

ISBN: 978-81-993182-2-9

SCIENCE, TECHNOLOGY AND SOCIETY: NEXT GEN RESEARCH VOLUME I



Editors:

Dr. Manoj P. Mahajan
Mr. Anand Kumar Mishra
Dr. Preyoshi Bose
Dr. Shivkumar Verma

Bhumi Publishing, India



First Edition: September 2025

SCIENCE, TECHNOLOGY AND SOCIETY: NEXT GEN RESEARCH VOLUME I

(ISBN: 978-81-993182-2-9)

DOI: <https://doi.org/10.5281/zenodo.17240674>

Editors

Dr. Manoj P. Mahajan

Department of Physics,
V. G. Vaze College of Arts, Science &
Commerce (Autonomous), Mulund, Mumbai

Mr. Anand Kumar Mishra

Department of Chemistry,
Deen Dayal Upadhyay
Gorakhpur University, Gorakhpur, U.P.

Dr. Preyoshi Bose

Department of Physics,
Smt. Chandibai Himathmal Mansukhani
College (Autonomous), Ulhasnagar, M.S.

Dr. Shivkumar Verma

Arunachal University of Studies,
Namsai,
Arunachal Pradesh



Bhumi Publishing

September 2025

Copyright © Editors

Title: Science, Technology and Society: Next Gen Research Volume I

Editors: Dr. Manoj P. Mahajan, Mr. Anand Kumar Mishra,

Dr. Preyoshi Bose, Dr. Shivkumar Verma

First Edition: September 2025

ISBN: 978-81-993182-2-9



DOI: <https://doi.org/10.5281/zenodo.17240674>

All rights reserved. No part of this publication may be reproduced or transmitted, in any form or by any means, without permission. Any person who does any unauthorized act in relation to this publication may be liable to criminal prosecution and civil claims for damages.

Published by Bhumi Publishing,

a publishing unit of Bhumi Gramin Vikas Sanstha



Nigave Khalasa, Tal – Karveer, Dist – Kolhapur, Maharashtra, INDIA 416 207

E-mail: bhumipublishing@gmail.com



Disclaimer: The views expressed in the book are of the authors and not necessarily of the publisher and editors. Authors themselves are responsible for any kind of plagiarism found in their chapters and any related issues found with the book.

PREFACE

The relationship between science, technology, and society has never been more significant than it is today. With rapid advancements across multiple disciplines, we are entering an era where scientific discoveries and technological innovations influence nearly every aspect of human life. From healthcare and agriculture to communication and environmental sustainability, these changes are reshaping the way we live, work, and interact with one another. The challenges and opportunities presented by such developments require thoughtful reflection, critical analysis, and responsible application.

*This book, *Science, Technology and Society: Next Gen Research*, has been envisioned as a platform to bring together diverse contributions from emerging and established researchers. The chapters compiled here reflect the latest trends, innovative methodologies, and transformative approaches that define contemporary research. More importantly, they highlight the importance of integrating science and technology with societal needs, ensuring that progress is aligned with sustainable development, ethical responsibility, and human welfare.*

An essential aim of this volume is to foster interdisciplinary understanding. The complexities of the modern world cannot be addressed in isolation; they require collaboration across fields and a willingness to explore new perspectives. By presenting research from varied domains, this book offers readers an opportunity to appreciate how interconnected our systems are and how innovation in one area can ripple across many others.

The book is intended for students, academicians, professionals, and anyone interested in the evolving landscape of science and technology. It encourages critical thinking and aims to inspire the next generation of scholars to contribute not just to the growth of knowledge but also to the betterment of society.

*We express our deep gratitude to all the contributors for their scholarly efforts and commitment in shaping this work. We also extend our thanks to the institutions, peers, and colleagues who supported the realization of this volume. It is our hope that *Science, Technology and Society: Next Gen Research* will serve as a valuable resource, stimulate dialogue, and inspire responsible innovation that addresses the needs of present and future generations.*

- Editors

TABLE OF CONTENT

Sr. No.	Book Chapter and Author(s)	Page No.
1.	EXPLORING ORGANIC THIN FILMS FOR ADVANCED DISPLAY TECHNOLOGIES Dhrubajyoti Saikia and Swagatam Deva Nath	1 – 7
2.	CHALLENGES OF NEXT-GEN RESEARCH: RISKS AND OPPORTUNITIES Sandeep Nivruttirao Niwadange, Hemraj Madhukar Meshram and Trupta Devrao Wakde	8 – 13
3.	HOW IMPORTANT IS THE USE OF MEDICAL APPLICATIONS IN LIFE TO STAY HEALTHY Raj Kumar Singh Bharti, Sushil Kumar, Asheesh Kumar Gupta, Dharamveer Singh, Swatantr Bahadur Singh, Amit Kumar and Anil Kumar	14 - 20
4.	FARMER RIGHTS IN THE MEDICINAL PLANT SECTOR Pooja Barthwal, Girish Chandra and Kamla Dhyan	21 – 29
5.	FISCHER CARBENE-MEDIATED ANNULATION REACTIONS TOWARD N-FUSED HETEROCYCLIC FRAMEWORKS Priyabrata Roy	30 – 47
6.	NEXT-GENERATION SCIENCE: SHAPING SOCIETY, OVERCOMING HURDLES, AND SHAPING FUTURE FRONTIERS K Janani and P Sivakami	48 – 52
7.	THE NUTRITIONAL ADEQUACY OF PLANT BASED DIETS Prachi Chaturvedi	53 – 59
8.	METAL-BASED ANTICANCER AGENTS: EXPLORING THE PROMISE OF TRANSITION COMPLEXES IN CANCER THERAPY Pawanjeet Kaur	60 – 71
9.	RENEWABLE ENERGY: A PATHWAY TO A SUSTAINABLE FUTURE Bindesh Kumar Shukla	72 – 77

10.	TRANSITION METAL OXIDES: STRUCTURAL INSIGHTS, UNIQUE PROPERTIES AND EMERGING APPLICATIONS FOR A SUSTAINABLE FUTURE Amarsinha Babasaheb Gorepatil	78 – 81
11.	MATHEMATICAL MODELING IN CHEMICAL SYSTEMS Anand Kumar Mishra and Shiv Kumar Verma	82 – 95
12.	ALCOHOL TECHNOLOGY FOR A SUSTAINABLE BIOFUEL FUTURE Gorepatil Pratapsinha	96 – 99
13.	RAINBOW CONNECTION NUMBER OF THE ENHANCED POWER GRAPH Richa Jain	100 – 105
14.	IMPACT OF GENETICALLY MODIFIED FOODS ON HUMAN HEALTH Krithika K, Gunavadhana S and Anu Swedha Ananthan	106 – 109
15.	NEXT-GENERATION CROP MONITORING WITH SMART TECHNOLOGIES IN PRECISION AGRICULTURE Yashaswini R, Sridhara M R, Prem Sagar S P, V C Raghavendra and Sharanabasava	110 – 131
16.	THE SCIENCE SHIFT Manasa C and Madhusudhan H S	132 – 135

EXPLORING ORGANIC THIN FILMS FOR ADVANCED DISPLAY TECHNOLOGIES

Dhrubajyoti Saikia¹ and Swagatam Deva Nath*²

¹Department of Physics, Joya Gogoi College, Khumtai, Golaghat, Assam, India

²Department of Physics, Nanda Nath Saikia College, Titabar, Assam, India

*Corresponding author E-mail: swgtmdvnth@gmail.com

Introduction to Organic Thin Film in Semiconductor-Based Devices

Organic semiconductors are carbon-based materials, usually composed of π -conjugated molecules or polymers, which can exist either as molecular crystals or amorphous films. Owing to their electronic properties, these materials play an essential role in the development of organic optoelectronic devices. Organic optoelectronics focuses on understanding and using organic small molecules or polymers with electronic properties. Unlike inorganic conductors and semiconductors, organic electronic materials are made from carbon-based small molecules or polymers. One of the biggest benefits of organic electronics is their potential for lower production costs compared to traditional inorganic electronics. [1–3].

Organic optoelectronic devices are electrical systems like light-emitting diodes (LEDs), photovoltaic cells (PVs), or thin-film transistors (TFTs). In these devices, organic materials with semiconducting properties serve as the active medium. The molecular units in organic materials are separate, so long-range order between adjacent molecules or polymer chains is unnecessary. This allows organic semiconductors to offer clear benefits over traditional inorganic semiconductor materials like silicon (Si) or gallium arsenide (GaAs). For example, we can create complex multilayer device structures with nanometer-scale thickness using organic materials through roll-to-roll printing or vacuum deposition techniques. However, it's important to point out a significant limitation of organic semiconductors. They have very few charge carriers (electrons or holes) and act like insulators until electrical charges are introduced [4, 5]. This characteristic shows that in practical devices, all charge carriers, including holes and electrons, must be injected from the anode and cathode. Therefore, the properties at the interface between the organic layers and the electrode surfaces significantly affect device performance, stability, and operational lifetime.

In this context, thin films are very important. A thin film is a material layer with a thickness that ranges from fractions of a nanometer to several micrometers. These films can be deposited using various methods, such as chemical deposition, physical deposition, controlled growth modes, and epitaxial techniques. Thin films are essential for both studying and using materials with innovative and unique physical and electronic properties. As low-cost integrated circuit technology has improved, the need for thin-film-based devices has also grown. Conventional integrated circuits, which combine many active and passive components on single-crystal silicon

wafers, do not work well for applications like flat-panel display addressing. This led to the search for different fabrication methods. Thin-film deposition techniques offer a viable alternative, allowing for the creation of various thin-film devices on both rigid and flexible surfaces for use in optoelectronics and display technologies. Among these devices, such as thin-film transistors and photovoltaic solar cells, the organic light-emitting diode (OLED) has become one of the most appealing and widely researched devices in physics and materials science over the past twenty years.

