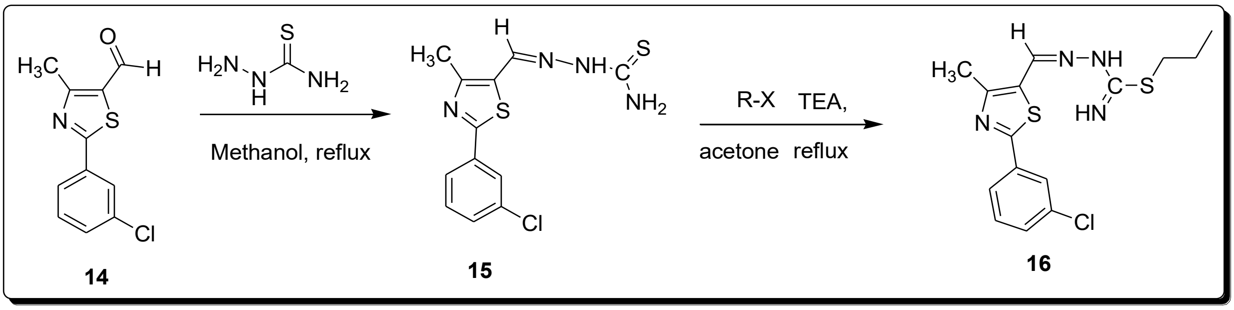
The reduction of ester **12** to (4-methyl-2-(3-chlorophenyl)thiazole-5-yl)methanol **13** was achieved by using lithium aluminium hydride in dry diethyl ether in 85 % yield. The structure of alcohol was confirmed by the spectral data. IR spectrum showed a strong absorption at 3290 cm^{-1} signifying the presence of the hydroxyl group with absence of absorption in the C=O region. The ^1H NMR spectrum of **13** revealed absence of quartet and the triplet corresponding to carboethoxy group as well as appearance of a singlet at δ 4.82 integrating for two protons ascribed to the –CH_2OH proton. Apart from this, the spectrum also revealed a peak corresponding to the three methyl protons at δ 2.42 and the aromatic protons appeared at δ 7.26 to 7.80 integrated for four aromatic protons. The mass spectrum of **13** showed the *m/z* peak at 239.5 $(M+H)^+$ which further confirms its structure.

Literature revealed the selective oxidation of the alcohol function into aldehyde[23] in (4-methyl-2-phenylthiazole-5-yl)methanol was achieved using transition metal oxidising agents. Accordingly the alcohol was selectively oxidized to aldehyde in 65 % using MnO_2. It was observed that when the alcohol **13** was treated with IBX in DMSO at 0 °C to room temperature furnished aldehyde **14** in 90 % yield within 20 minutes of reaction time (**Scheme 3**). The formation of 4-methyl-2-(3-chlorophenyl)thiazole-5-carbaldehyde **14** was confirmed by its spectral studies.



Scheme 3

The IR spectrum of **14** displayed the absorption bands at 2847, 2735 cm^{-1} and 1690 cm^{-1} due to stretching frequency of aldehyde C-H and C=O functional groups. ^1H NMR spectrum of **14** showed the singlet at δ 2.79 integrating for three protons are assigned for methyl group, four aromatic protons are appeared at δ 7.43 (m, 2H); 7.83 (d, 1H); 8.02 (s, 1H). The aldehyde proton resonated at δ 10.11. The ^{13}C NMR of aldehyde showed one signal at δ 18.8 corresponds to methyl group of thiazole ring. The phenyl and thiazole ring carbons are appeared at δ125.24, 127.0, 130.0 131.0, 133, 134, 135.0, 162.0 and 171.0, while a peak at δ 182.0 was attributed to the C=O of aldehyde group. Further the structure was confirmed by HRMS spectrum which showed the *m/z* peak at 270.0360 $(M+MeOH + H)^+$.



Scheme 4

The thiosemicarbazide was subjected to the condensation reaction with 4-methyl-2-(3-chlorophenyl)thiazole-5-carbaldehyde **14** using glacial acetic acid as catalyst in dry methanol afforded the thiosemicarbazone in 74 to 84 % yield. The thiosemicarbazone on nucleophilic substitution reaction with propyl bromide gave 1((2-(3-chlorophenyl)-4-methylthiazol-5-yl)methyleneamino)-2-propylisothiourea.

The IR spectrum of compound **16** showed absence of characteristic absorption peaks at 2550 cm^{-1} (S-H) indicated the formation of S-alkylation, which was further confirmed by its ^{1}H NMR data. The ^{1}H NMR spectrum of **16** displayed a peaks at δ 1.06 (t, 3H); 1.83 (m, 2H); 3.04 (t, 2H) confirms the presence of S-propyl group. The singlet at δ 2.56 integrated for three protons corresponds to three protons of methyl group. The aromatic protons are resonated at δ 7.39 to 8.51. Two -NH protons are showed bs at δ 5.5. The ^{13}C NMR of 16 Showed peaks at 13.4, 15.8, 22.9, 32.0, 124.5, 126.5, 130.2, 135.0, 141.1, 145.4, 155.1, 156.6, 162.1, 163.2, 165.7, 167.8, 174.0. The structure was further confirmed by LCMS spectrum which showed $(M + H)^+$ at 352.95 and 353.0 corresponds to 80% and 20 % E and Z isomers respectively.

Experimental

Ethyl-2-(3-chlorophenyl)-4-methylthiazole-5-carboxylate

Mixture of 2-choro-3-oxoethylbutanoate 13 (6.0 g; 0.037 mol) and 3-chlorothiobenzamide, 12 (5.0 g ; 0.037 mol) in ethanol (50 mL) was refluxed for 8 hours . After completion of the reaction (TLC), half of the solvent was distilled off and reaction mass cooled to room temperature . The product was filtered, washed with water and recrystallised from ethanol, yield 8.0 g (90 %).

MF: $C_{13}H_{12}NO_2SCl$

IR: 1728 cm^{-1}

1H NMR: 1.40 (t, 3H) ; 2.80(s, 3H); 4.38 (q , 2H); 7.39 (m , 2H); 7.82 (d, 1H);
7.98 (s, 1H)

LCMS: 281.76 $(M+H)^+$

(2-(3-chlorophenyl)-4-methylthiazol-5-yl)methanol

To a ice cold solution lithium aluminium hydride (2.3 g; 0.060 mol) in 50 mL dry diethyl ether, ethyl 2-(3-chorophenyl)-4-methylthiazole-5-carboxylate , 14 (7.5 g; 0.030 mol) was added dropwise over a period of 30 minutes and the mixture was further stirred for 1 hour at 0 ◦C . After completion of the reaction (TLC), the reaction mixture was quenched by saturated solution of sodium sulphate. The reaction mixture was filtered on sintered funnel. The aqueous was extracted with diethyl ether (2 x 30 mL), the combined organic layer was washed with water, then brine and dried over sodium sulphate. Solvent was removed by distillation furnished (2-(3-chlophenyl)-4-methylthiazol-5-yl)methanol, 5.40 g (87 %).

MF:$C_{11}H_{10}NOSCl$

IR: 3290 cm^{-1}

1H NMR : 2.42 (s , 3H) ; 4.80 (s, 2H) ; 7.39 (m , 2H) ; 7.82 (d, 1H) ; 7.98 (s, 1H).

LCMS : 239.72 $(M+H)^+$

(2-(3-chlorophenyl)-4-methylthiazol-5-yl) carbaldehyde

To a solution of (2-(3-chlorophenyl)-4-methylthiazol-5-yl)methanol, (5.0g , 0.020 mol) in DMSO 30 mL, IBX (6.3g , 0.023 mol) was added at 0 °C and the reaction mixture was stirred at 0 °C to room temperature. The progress of reaction was monitored on TLC. After completion of the reaction (20 minutes), water 90 mL was added in reaction mixture and extracted with diethyl ether (3 x 40 mL). The organic layer was washed with water, brine and dried over sodium sulphate. The solvent was distilled to afford white solid, 4.96g in 94% yield.

MF: $C_{12}H_{11}N_4S_2Cl$

IR : 2735, 2847 , 1690 cm^{-1}

^{1}H NMR: 2.79 (s , 3H) ; 7.43 (m , 2H) ; 7.83 (d , 1H, J=8Hz) ; 8.02 (s , 1H) ; 10.11 (s 1H)

^{13}CNMR: (CDCl3): 18.8, 125.24, 127.0, 130.0, 131.0,133.0,134.0, 135.0, 162.0,171.0,182.0

MASS : 237.71 $(M+H)^+$

1-((2-(3-chlorophenyl)-4-methylthiazol-5-yl)methylene) thiosemicarbazide

To a solution of with (2-(3-chlorophenyl)-4-methylthiazol-5-yl) carbaldehyde **17** (1.0 g; 0.005) thiasemicarbazide (30 mL), methanol (0.75 g, 0.006 mol) was added. The reaction mixture was allowed to stand & warmed on waterbath, cooled in ice water . the reaction was monitored by TLC, After completion of reaction, the product was filtered washed with cold water & recrystllised from methanol . The yield as (1.20g , 92%)

MF: $C_{12}H_{11}N_4S_2Cl$

IR :

^{1}H NMR:

LCMS: 310 $(M+H)^+$

1-((2-(3-chlorophenyl)-4-methylthiazol-5-yl)methyleneamino)-2propylisothiourea

To a solution 1-((2-(chlorophenyl)-4-methylthiazol-5-yl)methylene)thiosemicarbazide, Schiff's base (0.170g; 0.000584 mol) in dry acetone (20 mL), propyl bromide (0.080g; 0.000657 mol) was added and the reaction mixture was refluxed for 2-3 hours (TLC). After completion of reaction mixture cooled in ice water , product crystalised as white solid.The yield as o.150 g (77 %).

MF: $C_{15}H_{17}N_4S_2Cl$

IR: 3392 , 3093, 1593, 1516 cm^{-1}

NMR: 1.06 (t, 3H) ; 1.83 (m, 2H) ; 2.56 (s, 2H) ; 3.04 (t , 2H) ; 5.51 (s ,1H) ; 5.68 (s , 1H) ; 7.39 (m , 2H) ; 7.80 (d , 1H) ; 7.95 (d , 1H) ; 8.51 (s , 1H) .

LCMS: 352.91 $(M+H)^+$

SwissADME Data Table: 3-chlorophenyl thiazole thiosemicarbazone derivatives

Compound ID	**Mol. Weight (g/mol)**	**Log $P_{o/w}$ (Consensus)**	**TPSA (Å²)**	**GI Absorption**	**BBB Permeant**	**Lipinski Violations**
3-Cl-T1	331.82	3.12	88.45	high	No	0
3-Cl-T2	345.85	3.45	88.45	high	No	0
3-Cl-T3	375.87	3.20	97.68	high	No	0
3-Cl-T4	410.32	4.02	88.45	high	No	0

Synthesis of the 3-chlorophenyl thiazole series was achieved with high purity and moderate-to-excellent yields (**75–90%**). Structural analysis confirmed the successful formation of the thiazole ring and the (E)-geometry of the thiosemicarbazone linkage. SwissADME profiling revealed that all derivatives adhere strictly to Lipinski's Rule of Five with zero violations. The BOILED-Egg model predicted high gastrointestinal absorption for all compounds, while the 3-chloro substitution successfully optimised the lipophilicity (Log P approx. 3.12–4.02) compared to unsubstituted analogues. Furthermore, the compounds exhibited a favourable Synthetic Accessibility (SA) score, averaging 2.95.

Conclusion

The integration of the 3-chlorophenyl group into the thiazole-thiosemicarbazone framework yielded molecules with excellent "drug-like" characteristics and predictable pharmacokinetic profiles. These findings suggest that the synthesized derivatives are promising leads for further in vitro biological screening and lead optimization in drug discovery.

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NANOMATERIAL BASED PHOTOCATALYST FOR WATER TREATMENT AND CLEAN ENERGY

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Abstract

The increasing scarcity of clean water and the growing global demand for sustainable energy have emerged as critical challenges due to population growth, climate change, industrialization, and environmental pollution. Conventional water treatment and energy production technologies often suffer from high operational costs, limited efficiency, and secondary pollution. Nanotechnology and photocatalytic processes have gained significant attention as environmentally friendly and cost-effective solutions to these global issues. This work reviews recent advancements in nanomaterial-based technologies for water and wastewater treatment, with particular emphasis on photocatalytic mechanisms and applications. Various nanomaterials, including metal oxide nanoparticles, graphene-based materials, carbon nanotubes, and two-dimensional materials, are discussed for their roles in pollutant degradation, water purification, and hydrogen generation through photocatalytic water splitting. The fundamental mechanisms of photocatalysis, including oxidation and reduction pathways, along with factors affecting photocatalytic efficiency such as band gap energy, surface area, pH, temperature, light intensity, and catalyst loading, are critically examined. The study highlights the potential of nanotechnology-driven photocatalytic systems to address water pollution and energy shortages, offering sustainable pathways for environmental remediation and clean energy production.

Keywords: Water Treatment, Photocatalyst, Nanotechnology, Nanomaterials, Clean Energy Production.

1. Introduction

Ensuring affordable and reliable access to clean water for a rapidly growing global population represents one of the most critical challenges worldwide. Population growth, climate change, and escalating water pollution have significantly strained existing water supply systems [1]. According to World Health Organization projections published in 2014, nearly 50% of the global population is expected to experience water scarcity by 2025. Despite this growing demand, only about 20% of global wastewater was adequately treated as of 2015. Furthermore, a United Nations report in 2016 revealed that nearly 70% of industrial wastewater in developing countries is discharged into the environment without sufficient treatment. Contaminants such as pathogens, organic compounds, heavy metals, industrial effluents, and various inorganic ions persist in water bodies due to their resistance to natural degradation, thereby altering water quality and posing serious environmental and health risks [2].

Therefore, the urgent global need is for clean air, safe drinking water, and sustainable energy resources. Photocatalytic technology has demonstrated promising results in addressing these challenges by offering green, low-cost, and environmentally friendly solutions. In the energy sector, photocatalysis enables clean hydrogen production, while in environmental remediation it provides effective methods for water and air purification [2].

A wide range of nanomaterials including polymer-based nanomaterials, carbon nanotubes, nano-zeolites, graphene, graphene oxide (GO), graphene quantum dots, and metallic nanoparticles have been developed for water purification applications [3-5]. These nanomaterials are effective in removing pathogens, metal oxides, toxic metal ions, and organic and inorganic solutes from surface water, groundwater, effluents, and natural water sources. Treatment techniques such as nanofiber filtration, nanofiltration membranes, reverse osmosis, carbon nanotube-based systems, and ultrafiltration have shown considerable promise [6].