The interdisciplinary nature of OLED research has significantly fueled its quick growth and interest. This field combines synthetic chemistry, physical chemistry, device physics, and surface engineering, making it a vibrant area of study. Organic Light Emitting Diodes now stand out as a promising technology for the next generation of optoelectronic devices. OLEDs have several notable benefits, such as self-emissive operation, very low power consumption, wide viewing angles over 150 degrees, and fast response times. Fundamentally, an OLED is a device that produces light from organic semiconducting materials when an external electrical bias is applied. Because of these unique features, OLEDs have been extensively studied and optimized to improve their efficiency, stability, and performance, with applications including flat-panel displays and solid-state lighting.

The basic structure of an OLED generally consists of one or more organic semiconducting thin films placed between two electrodes. One of these electrodes, usually the anode, needs to be optically transparent to let the generated light pass through, while the cathode is typically reflective. When a voltage is applied, the anode supplies holes while the cathode introduces electrons into the organic layers. These charge carriers migrate through the film and eventually combine in the emissive region to form excitons, which release light upon recombination. The emitted photons are partially reflected by the metallic cathode and eventually escape through the transparent anode, resulting in the visible luminescence of the device.

Introduction to Display Technologies in Modern Life Style

Nowadays, most people around the world spend a lot of time using different display screens. With computer screens, you can browse the internet, enjoy games, and watch shows or movies. Displays are also essential for everyday tasks like managing office information, doing research projects, accessing online learning materials, and using various multimedia resources. So, the design, technology, and function of display systems play a big role in our daily lives across different generations and populations.

Over time, display technologies have advanced significantly, especially with the rise of flat-panel display (FPD) technologies like liquid crystal displays (LCDs) and plasma displays. These are quickly replacing traditional cathode ray tube (CRT) displays. Until recently, most televisions and computer monitors were based on CRT technology. Current display development marks a shift from bulky CRTs to slimmer, more modern flat-panel displays.

Cathode ray tubes (CRTs) are vacuum tubes that have a phosphorescent screen and one or more electron guns. These devices create and adjust images by accelerating and directing electron beams onto the screen [6]. They were commonly used in traditional televisions and computer monitors. In CRTs, electrons are created through thermionic emission at a heated cathode under high voltage. These electrons are then focused into a beam that hits a phosphorescent screen. This process happens inside a glass tube that is bulky, heavy, and relatively fragile. For safety, the faceplate of the CRT is usually made of thick lead glass, which provides strong shatter resistance and blocks most X-ray emissions. From the late 2000s onward, CRTs were mostly replaced by newer display technologies like LCDs, plasma displays, and OLEDs. These alternatives are lighter, less bulky, more energy-efficient, and cheaper to produce. In modern CRT monitors and televisions, the electron beams were deflected by different magnetic fields created by coils around the tube's neck. The study of cathode rays began in the 19th century, with Hittorf's initial observations in 1869. Later, contributions by Schuster, Crookes, and Thomson established their nature, with Thomson's experiments ultimately demonstrating that these rays consist of electrons—the first identified subatomic particles., the first known subatomic particles. The earliest version of the CRT was the “Braun tube,” invented by German physicist Ferdinand Braun in 1897 [7, 8]. This early tube was a cold-cathode diode. It was a modification of the Crookes tube and included a phosphor-coated screen. Color CRTs built on this idea by using three different phosphors that emit red, green, and blue light. These phosphors were arranged in clusters or stripes called “triads” [9]. To create excitement, color CRTs used three separate electron guns—one for each primary color—arranged either in a line or in an equilateral triangle. This innovation laid the groundwork for color display systems, which later influenced the development of new display technologies.

After CRTs, the focus shifted to plasma display technology, with OLEDs discussed earlier. Plasma displays were mainly used in large televisions and public information screens. Plasma screens function through the ionization of noble gases (commonly xenon and neon) contained in tiny cells. When electrically excited, these gases emit ultraviolet radiation, which in turn activates phosphor coatings to produce visible images. Plasma displays consist of many small cells stacked between two glass panels that hold inert noble gas mixtures.

The benefits of plasma technology include lightweight, flat panels with wide viewing angles, thin screens, and bright images. Plasma displays can also be made very large, reaching up to 381 cm diagonally. A standard plasma panel is about 6 cm thick, with the overall unit being under 10 cm thick. However, the power consumption of plasma displays varies based on image brightness. For instance, bright scenes use significantly more energy than dark ones. While a 50-inch (127 cm) plasma screen initially consumed around 400 W, models made after 2006 were improved to run at 220–310 W in cinema mode. The latest plasma displays can last up to 60,000 hours of actual use, which is equal to 27 years at six hours per day, before the brightness drops to half its original value.

People often measure plasma display performance by its contrast ratio, which shows the difference between the brightest and darkest parts of an image. Higher contrast ratios lead to more realistic image quality. For plasma displays, contrast ratios as high as 30,000:1 have been reported, providing a notable edge over other display technologies, except for OLEDs [10–13]. On the other hand, liquid crystal displays (LCDs) are commonly found in mobile phones, laptop screens, computer monitors, televisions, digital watches, and calculator displays. In LCDs, the backlight passes through liquid crystal cells that act as light gates alongside polarized filters. In general, a liquid crystal display (LCD) is an electronic visual technology that uses the light-modulating properties of liquid crystals. LCDs are versatile. They can show both detailed images, like those on computer monitors, and simple images, such as those on digital clocks. In some cases, specific characters, digits, or words are preset using coded addressing systems. Unlike other display technologies that use large elements to create images, LCDs depend on a grid of many small pixels to form pictures. This design approach makes LCD technology unique, although its basic operating principles are similar to those of other flat-panel technologies. From the 1970s onward, LCDs grew in popularity and eventually became the leading flat-panel display technology. Due to the fierce competition among display technologies, it is important to describe and compare LCDs with OLEDs.

Liquid crystals occupy an intermediate phase between solids and liquids. Their anisotropic molecules, typically elongated or disk-like, can be reoriented by external stimuli such as electric or magnetic fields, which makes them useful in display technologies. However, liquid crystals are also very sensitive to temperature: at low temperatures, they can freeze into solids, while at high temperatures, they lose their order and become completely liquid. Two main phases of liquid crystals are recognized: the nematic phase and the smectic phase. The nematic phase is the simplest and most fluid-like, with molecules moving freely while generally aligning in one direction. In contrast, the smectic phase is more solid-like, with liquid crystal molecules organized in distinct layers. Within these layers, the molecules can move freely side to side but not between adjacent layers, while still tending to align in the same direction [14–16].

Advantages of LCD Toward Modern Life

1. LCD panels are lighter and slimmer than CRTs, which simplifies transportation and installation, especially for large screens. For example, buyers of large-screen LCD televisions usually only need two family members to help move them into their homes, unlike the heavier and bulkier CRT televisions.
2. LCD technology uses relatively low power. Depending on brightness levels and the type of content shown, older backlit models generally consumed 30% to 50% of the power needed by CRT monitors. Modern LED-backlit LCD models typically use only 10% to 25% of the power of a similar CRT monitor.
3. Because they require less power, LCDs generate very little heat during use compared to CRTs.

4. LCD operation does not result in geometric distortion, which keeps the displayed image clear.
5. Sometimes, a slight flicker may occur based on the specific backlight technology used.
6. LCD pixels can hold their state between refresh cycles, which removes refresh-rate flicker. This is often an issue in CRT monitors.
7. As mentioned earlier, LCD technology is much thinner than CRT monitors. This feature allows LCD monitors to be placed farther away from the user and helps reduce eye strain during long periods of use.
8. LCDs can produce sharp images with minimal smearing when they operate at their native resolution.
9. During use, LCD technology emits much less unwanted electromagnetic radiation compared to CRT displays, making it safer for users.
10. According to the literature, there is no theoretical limit to the resolution that LCD technology can achieve. When multiple LCD panels are combined to create a single image, this setup is called “stacked resolution.”
11. LCD technology also allows for the production of very large display sizes, typically over 150 cm in diagonal measurement.

Disadvantages of LCD in Display Technology

1. In general, older LCD monitors exhibited a limited viewing angle. Even within the specified viewing range, both contrast and brightness tended to vary depending on the viewer’s position relative to the screen.
2. In earlier models, uneven backlighting was often observed, which contributed to noticeable brightness distortions, particularly toward the edges and boundaries of the display.
3. Since liquid crystal elements cannot completely obstruct backlight, LCDs sometimes display weak black levels, leading to reduced contrast in darker images.
4. A significant issue related to eye strain arises from the use of strobing backlights in LCDs. While strobing helps to reduce motion blur caused by the relatively slow response times of liquid crystals, it can simultaneously contribute to visual discomfort and fatigue.
5. Since 2012, most LCD backlighting systems have employed pulse-width modulation (PWM) to regulate screen brightness. However, PWM can produce flickering effects that are more noticeable than those of CRT displays operating at 85 Hz. For some users, this effect is particularly responsible for eye strain and visual discomfort.
6. LCDs typically support only one native resolution. Displaying any other resolution requires the use of a video scaler, which may introduce image fuzziness. Alternatively, running the display in a 1:1 pixel-mapping mode preserves image sharpness but fails to fill the entire screen area, leading to unused display space.

7. LCD technology also suffers from fixed bit depth limitations. Many commercially available low-cost LCDs are capable of displaying only 262,000 colors, which is significantly lower than the full 16.7 million colors supported by higher-quality displays.