Nanotechnology has emerged as a powerful solution to current challenges in water treatment [7, 8]. It enables efficient utilization of unconventional water resources and introduces innovative enhancements to conventional treatment methods. Its major roles in water treatment include pollutant remediation, water purification, real-time pollution monitoring using nanosensors, and pollution prevention. Significant progress has been achieved through molecular-level understanding of pollutants, which has facilitated the effective use of nanoparticles for water filtration.

Nanochemistry-driven treatment technologies are generally more efficient and economical than traditional purification methods. These approaches include the fabrication of advanced membranes and the use of mixed metal oxides, zeolites, bimetallic nanoparticles, and carbon-based nanocatalysts for pollutant degradation. Additionally, nano-zero-valent metals and magnetically responsive nanoparticles have been widely applied as nanosorbents for water remediation. This work focuses on recent developments in nanotechnology-assisted water treatment, emphasizing the role of various nanomaterials [9]. Due to their high surface-to-volume ratios, nanomaterials interact effectively with microorganisms and contaminants, thereby enhancing treatment efficiency [10]. Nanomaterials typically possess dimensions below 100 nm and exhibit significantly altered properties, offering extensive opportunities for sustainable water treatment solutions [11, 12].

1.1 Wastewater Treatment

Nanomaterials are defined as materials with at least one dimension below 100 nm. At this scale, materials exhibit unique size-dependent properties that make them highly suitable for water and wastewater remediation. Their uniform size distribution, large specific surface area, high reactivity, and rapid dissolution enhance processes such as adsorption and catalytic degradation. In addition, special characteristics such as surface plasmon resonance, superparamagnetism, and quantum confinement further expand their functional applications. The following sections discuss the role of nanomaterials in specific treatment processes [2].

1.2 Catalytic Wet Air Oxidation

The design of highly selective nanocatalysts with optimally arranged metal atoms and active sites remains challenging. However, organic functional polymers offer flexibility in tailoring nanocatalyst composition, enabling improved activity, selectivity, and stability. Platinum, palladium, and ruthenium nanoparticles embedded within hyper-crosslinked polystyrene matrices have demonstrated excellent catalytic performance in the catalytic wet air oxidation (CWAO) of phenolic compounds. High phenol conversion efficiencies have been achieved using platinum-loaded polymeric catalysts [13]. Compared to thermal incineration, platinum-based CWAO systems provide efficient oxidation at relatively low temperatures, particularly in bubble column reactors [14]. Due to its ability to completely oxidize toxic pollutants into harmless end products such as CO_2, H_2O, and N_2, CWAO has gained significant attention for industrial wastewater treatment [15].

1.3 Water Purification Using Two-Dimensional Graphene

Two-dimensional graphene-based materials—including pristine graphene, graphene oxide, and reduced graphene oxide—have emerged as critical nanomaterials for water purification [60]. These materials exhibit excellent adsorption capacity, antifouling behavior, and photocatalytic activity. Graphene membranes, owing to their atomically thin structure, often outperform conventional polyamide membranes in filtration efficiency [16,17]. Considerable research interest has focused on graphene-based desalination technologies [18–20], as these materials effectively remove salts due to their strong affinity for sodium ions [21]. Surface functionalization with nitrogen or hydrogen allows selective ion transport. While several studies report antimicrobial activity of graphene-based materials against microorganisms such as *E. coli*, *S. aureus*, *S. mutans*, and *Pseudomonas aeruginosa*, some reports indicate variability and debate regarding these antibacterial effects [22–24].

1.4 Photocatalysis

One of the major limitations of conventional water treatment technologies is their inability to remove non-biodegradable organic pollutants and waterborne viruses without generating harmful disinfection by-products. Consequently, there is a growing demand for cost-effective, environmentally friendly systems capable of eliminating these contaminants with minimal energy and chemical inputs. Advanced oxidation processes (AOPs) have emerged as reliable alternatives due to their ability to generate highly reactive oxidizing radicals [25,26].

Photocatalysis, a widely studied AOP, enhances the biodegradability of persistent pollutants and effectively inactivates emerging microbial pathogens. Photocatalytic oxidation involves light-activated catalysts that generate reactive species such as hydroxyl radicals, superoxide ions, ozone, and hydrogen peroxide, which non-selectively oxidize contaminants [27]. Techniques involving UV irradiation, solar light exposure, and combinations with oxidants such as H_2O_2 and O_3 have been extensively investigated [28–29]. Both homogeneous (photo-Fenton) and heterogeneous photocatalysis are considered effective, although heterogeneous systems are generally preferred due to simpler operation and lower cost [30].

1.5 Titanium Dioxide Nanoparticles for Water Purification

Photocatalysis using semiconductor nanoparticles is considered a promising oxidation technique for water treatment. Among various photocatalysts, titanium dioxide (TiO_2) nanoparticles are the most widely used due to their high photocatalytic activity, chemical stability, non-toxicity, and affordability. TiO_2 effectively degrades organic pollutants and dyes by breaking molecular bonds under UV or solar irradiation, leading to complete mineralization into CO_2 and H_2O.

TiO_2 nanoparticles synthesized via the sol-gel method and calcined at temperatures of 400 °C and 700 °C have demonstrated strong photocatalytic performance. Heat-treated TiO_2 nanoparticles, particularly those calcined at 700 °C, showed enhanced degradation efficiency for methyl orange under UV irradiation. Observable color changes during treatment further confirmed the photocatalytic degradation process. These findings indicate that heterogeneous TiO_2-based photocatalysis is an effective approach for removing azo dyes from wastewater [31].

1.6 General Mechanism of Photocatalytic Reactions

In photocatalysis, the reaction rate primarily depends on the catalyst's crystal structure and the energy of the incident light. Semiconductor materials act as photosensitizers, facilitating light-induced redox reactions based on their electronic band structure. When the energy of incoming photons equals or exceeds the band gap of the catalyst, electrons are excited from the valence band to the conduction band, leaving behind holes. These charge carriers drive oxidation and reduction reactions: holes oxidize donor molecules and generate hydroxyl radicals from water, while conduction-band electrons reduce oxygen to form superoxide radicals. Together, these processes enable the conversion of pollutants or water molecules into desired products [32].

1.7 Oxidation and Reduction Mechanisms

Upon light irradiation, electron–hole pairs are generated in the photocatalyst. The holes oxidize water molecules to produce hydroxyl radicals, which possess strong oxidizing ability and decompose organic pollutants. In the presence of oxygen, further chain reactions occur, ultimately mineralizing pollutants into carbon dioxide and water [32].

Reduction reactions primarily involve atmospheric oxygen, which readily accepts electrons from the conduction band to form superoxide radicals. These species may further react to form peroxides and eventually water. In systems containing high concentrations of organic matter, photocatalytic activity is enhanced due to reduced electron–hole recombination, improving overall efficiency [32].

2. Applications of Photocatalysis

2.1 Hydrogen Production via Water Splitting

Photocatalysis offers a sustainable method for hydrogen generation, producing clean energy without harmful by-products. Although water splitting using TiO_2 was first demonstrated in 1972, it gained widespread attention only after global energy crises highlighted the limitations of fossil fuels. Photocatalytic hydrogen production operates under solar irradiation, requires low energy input, and offers long-term sustainability, making it a promising alternative energy source for the 21st century.

Hydrogen generation depends on semiconductor photocatalysts such as TiO_2, ZnO, and Ag_2O. When photons excite the catalyst, electron–hole pairs are generated. For efficient hydrogen evolution, the conduction band must be sufficiently negative relative to the hydrogen reduction potential, while the valence band must be positive enough to oxidize water [32].

2.2 Wastewater Treatment

Although nearly two-thirds of the Earth’s surface is covered by water—amounting to approximately 330 million cubic miles—only a very small fraction is suitable for human use. Merely 3% of the planet’s water is freshwater, of which only about 1% is readily available as surface water, while the remainder is trapped in glaciers or underground reservoirs. As a result, access to clean drinking water remains a major global concern, with nearly one in six people lacking safe potable water. The global population continues to grow rapidly, increasing by approximately 83 million people annually, and it was estimated to reach 7.9 billion by 2020 [33].

Water pollution poses severe health risks worldwide. According to the World Health Organization (WHO), diarrheal diseases largely caused by contaminated water—ranked as the second leading cause of death in 2019, while cholera alone accounts for approximately 95,000 deaths each year [34]. In addition, nearly two billion people still lack access to basic sanitation facilities, and about one-quarter of healthcare institutions suffer from inadequate water services. If current trends persist, nearly half of the world’s population is expected to live in water-stressed regions by 2025 [35].

These statistics highlight that water pollution, water scarcity, and the need for effective purification technologies represent some of the most pressing global challenges today. The situation is particularly critical in developing countries such as Pakistan, India, and Bangladesh, where rapid population growth, limited resources, and ongoing energy crises further intensify the importance of water purification [36].

Several conventional water treatment techniques—such as chemical transformation, distillation, biological treatment, reverse osmosis, coagulation–flocculation, microfiltration, ultraviolet treatment, and ultrafiltration—are currently employed [37, 38]. However, each of these methods has inherent limitations, and none can independently ensure complete contaminant removal or provide universally safe drinking water. Moreover, many of these approaches are energy-intensive and costly, making them unsuitable for widespread application in developing regions.

In the context of the current global crisis, advanced water purification technologies are therefore critically needed. Nanomaterials used as photocatalysts have demonstrated promising, environmentally friendly outcomes. Photocatalysis is a green wastewater treatment technique that operates under light irradiation in the presence of an appropriate catalyst to degrade pollutants. The process involves light-induced excitation using ultraviolet, visible, or infrared radiation—depending on the catalyst's band structure—which generates electron–hole pairs. These charge carriers produce highly reactive oxidizing and reducing radicals at the valence and conduction bands, respectively, which subsequently react with organic or inorganic contaminants and degrade them through secondary reactions. Semiconductor nanoparticles are particularly suitable photocatalysts for wastewater treatment due to their wide band gaps and activity in the visible light region. The primary focus of current research is the development of low-cost, energy-efficient systems using visible-light-responsive catalysts.

2. 3 Factors Affecting Photocatalytic Wastewater Treatment

2.3.1 Electron–Hole Pair Separation

One of the most critical factors influencing photocatalytic efficiency is the separation rate of electron–hole pairs. In semiconductor catalysts, these charge carriers have very short lifetimes and tend to recombine rapidly. For effective photocatalysis, it is essential that electrons and holes participate in secondary redox reactions before recombination occurs. For instance, in TiO_2, valence-band holes act as strong oxidizing agents, while conduction-band electrons function as effective reducing agents, with redox potentials of approximately 1.0–3.5 V and 0.5–1.5 V, respectively, relative to the normal hydrogen electrode [39]. An ideal photocatalyst should therefore possess a wide band gap and a low recombination rate.

2.3.2 Catalyst Structure

The photocatalytic performance is strongly dependent on the structural characteristics of the catalyst. Titanium dioxide exists in three crystalline phases rutile, brookite, and anatase—among which anatase exhibits superior photocatalytic activity due to its stable structure, higher adsorption capacity, and favorable conduction-band position. Catalyst morphology also plays a crucial role; for example, spherical ZnO nanoparticles demonstrate higher degradation efficiency than rod-shaped structures because of their larger surface area. Photocatalysts are generally more effective in nanoscale form than in bulk form, as reduced particle size increases surface-to-volume ratio and provides more active sites for reactions. Consequently, nano-TiO_2 exhibits significantly higher activity compared to bulk TiO_2 [40].

2.3.3 pH of the Solution

Solution pH significantly affects photocatalytic efficiency by altering the surface charge of the catalyst and influencing electrostatic interactions between charged pollutants and the catalyst surface. Literature reports indicate that photocatalytic efficiency is relatively low under acidic conditions ($pH < 5$) due to high proton concentration, which limits hydroxyl radical formation. In the pH range of 5–10, photocatalytic activity increases, reaching a maximum in alkaline conditions around pH 10, where hydroxyl radicals readily react with organic pollutants. However, at very high pH values (11–13), efficiency decreases due to excessive hydroxyl ion scavenging, which reduces their availability for pollutant degradation [41].

2.3.4 Catalyst Loading

Photocatalytic degradation generally increases with catalyst dosage, as higher catalyst concentrations generate more reactive radicals, thereby enhancing reaction rates. However, beyond an optimal concentration, further increases in catalyst loading hinder light penetration, leaving portions of the catalyst inactive and reducing overall efficiency [42].

2.3.5 Temperature

Temperature also influences photocatalytic reaction rates. Studies have shown that for TiO_2-based systems, photocatalytic efficiency decreases at temperatures around 80 °C due to enhanced electron–hole recombination and reduced light absorption. Optimal reaction rates are typically achieved within the temperature range of 20–80 °C [43].

Conclusion

The growing challenges of water pollution, freshwater scarcity, and global energy crises demand innovative, sustainable, and environmentally friendly technological solutions. Nanotechnology-enabled photocatalytic processes have demonstrated exceptional potential in addressing these issues through efficient water purification and renewable hydrogen production. Nanomaterials, owing to their high surface-to-volume ratio, tunable band gap, and enhanced reactivity, significantly improve the efficiency of photocatalytic reactions compared to conventional bulk materials.

Photocatalysis provides a green and cost-effective approach for degrading persistent organic pollutants, eliminating pathogenic microorganisms, and mineralizing hazardous contaminants without producing harmful by-products. In addition, photocatalytic water splitting offers a promising route for clean hydrogen generation using solar energy, contributing to long-term energy sustainability. Factors such as catalyst structure, band gap engineering, surface morphology, pH, temperature, and light intensity play crucial roles in optimizing photocatalytic performance.

Despite notable progress, challenges related to catalyst stability, charge recombination, scalability, and real-world application remain. Continued research focused on material design, nanostructure optimization, and visible-light-active photocatalysts is essential to enhance efficiency and practical deployment. Overall, nanotechnology-based photocatalytic systems represent a powerful platform for addressing environmental pollution and energy demands, paving the way toward sustainable development and improved quality of life.

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MACHINE LEARNING APPROACHES FOR FAULT IDENTIFICATION IN ELECTRICAL POWER NETWORKS

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Abstract

Electrical power networks are critical infrastructures responsible for reliable energy transmission and distribution. Fault occurrence in transmission lines, transformers, and distribution systems may lead to power outages, equipment damage, and economic losses. Conventional protection techniques based on threshold settings and relay coordination often struggle to handle modern smart grids integrating renewable energy sources and distributed generation. Machine Learning (ML) has emerged as an intelligent data-driven solution capable of identifying faults rapidly and accurately. This chapter presents machine learning approaches for fault identification in electrical power networks, covering system architecture, data acquisition, feature extraction, classification algorithms, and performance evaluation methods. Recent advances including deep learning, ensemble learning, and predictive analytics for real-time fault diagnosis are also discussed. The chapter highlights challenges, practical implementation issues, and future research directions toward autonomous intelligent power networks.

Keyword: Machine Learning, Fault Identification, Power System Protection, Smart Grid, Fault Classification, Deep Learning, Predictive Maintenance.