Conclusions:

Thin films provide many benefits in semiconductor devices. They allow for the creation of both spherical and anisotropic nanoparticles with distinct functional properties. These nanoparticles are commonly used in various applications because they are low-cost, use less material, and have excellent electronic, magnetic, catalytic, and optical features. Additionally, it is possible to produce stable nanoparticle-based thin films, CNT-nanoparticle/nanocomposite films, hybrid nanoparticle/organic thin films, and hybrid nanoparticle/oxide thin films through wet-chemical methods, electrodeposition, and microwave techniques. These thin-film structures show better efficiency and improved control over surface properties, making them suitable for targeted applications.

The growth technique used to make thin films is very important. Different methods yield films with different physical and chemical properties, even when starting with the same precursor materials. Therefore, the overall properties of thin films depend not only on their composition but also on their structure, microstructure, and any impurities present. This emphasizes the need to carefully control process parameters to tailor the characteristics of thin films on various substrates. Research indicates that the performance improvements of thin films across various applications are closely related to their surface-to-volume ratio. However, managing the grain size of these thin films remains a significant research challenge. The long-term stability of nanocrystalline thin films is another critical issue currently being studied. Thus, both the application and performance of thin-film-based devices depend largely on the fabrication methods and growth techniques used.

Thin-film technology supports several device applications, including solar cells, chemical and biological sensors, organic photovoltaic devices, and thin-film transistors. Moreover, additive manufacturing processes for thin films offer numerous benefits, such as creating uniform circuit lines, enhancing electrical and mechanical performance, producing thinner and more flexible circuits, achieving high-density resolution patterns, and improving surface parameter control. These methods are also efficient and require less precious metal for device production while delivering superior physical and electrical performance.

From this discussion, it is evident that proper fabrication, structural adjustment, and device integration of thin films in optoelectronic applications lead to better performance control and enhanced characterization. These advancements are expected to bring significant changes to display technology and help develop commercially viable next-generation electronic and optoelectronic systems.

References:

1. Tang, C. W., Vanslyke, S. A., & Chen, C. H. (1989). Electroluminescence of doped organic thin films. *Journal of Applied Physics*, 65(9), 3610–3616.
2. Chun, H. Y., Gu, F. H., & Rong, Q. W. (2000). Properties of organic thin films prepared by vacuum deposition. *Thin Solid Films*, 363(1–2), 218–222.
3. Cao, Y., Parker, I. D., & Yu, G. (1998). Improved quantum efficiency for electroluminescence in semiconducting polymers. *Nature*, 397, 414–417.
4. Lu, Z. L., Yuan, T. S., & Zhu, W. G. (2000). Carrier injection in organic light-emitting diodes. *Chinese Physics Letters*, 17(11), 773–776.
5. Chen, X. H., Xu, Z., & Hou, Y. B. (2002). Interface studies in organic light-emitting diodes. *Chinese Physics Letters*, 19(2), 1697–1700.
6. About.com. (2009, October 4). History of the cathode ray tube. Retrieved from <https://www.about.com>
7. Braun, F. (1897). Ueber ein Verfahren zur Demonstration und zum Studium des zeitlichen Verlaufs variabler Ströme [On a process for the display and study of the course in time of variable currents]. *Annalen der Physik und Chemie*, 3(60), 552–559.
8. Advameg, Inc. (2008, April 27). Cathode ray tube. *Medical Discoveries*. Retrieved from <https://www.medicaldiscoveries.com>
9. bit-tech.net. (2009, October 4). How CRT and LCD monitors work. Retrieved from <https://www.bit-tech.net>
10. Pope, M., Kallmann, H. P., & Magnante, P. (1963). Electroluminescence in organic crystals. *Journal of Chemical Physics*, 38, 2042–2043.
11. Kido, J., & Lizumi, Y. (1998). Electroluminescent devices based on polymer blends. *Applied Physics Letters*, 73(19), 2721–2723.
12. Kido, J., & Matsumoto, T. (1998). Bright white light-emitting organic electroluminescent devices having a multilayer structure. *Applied Physics Letters*, 73(20), 2866–2868.
13. Deng, Z. B., Ding, X. M., & Lee, S. T. (1999). Efficient electroluminescence from doped organic light-emitting devices. *Applied Physics Letters*, 74(2), 2227–2229.
14. Wu, C. C., Wu, C. I., Sturm, J. C., & Kahn, A. (1997). Organic light-emitting devices with improved carrier injection using indium-tin-oxide anodes treated with oxygen plasma. *Applied Physics Letters*, 70(11), 1348–1350.
15. Nuesch, F., Rothberg, L. J., Forsythe, E. W., Le, Q. T., & Gao, Y. L. (1999). Charge injection and transport studies of organic light-emitting diodes with doped hole-transport layers. *Applied Physics Letters*, 74(6), 880–882.
16. Jabbour, G. E., Kippelen, B., Armstrong, N. R., & Peyghambarian, N. (1998). Photovoltaic cells based on dye-sensitized organic–inorganic composites. *Applied Physics Letters*, 73(9), 1185–1187.

CHALLENGES OF NEXT-GEN RESEARCH: RISKS AND OPPORTUNITIES

Sandeep Nivruttirao Niwadange*,

Hemraj Madhukar Meshram and Trupta Devrao Wakde

Department of Chemistry,

Shri Govindrao Munghate Arts & Science College, Kurkheda. Gadchiroli 441 209 M.S.

*Corresponding author Email: sandip.niwadange@gmail.com

Abstract:

Next-generation (Next-Gen) research, spanning artificial intelligence, biotechnology, nanotechnology, quantum computing, and space exploration, promises transformative benefits for humanity. These innovations can drive medical breakthroughs, sustainability, and digital progress, yet they also pose ethical, social, environmental, and security challenges. Risks include genetic manipulation, algorithmic bias, widening inequalities, workforce disruptions, and geopolitical tensions. This chapter examines the dual nature of Next-Gen research—its opportunities and inherent risks—through critical analysis and case studies such as CRISPR, AI in healthcare, renewable energy transitions, and COVID-19 vaccine development. It highlights strategies for ethical governance, inclusive innovation, and interdisciplinary collaboration, stressing that the success of Next-Gen research lies not only in technological advancement but in society's ability to manage its consequences responsibly and equitably.

Introduction:

The 21st century has witnessed an unprecedented acceleration in science and technology, reshaping economies, societies, and cultures at a global scale. Innovations in artificial intelligence (AI), biotechnology, quantum computing, nanotechnology, and space exploration promise transformative benefits for humanity. Yet, these advances are not without profound challenges. Next-generation (Next-Gen) research often involves high costs, ethical dilemmas, environmental concerns, and geopolitical tensions.

Scientific research is entering a transformative era marked by rapid advances in artificial intelligence, biotechnology, nanotechnology, quantum science, and space exploration. Collectively referred to as next-generation (Next-Gen) research, these innovations hold the potential to solve some of humanity's most pressing challenges, from curing genetic diseases to mitigating climate change and expanding sustainable energy resources. At the same time, such breakthroughs bring new risks and uncertainties. Ethical dilemmas surrounding genetic engineering, environmental impacts of advanced technologies, widening inequalities in access, and threats to global security all underscore the complexity of balancing progress with

responsibility. This chapter explores these opportunities and challenges, offering insights into how societies can harness the promise of Next-Gen research while addressing the risks that accompany it.

Defining Next-Gen Research:-

Next-Gen research refers to cutting-edge, interdisciplinary scientific inquiries and technological innovations that push the boundaries of existing knowledge. This includes:

- ❖ Artificial Intelligence (AI) and Machine Learning for automation and decision-making.
- ❖ Biotechnology and Genomics for personalized medicine and sustainable agriculture.
- ❖ Nanotechnology and Materials Science for smart devices and energy solutions.
- ❖ Quantum Computing for advanced problem-solving and cryptography.
- ❖ Space Exploration and Astrobiology for planetary colonization and resource utilization.
- ❖ Green and Sustainable Technologies for addressing climate change.

Opportunities in Next-Gen Research:

Next-generation (Next-Gen) research opens vast possibilities for scientific, technological, and social transformation. By integrating interdisciplinary approaches and harnessing advanced tools, it has the potential to address global challenges while improving quality of life. The key opportunities include:

Medical Breakthroughs and Healthcare Innovation:

Biotechnology, genomics, and nanomedicine are revolutionizing healthcare. Personalized medicine—tailored to an individual’s genetic makeup—promises more effective treatments with fewer side effects. CRISPR-Cas9 gene-editing technology has opened pathways to correct genetic disorders, while nanorobots are being explored for targeted drug delivery. Artificial intelligence (AI) is enhancing diagnostic accuracy and accelerating drug discovery, reducing the time and cost of bringing new medicines to market. These developments point toward a future where healthcare becomes more preventive, precise, and accessible.

Sustainable Development and Climate Action:

Next-Gen research plays a critical role in building a sustainable future. Advances in green chemistry, renewable energy technologies (solar, wind, hydrogen fuel cells), and energy storage solutions offer pathways to reduce dependence on fossil fuels. Carbon capture and utilization technologies, coupled with bio-inspired materials, provide innovative solutions to mitigate climate change. Additionally, biotechnology can improve agricultural productivity through drought-resistant crops and sustainable farming practices, directly supporting food security.

Digital Transformation and Smart Societies:

The rapid growth of AI, Internet of Things (IoT), big data analytics, and quantum computing is transforming industries, governance, and daily life. Smart cities equipped with sensor-based infrastructure can optimize energy usage, waste management, and transportation systems,

improving urban sustainability. In education, digital platforms and AI tutors are making personalized learning accessible across socio-economic divides. Quantum technologies further hold the promise of solving complex scientific problems, from materials discovery to advanced cryptography.