1. Introduction

Electrical power systems consist of generation units, transmission lines, substations, and distribution networks operating continuously under dynamic environmental and loading conditions. Faults such as short circuits, line-to-ground faults, and equipment failures significantly affect system stability.

Traditional protection schemes rely on

- Distance relays
- Overcurrent relays
- Differential protection

These rule-based methods depend on predefined thresholds and may fail under changing grid conditions. Increasing penetration of renewable energy and distributed resources introduces uncertainty, making intelligent monitoring essential.

Machine Learning enables automatic learning from historical and real-time operational data to detect abnormal behaviour. Recent studies show ML models can achieve fault detection accuracy above **99%** using algorithms such as Support Vector Machines and Random Forest classifiers in power networks.

2. Types of Faults in Electrical Power Networks

Faults in electrical systems are categorized as follows

2.1 Symmetrical Faults

- Three-phase fault
- Balanced system disturbance
- Rare but highly severe

2.2 Unsymmetrical Faults

- Single Line-to-Ground (LG)
- Line-to-Line (LL)
- Double Line-to-Ground (LLG)

Unsymmetrical faults constitute nearly 70–80% of transmission failures.

2.3 Equipment Faults

- Transformer insulation failure
- Cable degradation
- Generator winding faults

Rapid identification minimizes cascading failures and blackout risks.

3. Machine Learning Framework for Fault Identification

A typical ML-based fault detection architecture includes

3.1 Data Acquisition

Electrical parameters collected using:

- Current Transformers (CT)
- Potential Transformers (PT)
- Phasor Measurement Units (PMU)
- SCADA systems

Voltage, current magnitude, phase angle, and frequency signals are continuously monitored.

3.2 Data Pre-Processing

Raw signals contain noise and missing values. Processing steps include

- Signal normalization
- Noise filtering
- Feature scaling
- Outlier removal

Wavelet transforms and statistical filtering improve fault feature extraction.

3.3 Feature Extraction

Important fault features include:

- RMS current variation
- Voltage sag/swell
- Harmonic distortion
- Frequency deviation

Feature engineering significantly influences ML performance.

4. Machine Learning Algorithms for Fault Identification

4.1 Support Vector Machine (SVM)

SVM separates faulty and normal operating conditions using optimal hyperplanes.

Advantages:

- High accuracy
- Effective for small datasets
- Robust classification

Research demonstrates SVM achieving 99.6% fault detection accuracy in electrical systems.

4.2 Decision Tree and Random Forest

Decision Trees classify faults using hierarchical decision rules, while Random Forest improves reliability through ensemble learning.

Applications:

- Transmission line fault classification
- Fault localization
- Real-time monitoring

Ensemble ML models improve detection robustness under varying grid conditions.

4.3 Artificial Neural Networks (ANN)

ANN models learn nonlinear relationships between electrical parameters.

Capabilities:

- Pattern recognition
- Adaptive learning
- Complex fault classification

ANNs are widely used for transformer and distribution network monitoring.

4.4 Deep Learning Models

Advanced deep learning techniques include

- Convolutional Neural Networks (CNN)
- Long Short-Term Memory (LSTM)
- Hybrid CNN-LSTM models

Deep learning enables automatic feature extraction and accurate short-circuit fault diagnosis in modern distribution grids.

5. Fault Classification and Localization

Machine learning supports both

Fault Classification

Identifies fault type:

- LG
- LL
- LLG
- Three-phase faults

Fault Localization

Determines fault distance from substation.

Recent IEEE research demonstrates ML systems capable of identifying faulty transmission lines within milliseconds using real-time measurements.

6. Performance Evaluation Metrics

ML model effectiveness is evaluated using:

- Accuracy
- Precision
- Recall
- F1-Score
- Confusion Matrix

High-performance models report accuracy above 97–99% for transmission line fault detection using hybrid learning approaches.

7. Applications in Modern Power Networks

Machine learning-based fault identification is applied in

- Smart grids
- Renewable integrated systems
- Microgrids
- Power transformer monitoring
- Distribution automation

Predictive analytics improves system reliability by detecting incipient faults before failure occurs.

8. Challenges in ML-Based Fault Detection

Despite advantages, several challenges remain

- Lack of publicly available datasets
- Data imbalance problems

- Cyber-physical security risks
- Real-time computational constraints
- Model interpretability issues

Robustness against noisy or missing sensor data remains a major research focus in ML-assisted protection systems.

9. Future Research Directions

Future intelligent power networks will incorporate

- Explainable Artificial Intelligence (XAI)
- Edge AI-based protection relays
- Digital Twin power systems
- Federated learning for distributed grids
- Self-healing smart grids

Integration of AI with adaptive protection mechanisms will enable autonomous grid operation.

Conclusion

Machine Learning approaches provide transformative solutions for fault identification in electrical power networks. Compared to conventional protection schemes, ML-based systems offer faster detection, adaptive learning capability, and improved accuracy. Algorithms such as SVM, Random Forest, ANN, and deep learning models enable real-time monitoring and predictive fault diagnosis. As power systems evolve toward intelligent smart grids, ML-driven protection frameworks will play a vital role in ensuring reliability, resilience, and operational efficiency.

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SOCIAL MEDIA WHISPERS, AI ALERTS: PROTECTING HERBAL MEDICINE USERS

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Abstract

Herbal medicines are widely consumed globally and are frequently perceived as inherently safe due to their natural origin. However, increasing evidence indicates that herbal products are associated with adverse drug reactions (ADRs), including hepatotoxicity, nephrotoxicity, and herb–drug interactions. Traditional pharmacovigilance (PV) systems rely primarily on spontaneous reporting mechanisms, which are limited by under-reporting and delayed signal detection. With the rapid growth of digital communication platforms, social media has emerged as a real-time source of patient-reported health experiences. Artificial intelligence (AI), particularly natural language processing (NLP) and machine learning (ML), enables automated extraction of adverse event signals from unstructured text data. This review examines the limitations of herbal pharmacovigilance, evaluates the role of social media analytics in safety surveillance, discusses AI methodologies for adverse event detection, and proposes an integrated framework for digital herbal pharmacovigilance. Ethical considerations, regulatory implications, and future research directions are also addressed.

Keywords: Herbal Pharmacovigilance, Artificial Intelligence, Natural Language Processing, Social Media Analytics, Adverse Drug Reactions, Digital Health Surveillance.

1. Introduction

Herbal medicines constitute a major component of traditional and complementary medicine systems worldwide. The World Health Organization (WHO) estimates that a significant proportion of the global population depends on herbal products for primary healthcare [1]. Despite their widespread use, safety monitoring systems for herbal medicines remain underdeveloped.

Herbal products differ from synthetic drugs due to variability in plant sources, polyherbal formulations, and lack of strict regulatory harmonization. Consequently, adverse drug reactions associated with herbal products are often underreported [2]. Navarro et al. reported that herbal and dietary supplements are increasingly implicated in drug-induced liver injury cases, highlighting the importance of systematic monitoring [3].

Traditional pharmacovigilance systems, such as spontaneous reporting databases, are reactive and depend on voluntary submissions from healthcare professionals or patients [4]. These systems frequently fail to capture real-time signals.

The digital era has introduced new data streams. Social media platforms contain large volumes of patient narratives describing medication experiences. AI-based methods have demonstrated the ability to mine these unstructured datasets for safety signals [5,6].

2. Challenges in Herbal Pharmacovigilance

2.1 Under-Reporting

Choudhury et al. emphasized that herbal adverse events are significantly under-reported due to public perception of safety and lack of awareness about reporting systems [2].