Economic Growth and Industry 4.0:

Next-Gen technologies are fueling the Fourth Industrial Revolution (Industry 4.0), where automation, robotics, and advanced manufacturing reshape production systems. This transition creates new business models, startups, and global markets. Biotechnology-driven bioeconomies, renewable energy industries, and AI-powered enterprises are becoming engines of economic growth, opening opportunities for job creation in high-tech sectors, even as traditional employment patterns evolve.

Space Exploration and Resource Expansion:

Advancements in space science present opportunities beyond Earth. The Artemis program and private sector initiatives such as SpaceX are paving the way for lunar bases, Mars colonization, and interplanetary travel. Asteroid mining offers potential access to rare minerals, easing resource scarcity on Earth. Research in astrobiology expands our understanding of life in the universe, while space-based solar power concepts could provide sustainable energy solutions.

Social Transformation and Human Development

Beyond science and industry, Next-Gen research enhances human well-being and societal progress. Advanced communication technologies reduce barriers between people and nations, while breakthroughs in prosthetics, brain-computer interfaces, and assistive devices improve the quality of life for differently-abled individuals. Furthermore, equitable application of these innovations can help bridge social divides, empowering marginalized communities and creating more inclusive societies.

Opportunities in Next-Gen research lie at the intersection of scientific innovation and societal needs. From revolutionizing healthcare and enabling sustainable development to driving economic growth and exploring new frontiers in space, these advances carry the potential to redefine the human experience. If harnessed responsibly, Next-Gen research can guide humanity toward a more sustainable, equitable, and prosperous future.

Risks in Next-Gen Research:

While next-generation (Next-Gen) research offers groundbreaking opportunities, it also brings with it significant risks. These risks span across ethical, environmental, economic, social, and geopolitical dimensions, demanding careful attention to ensure innovation benefits humanity without causing harm.

1. Ethical and Moral Dilemmas:

Technologies like gene editing, artificial intelligence, and human enhancement raise profound ethical questions. CRISPR-based genetic modifications may lead to “designer babies,” raising concerns about altering human evolution. Similarly, AI systems often inherit biases from their training data, which can lead to discriminatory outcomes in areas such as hiring, law enforcement, and healthcare. Without strong ethical frameworks, these advances may undermine human dignity and justice.

2. Environmental Impacts:

Next-Gen innovations, while aimed at sustainability, can create new environmental burdens. The large-scale production of nanomaterials introduces unknown toxicological risks, potentially affecting ecosystems and human health. Energy-intensive technologies such as block chain and quantum computing can significantly increase carbon emissions if not powered by renewables. Additionally, growing electronic waste from rapid technological turnover poses a serious challenge to waste management and environmental protection.

3. Inequality and Accessibility Gaps:

There is a danger that advanced technologies will primarily benefit wealthy nations and individuals, widening the global digital divide. Developing countries may struggle to access cutting-edge healthcare, renewable energy systems, or AI-driven education. Within societies, the high cost of innovations may create a disparity between those who can afford them and those who cannot, leading to increased social stratification.

4. Economic and Employment Disruptions:

Automation, robotics, and AI-driven decision-making are rapidly transforming industries. While they increase productivity, they also displace traditional jobs. Millions of workers may require reskilling, and societies unprepared for these transitions risk rising unemployment, income inequality, and social unrest. Small businesses and traditional industries could struggle to compete in an AI-dominated economy.

5. Security and Geopolitical Risks:

Next-Gen research carries profound security implications. Quantum computing could render current encryption systems obsolete, threatening global cyber security. Advances in synthetic biology raise fears of bioterrorism through engineered pathogens. Meanwhile, technological supremacy may fuel geopolitical rivalries, with nations competing for dominance in AI, space exploration, and biotechnology, potentially destabilizing international relations.

6. Public Distrust and Misinformation:

Rapid scientific progress often outpaces public understanding, creating fear and resistance. For example, vaccine hesitancy during the COVID-19 pandemic highlighted the risks of misinformation undermining public health. A lack of transparency in AI systems (the “black box

problem”) also fuels distrust. If societies do not engage the public in open dialogue about emerging technologies, resistance and skepticism may block beneficial innovations.

7. Unintended Consequences of Innovation:

Many Next-Gen technologies are still in their infancy, making their long-term impacts uncertain. For instance, while autonomous vehicles promise safer transportation, they may introduce new vulnerabilities such as system failures or cyberattacks. Similarly, human–AI collaboration may result in unforeseen behavioral, psychological, or social shifts that societies are unprepared to address.

Table 1: Opportunities vs Risks in Next-Gen Research

Opportunities	Risks
Medical Breakthroughs – Personalized medicine, gene editing (CRISPR), nanomedicine, and AI-driven diagnostics improve healthcare and life expectancy.	Ethical Dilemmas – Genetic manipulation may lead to 'designer babies,' AI bias raises fairness issues, and human enhancement challenges moral boundaries.
Sustainable Development – Renewable energy, green chemistry, and sustainable agriculture help mitigate climate change and ensure food security.	Environmental Impacts – Production of nanomaterials, electronic waste, and high energy use in quantum computing may harm ecosystems.
Digital Transformation – AI, IoT, big data, and quantum computing enhance smart cities, personalized learning, and scientific discovery.	Inequality & Accessibility Gaps – Developing nations and marginalized groups may lack access to advanced technologies, widening the digital divide.
Economic Growth (Industry 4.0) – Automation, robotics, and biotechnology create new industries, startups, and global markets.	Job Disruptions – Automation displaces traditional jobs; millions may require reskilling, risking unemployment and inequality.
Space Exploration & Resource Expansion – Asteroid mining, Mars colonization, and space-based energy solutions expand human frontiers and resources.	Geopolitical & Security Threats – Quantum computing threatens cybersecurity, synthetic biology risks bioterrorism, and technology races may fuel conflicts.
Social Transformation – Assistive technologies, brain-computer interfaces, and inclusive digital platforms improve quality of life and accessibility.	Public Distrust & Misinformation – Lack of transparency and misinformation (e.g., vaccine hesitancy) reduce public trust in science.
Human Development & Global Collaboration – Interdisciplinary research fosters innovation and global problem-solving.	Unintended Consequences – Emerging technologies may have unpredictable long-term impacts (e.g., autonomous vehicles, AI dependency).

The risks of Next-Gen research demonstrate that innovation cannot be separated from responsibility. Ethical challenges, ecological pressures, inequalities, and security threats must be proactively managed through strong governance, inclusive access, and global cooperation. Only then can humanity ensure that the benefits of Next-Gen research outweigh its dangers.

Conclusion:

Next-generation research is a powerful force reshaping the trajectory of science, technology, and society. From medical breakthroughs and sustainable innovations to space exploration and digital transformation, the opportunities are immense and far-reaching. Yet, these advancements are accompanied by risks—ethical dilemmas, environmental impacts, social inequalities, and security concerns—that cannot be ignored. The challenge lies in striking a balance between innovation and responsibility, ensuring that progress benefits humanity while minimizing harm. By fostering global collaboration, embedding ethical frameworks, and prioritizing inclusivity, societies can harness the potential of Next-Gen research to create a future that is both transformative and sustainable.

References:

1. Brynjolfsson, E., & McAfee, A. (2017). *Machine, Platform, Crowd: Harnessing Our Digital Future*. W.W. Norton & Company.
2. Doudna, J. A., & Charpentier, E. (2014). The new frontier of genome engineering with CRISPR-Cas9. *Science*, 346(6213), 1258096.
3. Fukuyama, F. (2002). *Our Posthuman Future: Consequences of the Biotechnology Revolution*. Farrar, Straus and Giroux.
4. McKinsey Global Institute. (2017). *Jobs lost, jobs gained: Workforce transitions in a time of automation*.
5. NASA. (2020). *NASA's Artemis Program*. Retrieved from <https://www.nasa.gov>.
6. National Academies of Sciences, Engineering, and Medicine. (2018). *Globalization of Science and Security Risks*. Washington, DC: The National Academies Press.
7. Royal Society & Royal Academy of Engineering. (2004). *Nanoscience and nanotechnologies: Opportunities and uncertainties*.
8. UNESCO. (2021). *UNESCO Science Report: The Race Against Time for Smarter Development*.
9. World Bank. (2019). *World Development Report 2019: The Changing Nature of Work*.
10. World Health Organization (WHO). (2020). *Vaccine Hesitancy: A Growing Challenge*.

HOW IMPORTANT IS THE USE OF MEDICAL APPLICATIONS IN LIFE TO STAY HEALTHY

**Raj Kumar Singh Bharti*¹, Sushil Kumar¹, Asheesh Kumar Gupta¹,
Dharamveer Singh², Swatantr Bahadur Singh¹ Amit Kumar³ and Anil Kumar⁴**

¹Faculty of Pharmacy, School of Pharmaceutical Sciences,
IFTM University Lodhipur Rajput, Moradabad, Uttar Pradesh, India. Pin 244102.

²Shree ji institute of Pharmaceutical Education & Research Sikarpur Sarai Road,
Vill- Bichola Dhooki, Moradabad, Uttar Pradesh, India. Pin 244411.

³MIT College of Pharmacy, Ram Ganga Vihar Phase II, Moradabad. 244001.

⁴Maa Gayatri College of Pharmacy College of Pharmacy,
Kanth road Moradabad Pin- 244001

*Corresponding author E-mail: rajroy.ars@gmail.com

Abstract:

Health technology apps that address a variety of needs, from mental health assistance and chronic disease monitoring to fitness tracking and food management, have proliferated in the Indian market. With its all-inclusive approach to healthy living, which includes individualized meal programs, workout regimens, and professional advice from licensed dietitians and fitness instructors, one such app, HealthifyMe, has been incredibly popular. Similar to this, the highly regarded app Practo has made it easier for people to identify and schedule appointments with doctors, providing a practical way for them to get high-quality medical care.

Keyword: Fitness, Doctors, Medical Application, Mental and Technology

Introduction:

Healthcare Software refers to diagnostic products, therapeutic and prophylactic drugs, or vaccines intended for the diagnosis, prevention, or treatment of disease in humans, animals, or plants, as well as all discovery, research, development, and marketing efforts to support those uses, including but not limited to gene function elucidation and target validation. These apps provide numerous and significant tangible health benefits. First, they promote a proactive approach to wellness by encouraging people to live better lives. Apps like Cure. fit and HealthifyMe offer tailored exercise programs and nutrition plans, empowering users to make informed choices about their physical activity and dietary habits.

A 'Healthcare Software' is a software program designed for smart mobile devices that employs behavioral intervention technologies to assist a patient-centered approach to healthcare management.



Figure 1: Healthcare application

Healthcare Application

A healthcare application is a digital tool that can be used on a mobile phone or tablet PC to gather, manage, exchange, and save personal health information in order to improve health service understanding, technique, and delivery. Healthcare applications come in a variety of products and uses to support and promote high-quality public health. They connect patients with essential health services, facilities, and treatment needs. Examples include-

Aarogya Setu

Aarogya Setu is an Indian COVID-19 "contact tracing, syndromic mapping, and selfassessment" digital application, principally a smartphone app, created by the National Informatics Centre of the Ministry of Electronics and Information Technology. In just 40 days, the software received over 100 million installs. Aarogya Setu is a smartphone application produced by the Indian government that connects the country's population to numerous critical health services.

HealthifyMe

Healthify offers personalised diet plans from experienced nutritionists as well as customised workout routines from certified fitness instructors.

Talkspace

Talkspace is an online treatment platform that provides people access to professional therapists and psychiatrists from anywhere using their mobile app and internet by computer.

Cure.fit

Cure.fit is a healthcare firm that uses technology and data to help people live healthier lives and gain access to affordable healthcare. It provides both online and offline experiences in exercise, nutrition, and mental health through four verticals that are holistically linked.

Practo

The Practo app gives you access to a large network of clinics and doctors who offer online consultations to patients around the country. Patients can communicate directly with the doctors they consult. The software uses Google Maps to locate doctors near patients.

Healthians

Healthians is India's largest Health Test at Home service provider, delivering medical exams and health test packages to your home.

Sleep Cycle: Sleep Tracker

Relieve tension, sleep better, and wake up refreshed. Sleep Cycle is your personal sleep tracker and smart alarm clock with a variety of functions (including a snore recorder, sleep calculator, and sleep assistance - complete with bedtime stories and sleep music) to help you get a good night's sleep and wake up more easily. You will be in a better mood, feeling refreshed and focused throughout the day.



Figure 2: Sleep Cycle app

Medical Records

The Android Medical data App allows you to effortlessly preserve anamnesis, medical data, patient history, and medical records.

BetterHelp

BetterHelp is a psychological wellness (Mental health) platform that offers direct online counselling and therapy through web or phone text contact.

MyFitnessPal



Figure 3: myfitnesspal

MyFitnessPal is a smartphone app and website for measuring your health and fitness levels.

MyFitnessPal is one of the best weight loss apps and fitness apps, helping nearly 1 million members reach their nutrition and fitness.

Lifesum

Lifesum improves your well-being by providing food and nutrition insights while developing sustainable habits - begin your health journey today.

Calm

Calm is the #1 mental health app that helps you handle anxiety, rest more effectively, and live a more joyful, healthier lifestyle. Research-based tools can help you develop life-changing habits to improve your mental health. It offers meditation goods like as guided meditations and Sleep Stories through its subscription-based app.

Headspace

Headspace is an all-in-one emotional health app. Whether you want to enhance your sleep, handle daily worry, or communicate with a mental health coach, these tried-and-true tools will help you care for your mind. Text with mental health coaches to set goals and receive daily assistance.

Anytime Workouts

As an Anytime Fitness club participant, you will receive dozens of goal-based multi-week fitness plans, a library of over 1,100 exercises, and access to over 7,000 exercise images and videos to create your sessions.

mySugr app

The mySugr app allows users to log crucial therapeutic data such as blood sugar, meals, activity, insulin, and much more. It also assists in calculating the appropriate amount of insulin for corrections and mealtimes.

Clue

Track your monthly cycle with Clue, the 1 doctor-recommended free period monitor app created in conjunction with top health researchers.

Health & Fitness Tracker

Health Infinity is an all-in-one health and fitness tracker that helps you achieve your health goals, lose weight, make healthier food choices, and stay healthy. Weight loss tracker, water intake reminders, calorie counter, activities, exercise and workout tracker, sleep tracker, heart rate monitor, step counter (pedometer), medicine reminder, and much more all in one app.

The proliferation of health technology apps has also eased the incorporation of preventative care and wellness promotion into daily routines. Apps such as Health Kart and Practo Healthfeed gather content from medical specialists on diet, fitness, mental health, and illness prevention. These apps support informed decision-making and improve health literacy by spreading credible and accessible health information to users. Some applications also provide personalised wellness coaching, which assists people in developing long-term habits and lifestyles.

Now days, the patients who utilise mobile healthcare apps can participate in telemedicine, such as doctor-on-demand, and receive expert medical advice and diagnosis via live video. These platforms help patients schedule appointments easily and communicate with healthcare practitioners in real time, making care more accessible. The medical history can be swiftly evaluated to gain a better grasp of the patient's symptoms and approve treatment recommendations faster. Healthy lifestyle apps can monitor weight goals, sleep-wake cycles, women's health, and anxiety levels. Patients might also benefit from apps that offer instructional information about drug responses, trauma events, medicine combinations, and other issues. Assessment of risk programs let clinicians evaluate innovative clinical techniques for patients with chronic conditions. Risk circumstances are evaluated using specialized computation methods that examine several variables that influence patient health outcomes, allowing doctors to make more accurate treatment decisions.

Application Development Process

Creating a healthcare app follows a structured process that includes market research and planning, defining app features, selecting technology, designing the UI/UX, building and testing, defining monetization, and lastly deploying, supporting, and updating the app.

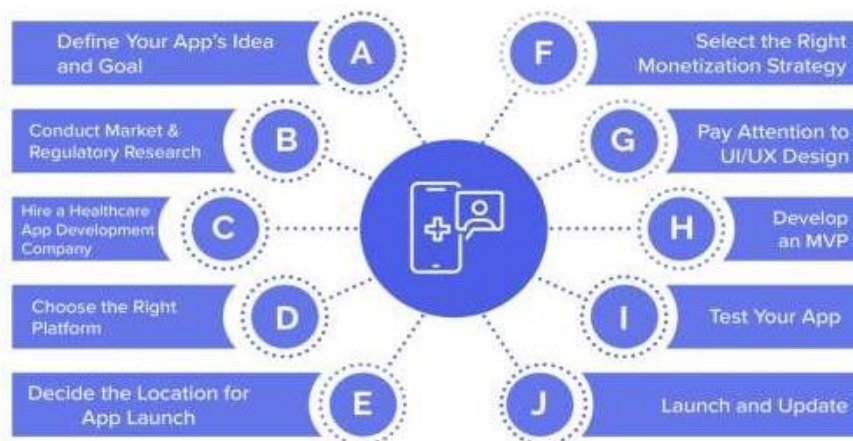


Figure 4: App Development Process

The Benefits of Medical Applications

3.1. Increased Patient Loyalty: Consumers are increasingly turning to technology to personalise treatment for their unique requirements. Patient loyalty is increased by fast digital medical services that deliver high-quality care outcomes. Patients believe their health concerns are being addressed effectively and with minimal effort.

3.2. Easy Access to Individual Care: Applications for healthcare are easy to use and allow patients to select a provider that meets their individual needs. Patients get immediate access to physicians or specialists as soon as their health problems indicate bad indicators, and symptoms are effectively managed with health advice or medications.

3.3. Chronic Disease Management: People with long-term conditions, such as heart disease and high blood pressure, can easily manage daily symptoms and monitor medication adherence. The program allows providers to monitor patient data and provide input on treatment regimens to enhance health outcomes.

3.4. Better Patient Enablement: Healthcare applications provide patients with simple medical information, allowing them to learn how to cure a variety of symptoms and diseases. Patients are provided with expert knowledge in an easy-to-use format, which can help them navigate better treatment journeys.

3.5. Provide Fast Medical Services: Instead of requiring in-person visits, patients can rapidly communicate with clinicians. Patients spend less time waiting for therapy and can easily begin taking new medications or schedule in-person scans, ultrasounds, and blood tests.

3.6. Reduced Medical Costs: Healthcare applications allow patients to pay per service or have visits covered by insurance plans, which lower the overall cost of medical visits. Patients pay for healthcare when they need it most and receive the same high-quality care.

3.7. Integration with Wearable's: Wearable gadgets collect critical data on health vitals, ailments, and symptoms, which physicians utilise to tailor patient treatment programs. Healthcare applications can be digitally connected to wearable insights, allowing patients to monitor real-time health data and make necessary modifications.

3.8. Improved Data Collection: Provider applications for healthcare collect data from patients' medical histories and allow physicians to quickly make better diagnoses and treatment recommendations. Providers can easily update, view, and share patient health information with other healthcare professionals, allowing them to better manage test results and prescription histories.