2.2 Complexity of Herbal Formulations

Polyherbal formulations contain multiple phytoconstituents, complicating causality assessment. Unlike synthetic drugs, standardization is often inadequate [2].

2.3 Regulatory Variability

Different countries classify herbal products as dietary supplements, traditional medicines, or pharmaceuticals, resulting in inconsistent safety surveillance frameworks [1].

Herbal pharmacovigilance presents unique challenges compared to conventional drug safety monitoring. Factors such as variability in plant composition, lack of standardized formulations, underreporting of adverse events, and weak regulatory frameworks contribute to difficulties in detecting and managing safety signals. Additionally, consumers frequently self-medicate with herbal products without professional supervision, increasing the risk of adverse herb–drug interactions. A structured summary of the key challenges associated with herbal pharmacovigilance is presented in Table 1.

Table 1: Key Challenges in Herbal Pharmacovigilance

Challenge	**Consequence**
Under-reporting	Delayed detection of adverse drug reactions (ADRs)
Polyherbal complexity	Difficulty in causality assessment due to multiple phytoconstituents
Self-medication practices	Lack of formal documentation and clinical traceability
Regulatory variability	Inconsistent monitoring and safety evaluation frameworks

3. Social Media as a Source of Safety Signals

Patients frequently share health experiences on Twitter, Reddit, Facebook groups, and online forums. These platforms provide real-time, patient-generated data.

Fan et al. (2025) demonstrated that social media monitoring enhances pharmacovigilance by identifying emerging safety trends [5]. Sarker et al. showed that NLP techniques can extract adverse drug reactions from social media posts with moderate to high accuracy [6].

However, data extracted from social media is noisy, informal, and context-dependent.

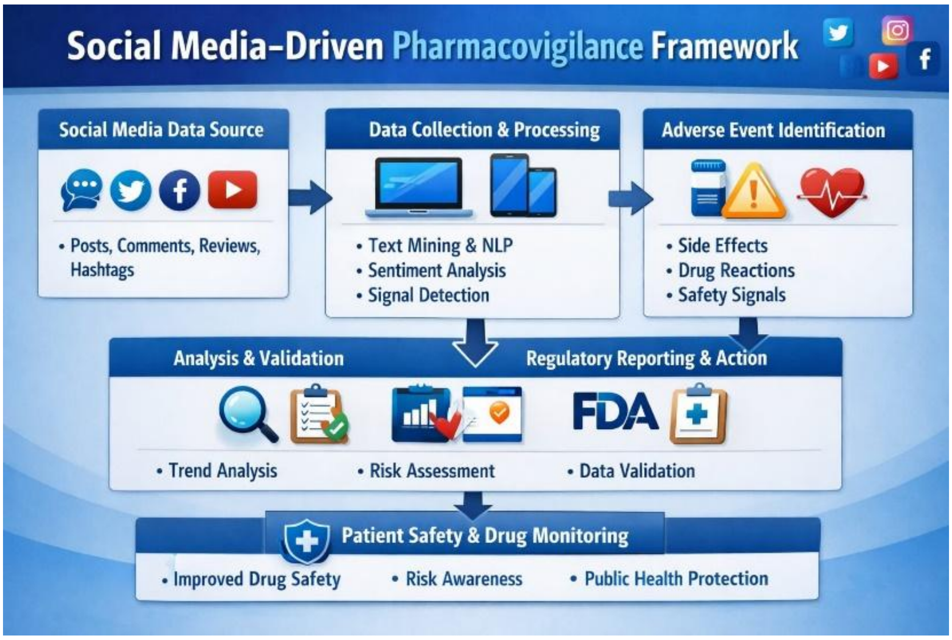

Figure 1: Social Media–Driven Pharmacovigilance Framework

Figure 2: AI Techniques Used in Pharmacovigilance

4. Artificial Intelligence in Digital Pharmacovigilance

4.1 Natural Language Processing (NLP)

NLP enables automated extraction of entities such as drug names, symptoms, and adverse events from text. Scaboro *et al.* (2022) demonstrated improvements in ADR extraction robustness using transformer-based models [7].

4.2 Machine Learning & Deep Learning

Deep learning architectures such as convolutional neural networks (CNN) and recurrent neural networks (RNN) improve detection accuracy in large datasets [4].

Roche *et al.* proposed a holistic AI-based pharmacovigilance optimization model using social media behavior analysis [8].

Nagar *et al.* (2025) discussed regulatory integration of AI-driven pharmacovigilance tools [9].

The transition from traditional pharmacovigilance systems to AI-enabled digital pharmacovigilance represents a paradigm shift in drug safety monitoring. While conventional systems depend on voluntary reporting and structured databases, AI-driven approaches leverage real-time, unstructured data sources such as social media and online forums. A comparative overview of these two approaches is presented in table 2.

Table 2: Traditional vs AI-Enabled Pharmacovigilance

Parameter	Traditional Pharmacovigilance	AI-Enabled Digital Pharmacovigilance
Data Source	Voluntary/Spontaneous reporting (HCPs, patients)	Multi-channel: Social media, wearables, EHRs, & digital forums
Timeliness	**Reactive:** Often delayed (weeks to months)	**Proactive:** Near real-time monitoring and alerts
Data Type	Structured clinical reports (ICSRs)	Unstructured text, audio, and big data sets
Scalability	**Limited:** Dependent on manual labor	**High:** Automated ingestion and case processing
Signal Detection	Manual review & basic statistical methods	Machine Learning (ML) & predictive pattern recognition
Causality	Expert-based case-by-case assessment	AI-assisted triage with high-speed correlation

5. Ethical and Regulatory Considerations

AI-based social media monitoring raises concerns regarding:

- Data privacy
- User consent
- Algorithm bias
- False positive alerts

Jain *et al.* (2025) highlighted the need for ethical governance frameworks in AI-enabled pharmacovigilance [10].

6. Future Directions

- Development of herbal-specific ADR ontologies
- Multilingual NLP systems
- Integration with WHO VigiBase
- Hybrid validation models combining AI alerts with clinical evidence

Conclusion

Digital pharmacovigilance powered by AI offers a transformative approach to protecting herbal medicine users. By leveraging real-time social media data, early detection of adverse events becomes possible. Although challenges related to validation and ethics persist, integration of AI alerts with traditional systems represents a promising advancement in herbal safety monitoring.

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SMART RESPONSIVE BUCCAL FILMS FOR ON-DEMAND DRUG RELEASE: NEXT-GENERATION ORAL DRUG DELIVERY SYSTEMS

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Abstract

Buccal drug delivery systems have emerged as a promising alternative to conventional oral and parenteral routes due to their ability to bypass hepatic first-pass metabolism and improve patient compliance. Recent advancements in smart and stimuli-responsive polymers have enabled the development of intelligent buccal films capable of on-demand drug release in response to physiological triggers such as pH, temperature, glucose levels, enzymes, and external stimuli. These smart responsive buccal films integrate mucoadhesive polymers with functional nanomaterials, enabling controlled, site-specific, and patient-tailored therapy. This review discusses the fundamentals of buccal drug delivery, smart polymer mechanisms, fabrication technologies, biomedical applications, clinical relevance, challenges, and future prospects. Emphasis is placed on innovative polymer systems such as chitosan derivatives, poly(N-isopropylacrylamide), Eudragit®, poloxamers, and enzyme-responsive materials. Smart buccal platforms represent a transformative step toward personalized, non-invasive, and digitally integrated therapeutic systems.

Keywords: Buccal Films, Smart Polymers, Stimuli-Responsive Systems, Mucoadhesion, On-Demand Release, Personalized Drug Delivery.