Conclusion:

The use of personal mobile devices in work and learning organizations is predicted to increase due to possible benefits in medical healthcare. Now day's use of these mobile devices is increasing very rapidly. Every person has his own smartphone. Many diseases can be treated and cured by downloading medical health related apps such as Lifesum, Calm, Headspace, Healthifyme, talkspace, curefit, Practo and Healthians in the smartphone. So people should use mobile phones for good deeds and download medical application related apps.

References:

1. PwC India. (n.d.). *Digital healthcare*. <https://www.pwc.in/industries/healthcare/digitalhealthcare.html>. Accessed May 19, 2024.
2. Onsurity. (n.d.). *Fitness apps in India*. <https://www.onsurity.com/blog/fitnessapps/>. Accessed May 19, 2024.

3. Healthline. (2024). *Talkspace review 2024: Our testers talk features, cost, and more.* <https://www.healthline.com/health/talkspace-reviews#how-it-works>. Accessed May 19, 2024.
4. Beato App. (n.d.). *Continuous glucose monitoring | Transforming diabetes management with CGM devices.* <https://www.beatoapp.com/blog/continuous-glucose-monitoring-transforming-diabetes-management-with-cgm-devices/>. Accessed May 19, 2024.
5. Gupta, P., Choudhury, R., & Kotwal, A. (2023). Achieving health equity through healthcare technology: Perspective from India. *Journal of Family Medicine and Primary Care*, 12(9), 1814–1817.
6. Ventola, C. L. (2014). Mobile devices and apps for health care professionals: Uses and benefits. *P & T*, 39(5), 356–364.
7. Faulds, M. C., Bauchmüller, K., Miller, D., Rosser, J. H., Shuker, K., Wrench, I., Wilson, P., & Mills, G. H. (2016). Feasibility of using “bring your own device” (BYOD) technology for electronic data capture in multicentre medical audit and research. *Anaesthesia*, 71, 58–66.
8. Kehoe, B. (2013). Mobility matters: BYOD—Proceed with caution. *Hospital & Health Networks*, 87, 17.

FARMER RIGHTS IN THE MEDICINAL PLANT SECTOR

Pooja Barthwal*, Girish Chandra and Kamla Dhyani

SGRR University, Dehradun

Corresponding author E-mail: poojabarthwal30@gmail.com

Abstract:

The growing demand for medicinal plants presents both opportunities and challenges for the farmers who cultivate them. These plants, integral to traditional medicine and modern wellness industries, are often produced by farmers in rural and indigenous communities, who possess extensive knowledge and skills passed down over generations. However, the rights of these farmers are increasingly threatened by issues such as inadequate land access, unfair trade practices, and exploitation of traditional knowledge and genetic resources. Farmers frequently find themselves excluded from the economic benefits generated by the commercialization of medicinal plants, while facing legal and regulatory barriers that undermine their intellectual property rights. This chapter explores the complex landscape of farmer rights in the medicinal plant sector, focusing on the legal, economic, and social challenges they encounter. It discusses the significance of intellectual property rights (IPR), land tenure, fair trade practices, and international frameworks such as the Convention on Biological Diversity (CBD) and the Nagoya Protocol. This chapter emphasizes the need for legal reforms and empowerment strategies to ensure farmers receive fair compensation and recognition for their contributions to the sector. The chapter argues that protecting farmer rights is not only essential for the welfare of the farmers but also for the sustainable and equitable development of the global medicinal plant industry.

Keywords: Traditional Knowledge, Medicinal, Farmer Rights, Farmer, Plant

Introduction:

The cultivation of medicinal plants plays a critical role in both global healthcare systems and local economies, as these plants are integral to traditional medicine, holistic health practices, and the emerging wellness industry. Farmers, especially those in rural and indigenous communities, are often the unsung stewards of this sector, possessing valuable traditional knowledge and agricultural expertise that has been passed down through generations. Medicinal plants are used for a variety of purposes, ranging from pharmaceuticals and dietary supplements to natural remedies and cosmetics. These plants are increasingly sought after in the global market, leading to growing economic opportunities for farmers who engage in their cultivation.

However, alongside these opportunities, there are a number of challenges regarding the rights of farmers involved in the production of medicinal plants. Farmers frequently face issues related to land access, intellectual property rights (IPR), fair trade, and the commercialization of plants and

their associated traditional knowledge (Sharma, 2018). In many cases, the benefits derived from medicinal plant commercialization fail to adequately reach the farmers who are the primary cultivators. Moreover, there is growing concern over biopiracy, where companies exploit genetic resources and traditional knowledge without offering fair compensation to local communities (Shiva, 2017). As demand for medicinal plants increases, ensuring the rights of farmers becomes more critical, not only for their economic welfare but also for the sustainable use of plant biodiversity.

This chapter examines the rights of farmers within the medicinal plant sector, exploring their role in the production of these plants, the challenges they face, and the legal frameworks that aim to protect their interests. Special attention is given to issues such as land tenure, intellectual property, and fair trade, as well as the importance of legal and policy mechanisms that ensure equitable benefit-sharing from the commercialization of medicinal plants (López-Carr *et al.*, 2020). The chapter also highlights potential pathways for empowering farmers and ensuring that their contributions to the medicinal plant sector are recognized and protected.

The Role of Farmers in Medicinal Plant Production

Farmers are essential to the medicinal plant industry, acting as the primary cultivators, knowledge keepers, and protectors of plant biodiversity. Their expertise in sustainable agricultural practices ensures a steady supply of raw materials for the pharmaceutical, herbal, and cosmetic industries. The rising global demand for medicinal plants offers both opportunities and challenges, particularly for farmers in rural and indigenous communities. This section highlights the significant contributions of farmers in medicinal plant production, including their roles in cultivation, biodiversity conservation, and knowledge preservation.

1. Cultivation and Sustainable Agricultural Practices

At the core of medicinal plant production, farmers utilize a blend of traditional and modern agricultural techniques to optimize growth and yield. Since many medicinal plants require specific soil and climate conditions, farmers rely on their extensive knowledge of local ecosystems to cultivate them effectively (Sharma & Kumar, 2020). Traditional methods such as organic farming, crop rotation, and intercropping help maintain soil health while minimizing dependence on chemical fertilizers and pesticides. These sustainable practices are essential for ensuring a continuous supply of medicinal plants while reducing environmental harm (Kumar *et al.*, 2021).

2. Biodiversity Conservation of Medicinal Plants

The increased commercialization of medicinal plants has raised concerns about biodiversity loss due to overharvesting. Farmers play a crucial role in conservation by domesticating and cultivating plant species at risk of extinction (Singh *et al.*, 2019). Through initiatives like seed banks and agroforestry, farmers help preserve genetic diversity and adopt sustainable harvesting

techniques. These conservation efforts align with global biodiversity policies, such as the Convention on Biological Diversity (CBD), which underscores the importance of local communities in protecting plant species (United Nations, 2022).

3. Safeguarding Traditional Knowledge

Many farmers, particularly in indigenous communities, possess deep-rooted traditional knowledge about medicinal plants, including their healing properties, cultivation methods, and processing techniques (Gupta & Verma, 2018). However, with the commercialization of medicinal plants, concerns regarding biopiracy and the unauthorized exploitation of traditional knowledge have emerged. Regulatory frameworks like the Nagoya Protocol aim to protect farmers and indigenous communities by ensuring they receive fair benefits from the use of their knowledge and natural resources (CBD Secretariat, 2021).

4. Economic Impact and Livelihood Opportunities

The cultivation of medicinal plants provides a vital source of income, particularly in developing nations where agricultural diversification is necessary for economic stability. Many small-scale farmers engage in medicinal plant farming as an alternative livelihood, capitalizing on both local and global markets (Patel *et al.*, 2020). However, barriers such as limited market access, price instability, and exploitation by intermediaries often prevent farmers from earning fair compensation. Cooperative farming models and fair trade initiatives have been introduced to improve farmers' earnings and ensure a fairer distribution of profits along the supply chain (Choudhary & Mishra, 2021).

5. Challenges Faced by Farmers in Medicinal Plant Cultivation

Despite their significant contributions, farmers involved in medicinal plant cultivation encounter several challenges, including:

- **Limited Access to Land and Resources:** Small-scale farmers often struggle with land ownership rights and restrictive policies that limit their ability to expand cultivation (Rao *et al.*, 2022).
- **Regulatory Hurdles:** Complex legal systems governing medicinal plant trade and intellectual property rights frequently prevent farmers from reaping the full economic benefits of their crops (Shiva, 2019).
- **Environmental and Climate Risks:** Changes in climate, unpredictable weather patterns, and soil degradation negatively affect medicinal plant production and farmer livelihoods (Meena *et al.*, 2020).

6. Policy Measures to Strengthen Farmers' Role

To enhance farmers' contributions to medicinal plant production, the following policy measures should be implemented:

- **Recognition of Traditional Knowledge:** Strengthening legal frameworks to ensure fair compensation for traditional knowledge holders.
- **Training and Capacity Building:** Providing farmers with education on sustainable cultivation methods and improved market access.
- **Cooperative Farming Models:** Encouraging farmers to join cooperatives to strengthen their bargaining power and enhance economic opportunities.
- **Fair Trade Certification:** Implementing ethical trade practices to ensure that farmers receive equitable pricing for their produce.

Legal Frameworks and Protection of Farmer Rights

Various international agreements and national policies have been established to safeguard the rights of farmers involved in the cultivation of medicinal plants.

- **Convention on Biological Diversity (CBD) and the Nagoya Protocol**

The CBD, along with its Nagoya Protocol, sets out regulations regarding access to genetic resources and equitable sharing of benefits. These frameworks stress the importance of acknowledging traditional knowledge holders and ensuring they receive appropriate compensation for their role in medicinal plant research and commercialization (López-Carr *et al.*, 2020).

- **The International Treaty on Plant Genetic Resources for Food and Agriculture (ITPGRFA)**

Although primarily designed for food crops, the ITPGRFA offers a foundation for securing farmers' access to plant genetic resources and ensuring their involvement in biodiversity conservation decision-making (Tripathi & Pandey, 2019).

- **National Policies and Farmer Rights Acts**

Certain countries, such as India, have enacted specific legislation to protect farmers' rights. The Protection of Plant Varieties and Farmers' Rights Act (PPVFR Act, 2001) aim to preserve traditional agricultural practices by granting farmers legal rights over the plant varieties they cultivate and develop. This law acknowledges farmers as key contributors to biodiversity conservation (Gupta, 2021). However, challenges persist in enforcing these policies and increasing awareness among farming communities.

Challenges and Opportunity:

The medicinal plant sector presents a unique set of challenges and opportunities for farmers. While growing demand for herbal and natural remedies has increased economic prospects, many farmers, particularly those in rural and indigenous communities, face significant barriers related to land tenure, intellectual property rights, fair trade, and environmental sustainability. This section explores the key challenges and opportunities with relevant data and references.

Opportunities:

1. Rising Global Demand for Herbal Medicines

The global herbal medicine market is experiencing rapid growth, offering farmers new economic opportunities. According to Grand View Research (2023), the global herbal medicine market was valued at \$151 billion in 2022 and is projected to grow at a CAGR of 11.2% from 2023 to 2030. This increasing demand creates a lucrative market for medicinal plant farmers, especially those who adopt sustainable and organic cultivation methods.

2. Fair Trade and Organic Certification Programs

Initiatives such as the FairWild certification and organic labeling schemes offer farmers better prices and access to premium markets. A study by FAO (2022) found that farmers participating in organic certification programs earned 30–50% higher prices compared to those selling uncertified products. Countries such as India and Peru have seen successful implementation of fair-trade models that empower smallholder farmers in the medicinal plant industry (ITC, 2021).

3. Government and International Support for Farmers

Several governments and international organizations are implementing policies to protect farmer rights in the medicinal plant sector. For example, India's National AYUSH Mission provides financial incentives for farmers cultivating medicinal plants, benefiting over 500,000 farmers since its launch (NMPB, 2021). Similarly, the Nagoya Protocol on Access and Benefit Sharing (ABS) under the Convention on Biological Diversity (CBD) promotes equitable sharing of benefits arising from the commercial use of medicinal plants (CBD Secretariat, 2020).

4. Technological Advancements and Agroforestry Models

Advancements in sustainable agriculture, such as agroforestry and vertical farming, are creating new opportunities for medicinal plant farmers. A study by Lal *et al.* (2022) found that integrating medicinal plants into agroforestry systems increased farm productivity by 40% while reducing soil degradation. Mobile technology and block chain solutions are also helping farmers track supply chains, ensure fair pricing, and reduce exploitation by intermediaries (ITC, 2021).

Challenges:

1. Land Tenure and Resource Access

One of the major challenges for medicinal plant farmers is securing access to land and resources. Many medicinal plant-producing regions are located in forested or ecologically sensitive areas, leading to conflicts between conservation policies and agricultural activities (Ghosh & Sinha, 2020). In India, for example, approximately 60% of medicinal plant species are collected from the wild, with farmers facing restrictions due to conservation laws (National Medicinal Plants Board [NMPB], 2021). Additionally, in several African countries, unclear land ownership policies prevent small farmers from investing in long-term cultivation of medicinal plants (FAO, 2022).

2. Intellectual Property Rights (IPR) and Biopiracy

Biopiracy—the unauthorized commercial use of traditional knowledge—remains a significant issue for medicinal plant farmers. Large pharmaceutical and cosmetic companies have patented medicinal plant-based products without recognizing or compensating the communities that have traditionally used these plants (Shiva, 2017). A study by the World Intellectual Property Organization (WIPO, 2021) found that over 70% of medicinal plant patents filed globally fail to acknowledge the contributions of traditional knowledge holders. For example, the patenting of neem (*Azadirachta indica*) and turmeric (*Curcuma longa*) derivatives sparked global controversies, as these plants have been used in Ayurvedic medicine for centuries.

3. Exploitation and Unfair Trade Practices

Farmers in the medicinal plant sector often receive low prices for their products due to a lack of bargaining power and market access. A study by the International Trade Centre (ITC, 2021) showed that while the global trade in medicinal plants is valued at over \$60 billion annually, farmers in developing countries receive less than 10% of the final retail price. Middlemen and exporters frequently exploit small-scale farmers, preventing them from accessing fair markets. Additionally, certification requirements (such as organic and fair-trade labels) are often expensive and difficult for small farmers to obtain (Sharma & Gupta, 2019).

4. Environmental and Sustainability Issues

Overharvesting and unsustainable cultivation practices have led to the depletion of wild medicinal plant species. The International Union for Conservation of Nature (IUCN, 2022) reports that over 20% of medicinal plant species are at risk of extinction due to habitat destruction and overexploitation. For instance, wild-harvested plants like Jatamansi (*Nardostachys jatamansi*) and Sarpagandha (*Rauvolfia serpentina*) are critically endangered in parts of the Himalayas (Kala, 2021). Climate change further exacerbates these challenges by altering plant growth patterns and reducing yields.

Future Directions

The future of farmer rights in the medicinal plant sector depends on an approach that values traditional knowledge, promotes sustainability, and ensures fair access to resources. Several key areas will influence the advancement of farmer rights in this field:

1. Strengthening Legal Protections for Farmers

While international treaties like the Convention on Biological Diversity (CBD) and the Nagoya Protocol provide some protection, national governments must implement more robust legal frameworks that specifically address the rights of farmers in the medicinal plant sector. This includes securing land tenure for small-scale farmers and indigenous communities, as well as creating legal mechanisms to prevent biopiracy and the misuse of traditional knowledge.

2. Promotion of Fair Trade and Certification Models

Expanding fair trade practices and certification systems (such as organic certification) will allow farmers to receive fair compensation for their efforts. Increasing the visibility of medicinal plants in sustainable and ethical trade networks can empower farmers by providing them access to global markets while ensuring fair wages and conditions.

3. Integration of Traditional Knowledge into Modern Legal Frameworks

As biotechnological advances in the medicinal plant sector continue, it will be crucial to integrate traditional ecological knowledge into modern patent and intellectual property systems. Collaborative models between farmers, indigenous groups, and biotech companies can provide fair mechanisms for profit-sharing and intellectual property protection. Additionally, education and legal reforms that support farmers in navigating these systems will ensure that they can capitalize on the economic opportunities presented by medicinal plant markets.

4. Support for Sustainable Farming Practices

There is a growing demand for medicinal plants cultivated sustainably. Governments and NGOs should invest in training and resources to help farmers adopt sustainable farming practices that preserve biodiversity and ecosystems. Additionally, promoting agroecological methods that enhance soil health and water management could lead to long-term ecological benefits, ensuring the viability of medicinal plant production.

5. Increased Investment in Research and Development (R&D)

Investment in research that supports sustainable practices, better yields, and the development of new plant-based medicines will benefit farmers by improving productivity and marketability. Collaborative research between farmers, researchers, and healthcare professionals can foster innovations that better meet market demands while benefiting the environment and local communities.

Conclusion:

The medicinal plant sector offers a valuable opportunity to empower farmers, protect traditional knowledge, and promote sustainable farming practices. However, it also faces challenges related to intellectual property, access to markets, and legal protections. Moving forward, it is essential to create a framework that not only safeguards farmers' rights but also acknowledges their contributions to global biodiversity and healthcare.

The implementation of fair-trade initiatives, legal reforms, and sustainable farming practices will be crucial in supporting farmers in this sector. Furthermore, incorporating traditional knowledge into modern intellectual property frameworks can bridge the divide between indigenous communities and the global market, ensuring fair benefits for both farmers and corporations. By fostering collaboration, enhancing legal protections, and supporting sustainable farming

practices, the medicinal plant sector can flourish, ensuring that farmers are properly recognized, supported, and compensated for their invaluable contributions.