1. Introduction

Buccal drug delivery utilizes the inner cheek mucosa for systemic or local drug administration. Compared to oral tablets, it avoids first-pass hepatic metabolism and offers rapid systemic absorption [1]. The buccal mucosa has a rich vascular network and relatively permeable epithelium, making it suitable for peptide, hormone, and cardiovascular drug delivery [2].

Traditional buccal films provide controlled release but lack environmental responsiveness. The integration of smart polymers has enabled stimuli-triggered drug release, improving therapeutic precision [3].

2. Buccal Mucosa and Drug Transport

- The buccal epithelium consists of:
- Stratified squamous epithelium
- Basement membrane

- Lamina propria
- Drug permeation occurs via:
- Transcellular pathway
- Paracellular pathway
- Mucoadhesion is achieved by hydrogen bonding, electrostatic interaction, and polymer chain interpenetration [4].

3. Smart Responsive Polymers in Buccal Films

Smart polymers alter their physicochemical properties in response to environmental stimuli [5].

3.1 pH-Responsive Polymers

These polymers swell or dissolve at specific pH levels.

Examples:

- Eudragit® L100, S100
- Poly(acrylic acid)
- Carbopol

They are useful in inflammatory oral conditions and ulcer-targeted therapy [6].

3.2 Thermoresponsive Polymers

Poly(N-isopropylacrylamide) (PNIPAM) exhibits phase transition at ~32°C [7]. At body temperature, polymer contraction can trigger drug release.

Poloxamer-based systems also exhibit temperature-dependent gelation [8].

3.3 Glucose-Responsive Polymers

Phenylboronic acid-functionalized polymers detect glucose changes and alter swelling behavior [9].

These are promising for:

- Buccal insulin delivery
- Diabetes-responsive films

3.4 Enzyme-Responsive Polymers

Certain polymers degrade in presence of oral enzymes such as lysozyme [10].Chitosan derivatives show enzyme-triggered breakdown.

3.5 Electrically or Light-Responsive Systems

Incorporation of nanoparticles allows remote-triggered release [11].

Applications include:

- Photothermal drug release
- Smart oral cancer therapy

4. Mucoadhesive Polymers Used in Smart Buccal Films

Commonly used smart mucoadhesive polymers:

- Chitosan and trimethyl chitosan [12]
- Hydroxypropyl methylcellulose (HPMC)
- Polyvinyl alcohol (PVA)
- Sodium alginate
- Thiolated polymers

Chitosan enhances permeation by transiently opening tight junctions [13].

5. Formulation Strategies

5.1 Film-Forming Polymers

Cellulose derivatives and synthetic polymers provide structural integrity and controlled drug release characteristics.

5.2 Nanotechnology Integration

Nanoparticles embedded within polymer matrices enhance stability, permeability, and controlled release. Nano-enabled buccal systems improve drug solubility and facilitate triggered release.

5.3 Manufacturing Techniques

- Solvent Casting: Most common laboratory method.
- Hot-Melt Extrusion: Solvent-free method suitable for scale-up [14].
- 3D Printing: Allows patient-specific dosing [15].

Table 1: Smart Polymers Used in Buccal Films and Their Mechanisms

Polymer	Stimulus	Mechanism	Typical Application
Eudragit L100	pH	Ionization of carboxyl groups leading to polymer swelling and dissolution.	Enteric coating for intestinal drug release.
PNIPAM	Temperature	Reversible coil-to-globule phase transition at its Lower Critical Solution Temperature (LCST).	On-demand release via local hyperthermia.
Chitosan	Enzyme / pH	Protonation of amino groups in acidic media or degradation by lysozymes.	Mucoadhesive and colon-specific delivery.
Poloxamer	Temperature	Thermally induced micellization and gelation (sol-to-gel transition).	In-situ forming injectable drug depots.
Phenylboronic Acid	Glucose	Reversible covalent bonding with glucose, changing the hydrogel's hydration.	Self-regulating insulin delivery systems.

6. Therapeutic Applications

6.1 Diabetes Management

Glucose-responsive buccal films are being explored for insulin delivery [9].

6.2 Pain Management

Fentanyl buccal systems demonstrate rapid systemic absorption [16].

6.3 Hormonal Therapy

Buccal films improve bioavailability of peptides and hormones [17].

6.4 Oral Cancer Therapy

Localized smart films reduce systemic toxicity [18].

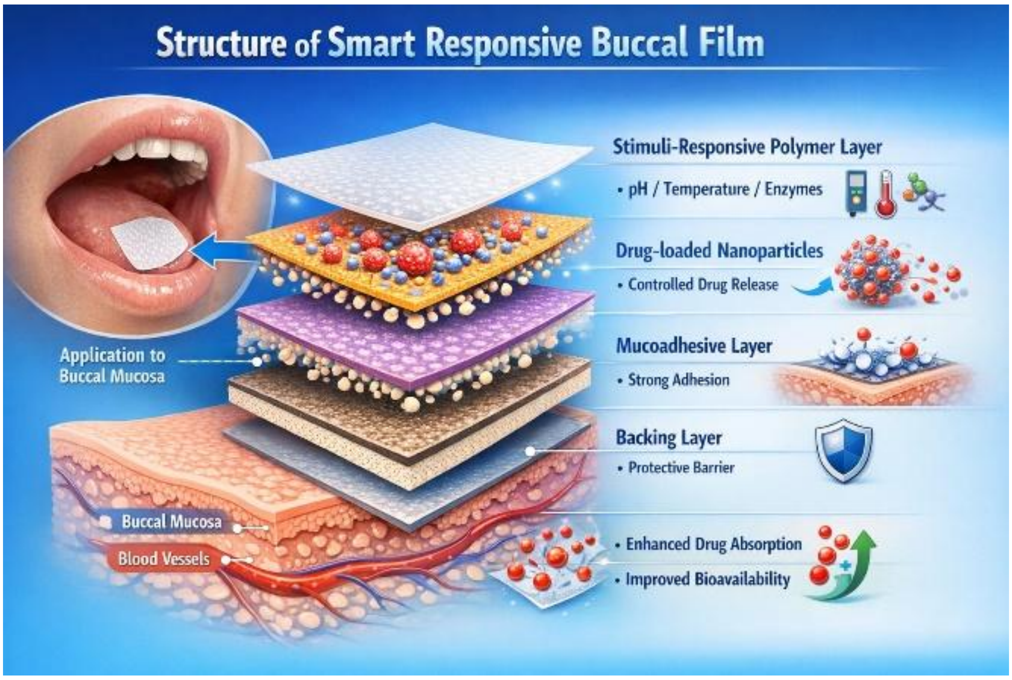

Figure 1: Structure of Smart Responsive Buccal Film

7. Advantages Over Conventional Systems

- Avoid first-pass metabolism
- Rapid onset
- Non-invasive
- Personalized therapy
- Reduced systemic toxicity

Table 2: Traditional vs Smart Buccal Drug Delivery

Parameter	Traditional Film	Smart Responsive Film
Drug Release	Passive	Trigger-based
Precision	Limited	High
Personalization	No	Yes
Adaptability	No	Yes

8. Challenges

- Limited drug loading capacity
- Stability of biological drugs
- Manufacturing scale-up
- Regulatory concerns

9. Future Perspectives

- Future research includes:
- AI-integrated smart films
- Biosensor-embedded systems
- Nanocomposite buccal platforms
- Digital health monitoring integration

Smart buccal films may become part of wearable-digital therapeutic systems.

Discussion

Smart responsive buccal films represent a shift from passive drug release toward intelligent therapeutic systems. Compared to conventional mucoadhesive films, they provide dynamic adaptability to patient physiology. Integration of nanotechnology, 3D printing, and bioresponsive polymers enhances precision dosing. However, translation to commercial scale requires stability validation and regulatory standardization. Collaboration between pharmaceutical scientists, polymer chemists, and biomedical engineers will accelerate clinical adoption.

Conclusion

Smart responsive buccal films are next-generation drug delivery platforms that combine mucoadhesion, stimuli responsiveness, and personalized medicine. Their ability to provide on-demand drug release improves therapeutic efficacy and patient compliance. Although challenges remain, rapid progress in smart polymers and fabrication technologies indicates strong potential for clinical translation.

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NEXT-GENERATION SMART AND SELF-RESTORATIVE MATERIALS

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Abstract

Smart and self-healing materials are advanced functional systems capable of responding to environmental stimuli and autonomously repairing damage. These materials integrate stimuli-responsiveness with reversible or embedded healing mechanisms to enhance durability, sustainability, and functional performance. This chapter provides an in-depth discussion of classification, mechanisms, material chemistry, fabrication strategies, nanotechnology integration, applications across biomedical, aerospace, electronics, and construction sectors, as well as current challenges and future perspectives.

Keywords: Self-Healing, Stimuli Responsive, Nanotechnology, Biomedical.

1. Introduction

The rapid advancement of materials science in the twenty-first century has led to the development of intelligent materials capable of performing beyond the limitations of traditional structural systems. Conventional materials are passive in nature; once damaged, their properties deteriorate permanently, leading to structural failure, increased maintenance costs, and safety risks. In contrast, smart and self-healing materials represent a paradigm shift toward adaptive and autonomous material systems that can sense environmental changes, respond dynamically, and restore functionality after damage.

Smart materials are defined as materials that exhibit controlled and reversible changes in their physical, chemical, or mechanical properties when exposed to external stimuli such as temperature, pH, light, electrical fields, magnetic fields, moisture, or mechanical stress [1]. These materials integrate sensing and actuation within the same system, enabling real-time adaptation to environmental conditions. Their behavior may include shape transformation, color change, volume expansion or contraction, variation in stiffness, or modulation of electrical conductivity.

Self-healing materials extend this concept further by incorporating mechanisms that allow the autonomous repair of microcracks, fractures, or surface damage without external human intervention [2]. Inspired by biological healing processes such as blood clotting and tissue regeneration, these materials are engineered to restore structural integrity and functional performance after damage. The healing process may be triggered automatically upon crack formation or activated by specific stimuli such as heat, light, or chemical changes.

The growing interest in smart and self-healing materials is driven by increasing demands for sustainability, durability, and safety across industries. Infrastructure deterioration, corrosion in aerospace systems, fatigue failure in automotive components, and mechanical damage in electronic devices highlight the need for materials capable of long-term resilience. By extending service life and reducing maintenance requirements, self-healing systems contribute significantly to cost efficiency and environmental sustainability.

At the molecular level, the design of smart self-healing materials involves advanced polymer chemistry, dynamic covalent bonding, supramolecular interactions, and microencapsulation techniques. These strategies enable reversible network formation, controlled release of healing agents, and multi-functional responsiveness. The integration of nanotechnology has further enhanced mechanical strength, healing efficiency, and responsiveness by improving interfacial interactions and network stability.

Interdisciplinary research plays a crucial role in the advancement of these materials. Contributions from chemistry, physics, materials engineering, nanotechnology, biomedical science, and artificial intelligence have accelerated the discovery and optimization of intelligent material systems. Emerging computational modeling and AI-driven design tools now allow prediction of healing kinetics, mechanical behavior, and stimulus-response efficiency, thereby reducing experimental trial-and-error approaches.

The convergence of smart functionality and self-healing capability has led to the development of next-generation materials with combined sensing, actuation, and repair features. Such materials are being explored in flexible electronics, biomedical implants, aerospace composites, self-healing coatings, and energy storage devices. Their multifunctional nature positions them as a cornerstone of future sustainable and adaptive technologies. [2].

2. Classification of Smart and Self-Healing Materials

- Smart and self-healing materials can be broadly classified into extrinsic and intrinsic systems [2].
- Extrinsic Systems: These systems incorporate microcapsules, hollow fibers, or vascular networks filled with healing agents. Upon crack formation, capsules rupture and release healing chemicals that polymerize and seal the damage [3].
- Intrinsic Systems: These rely on reversible chemical bonds such as hydrogen bonding, disulfide exchange, Diels–Alder reactions, ionic interactions, and metal-ligand coordination. These materials can heal multiple times due to dynamic bond reformation [4].

- Stimuli-Responsive Smart Materials: These materials respond to specific triggers such as temperature (thermo-responsive), pH (pH-responsive), light (photo-responsive), and electricity (electro-responsive) [3,4].

3. Mechanisms of Smart Behavior and Healing

Smart behavior arises from structural rearrangements, phase transitions, or ionization changes within polymer networks. Thermo-responsive polymers exhibit lower critical solution temperature (LCST) behavior, where polymer chains collapse or expand upon heating [5].

Self-healing mechanisms involve dynamic covalent chemistry and supramolecular interactions. Dynamic covalent bonds such as Diels–Alder linkages provide reversible cross-linking under heat. Disulfide bonds undergo exchange reactions under redox conditions [4].

Supramolecular forces including hydrogen bonding, π–π stacking, and ionic interactions enable rapid and repeatable healing. These non-covalent interactions allow structural recovery without significant energy input [6].

4. Materials and Fabrication Strategies

Polymers are the most widely used matrices for smart self-healing materials due to their versatility and tunable chemistry. Elastomers, hydrogels, epoxy resins, and polyurethane systems dominate current research [2].

Nanomaterials such as graphene, carbon nanotubes, silica nanoparticles, and nanoclays enhance mechanical strength and improve healing efficiency by reinforcing polymer networks [5].

Advanced fabrication techniques include microencapsulation, electrospinning, 3D printing, and layer-by-layer assembly. Additive manufacturing enables customized vascular healing networks and multifunctional architectures [5,7].

5. Applications

- Biomedical Applications: Self-healing hydrogels are used in wound dressings, drug delivery systems, and tissue engineering scaffolds. These materials maintain moist environments and adapt to physiological conditions [6].
- Electronics and Wearables: Conductive self-healing polymers are applied in flexible circuits, electronic skin, and stretchable sensors, enhancing device longevity [3].
- Aerospace and Automotive: Self-healing composites and coatings reduce crack propagation and corrosion, improving structural safety [7].
- Construction Industry: Self-healing concrete incorporating bacteria or microcapsules enables crack sealing and enhanced durability in infrastructure [7].

6. Challenges and Limitations

Despite remarkable progress, several challenges persist. High material and processing cost limits large-scale commercialization. Mechanical strength may decrease in highly dynamic polymer systems. Environmental stability and long-term durability remain critical concerns [2,4].

7. Future Perspectives

Future research focuses on biodegradable self-healing polymers, multi-stimuli responsive systems, AI-assisted material design, and integration with energy storage devices [5,8]. The convergence of nanotechnology, artificial intelligence, and sustainable chemistry is expected to accelerate innovation in smart materials.

Conclusion

Smart and self-healing materials represent a transformative direction in materials science. Their ability to adapt, sense, and autonomously repair damage provides enhanced durability, sustainability, and performance across multiple sectors. Continued interdisciplinary research will further expand their technological impact.

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