References:

1. CBD Secretariat. (2021). *The Nagoya Protocol on Access and Benefit-sharing: Global implementation and challenges*. United Nations Environment Programme.
2. Choudhary, R., & Mishra, S. (2021). *Fair trade and the economic empowerment of medicinal plant farmers: A case study from India*. *Agricultural Economics Journal*, 56(3), 189-204.
3. Gupta, A. K. (2021). *Protecting traditional knowledge in the age of biopiracy: Policy perspectives and farmer rights*. *Journal of Intellectual Property Law*, 27(3), 210-233.
- López-Carr, D., Sarmiento, J. F., & García, L. (2020). *Traditional knowledge and intellectual property rights: A look at the medicinal plant industry*. *Journal of Sustainable Agriculture*, 45(2), 210-222.
- Patwardhan, B., Gautam, M., & Sharma, A. (2020). *Medicinal plants, traditional knowledge, and sustainable development: Policy implications and future directions*. *Phytomedicine*, 78, 153-164.
4. Gupta, P., & Verma, R. (2018). *Traditional knowledge and medicinal plant cultivation: The role of indigenous communities*. *Ethnobotany Journal*, 14(2), 112-127.
5. Kumar, V., Sharma, A., & Reddy, M. (2021). *Sustainable cultivation of medicinal plants: A pathway to biodiversity conservation and economic growth*. *Journal of Herbal Studies*, 32(4), 76-91.
6. López-Carr, D., Sarmiento, J. F., & García, L. (2020). *Traditional knowledge and intellectual property rights: A look at the medicinal plant industry*. *Journal of Sustainable Agriculture*, 45(2), 210-222. <https://doi.org/10.1080/1531234X.2020.1743881>
7. Meena, S., Rao, P., & Singh, K. (2020). *Climate change impact on medicinal plant cultivation: Adaptation and mitigation strategies*. *Environmental Studies Journal*, 28(1), 55-72.
8. Patel, D., Joshi, M., & Shah, R. (2020). *Market access and pricing challenges for medicinal plant farmers: A review of economic barriers*. *International Journal of Agricultural Economics*, 48(2), 94-108.
9. Rao, G., Kumar, S., & Das, P. (2022). *Land tenure and resource access issues in medicinal plant farming: Implications for rural development*. *Journal of Agrarian Studies*, 39(1), 45-63.
10. Sharma, P. (2018). *Fair trade and the empowerment of farmers in the medicinal plant sector: Challenges and opportunities*. *Journal of Agricultural Economics*, 49(3), 118-134. <https://doi.org/10.1007/s12561-018-9262-9>

11. Sharma, P. (2018). *Fair trade and the empowerment of farmers in the medicinal plant sector: Challenges and opportunities*. Journal of Agricultural Economics, 49(3), 118-134.
12. Shiva, V. (2017). *Biopiracy: The plunder of nature and knowledge*. Zed Books.
13. Sharma, P., & Kumar, N. (2020). *Sustainable practices in medicinal plant farming: The role of organic agriculture*. Asian Journal of Agriculture, 15(3), 210-225.
14. Shiva, V. (2017). *Biopiracy: The plunder of nature and knowledge*. Zed Books.
15. Shiva, V. (2019). *Intellectual property rights and the exploitation of traditional knowledge in the medicinal plant industry*. Zed Books.
16. Singh, A., Verma, S., & Chatterjee, R. (2019). *Biodiversity conservation through medicinal plant cultivation: Case studies from rural India*. Environmental Conservation Journal, 26(2), 88-104.
17. Tripathi, S., & Pandey, R. (2019). *Biodiversity conservation and sustainable agriculture: The role of medicinal plant farmers*. Environmental Management Journal, 32(1), 45-61.
18. United Nations. (2022). *Convention on Biological Diversity: Progress and future directions*. United Nations Environmental Programme.

FISCHER CARBENE-MEDIATED ANNULATION REACTIONS TOWARD N-FUSED HETEROCYCLIC FRAMEWORKS

Priyabrata Roy

Department of Chemistry,
Victoria Institution (College), 78B, A.P.C. Road, Kolkata 700009, India

Corresponding author E-mail: priyo_chem@yahoo.co.in

Abstract:

This chapter presents a comprehensive exploration of novel synthetic strategies for the construction of nitrogen-containing fused heterocycles, including quinoxalines, phenazines, furoquinolines, and azahomosteroids, utilizing multicomponent reactions (MCRs) and Fischer carbene complexes (FCCs). Emphasis is placed on the one-pot generation and trapping of reactive azaisobenzofuran intermediates derived from o-alkynylheteroaryl carbonyl compounds and chromium carbene complexes. The developed methodologies facilitate the efficient and atom-economical assembly of complex polycyclic frameworks through [4+2] and unprecedented [8+2] cycloaddition reactions. Particular focus is given to the synthesis of biologically relevant scaffolds such as furoquinolinones and azahomosteroids, the latter constructed via strategic coupling of pre-functionalized A and D ring precursors, followed by in situ formation of intermediates leading to the B and C rings. The utility of these protocols is underscored by their operational simplicity, structural diversity, and potential in drug discovery and natural product synthesis.

Keywords: Fischer Carbene Complexes, Multicomponent Reactions (MCRs), Azaisobenzofuran Intermediates, [4+2] and [8+2] Cycloadditions, Fused Nitrogen Heterocycles, Azahomosteroids.

Introduction:

Heterocyclic compounds occupy a central position in organic chemistry due to their widespread occurrence in bioactive natural products, pharmaceuticals, agrochemicals, and functional materials¹. Among them, fused aza-heterocycles—structures in which nitrogen atoms are incorporated into fused ring systems—have attracted significant attention owing to their diverse biological properties and synthetic versatility². In particular, frameworks such as phenazine, quinoxaline, furoquinoline/isoquinoline, pyranoquinolinone, azahomosteroid, and aza-analogues of furanophanes serve as important scaffolds for the development of new drugs and agrochemicals².

Traditional methods for constructing these complex ring systems often rely on stepwise synthetic routes, which, while effective, are time-consuming and may involve multiple purification steps, harsh conditions, or low atom economy³. In contrast, one-pot strategies—where multiple bond-

forming transformations are executed in a single synthetic operation—offer a more efficient and sustainable alternative³. These methods reduce waste, minimize purification steps, and often improve overall yields⁴.

Among various reagents and strategies available for one-pot heterocyclic synthesis, Fischer carbene complexes have emerged as exceptionally powerful intermediates⁵. Their ability to participate in alkyne–carbene complex coupling and subsequent annulation reactions has enabled the rapid assembly of fused heterocyclic frameworks from relatively simple and accessible starting materials⁵. Notably, while most annulation strategies focus on constructing heterocyclic rings fused to a pre-existing benzene ring, fewer approaches have explored annulation onto pre-existing nitrogen-containing heterocycles—a direction that offers unique synthetic challenges and opportunities⁵.

This chapter aims to highlight a series of ring annulation strategies that utilize Fischer carbene complexes for the efficient synthesis of selected fused aza-heterocycles via one-pot or cascade reaction pathways. The discussion is organized into five major sections:

Part 1: Explores three-component one-pot syntheses of quinoxaline and phenazine ring systems.

Part 2: Focuses on the one-pot assembly of furo[2,3-h]quinoline and furo[2,3-h]isoquinoline derivatives.

Part 3: Delves into [8+2] cycloaddition reactions involving dienzylazaisobenzofurans to access furan-bridged 10-membered aza-heterocycles.

Part 4: Describes an intramolecular [4+2] cycloaddition strategy involving azaisobenzofuran intermediates to achieve aza-homosteroid skeletons in a convergent one-step fashion.

Together, these studies demonstrate the versatility and synthetic utility of Fischer carbene complexes in promoting novel heterocyclic transformations, particularly in the context of nitrogen-rich fused systems. This approach not only expands the synthetic toolbox for heterocyclic chemistry but also underscores the value of metal-carbene chemistry in modern organic synthesis.

Part 1: Explores three-component one-pot syntheses of quinoxaline and phenazine ring systems.

Literature Review / Previous Work

Quinoxaline-based compounds have garnered significant attention in the pharmaceutical field owing to their diverse therapeutic activities, including antiviral, antibacterial, anti-inflammatory, antiprotozoal, and kinase-inhibiting properties.⁶ They have also been explored for potential uses as anticancer, anthelmintic, antifungal, and insecticidal agents.⁷ Notably, the quinoxaline core forms an essential part of various antibiotic molecules such as echinomycin, levomycin, and actinomycin, which exhibit potent activity against gram-positive bacteria and show effectiveness against several transplantable tumors. Beyond biomedical applications, quinoxaline derivatives

are also utilized in functional materials such as dyes, electroluminescent devices, organic semiconductors, cavitands, molecular switches, and DNA-cleaving agents. Given this wide range of biological activities, quinoxalines are recognized as privileged scaffolds in the development of combinatorial libraries for drug discovery. Pharmaceutical formulations containing quinoxaline motifs—like lamprene for the treatment of leprosy, BMS-238497 as a kinase inhibitor, and XK-469 for anticancer therapy—are already in clinical use (Figure 2.1).

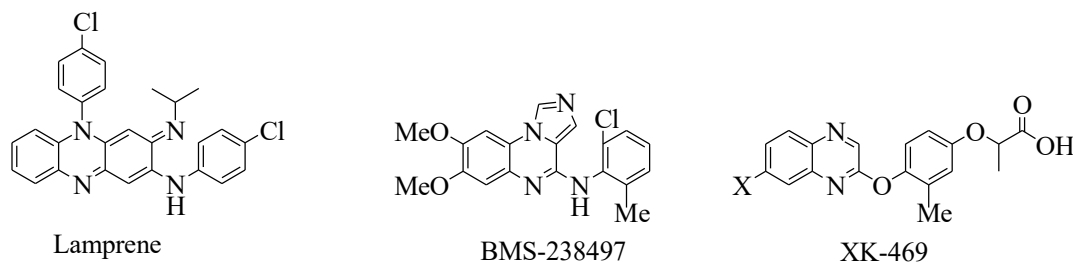


Figure 2.1: Biologically active quinoxalines

Phenazine-based natural products are primarily produced as secondary metabolites by microorganisms such as *Pseudomonas*, *Streptomyces*, and several other soil- and marine-dwelling genera. These compounds exhibit a wide range of biological functions, including antimicrobial, anticancer, antimalarial, and antiparasitic effects.⁸ The dual role of phenazine pigments as both antibiotics and virulence factors has been discussed in recent reviews.⁹ Owing to their redox-active nature, phenazines can reduce molecular oxygen to generate reactive oxygen species, which explains their broad-spectrum antimicrobial efficacy. Additionally, phenazines contribute to pathogenicity in human diseases. For instance, pyocyanin can trigger apoptosis in neutrophils, and *Pseudomonas aeruginosa* strains lacking pyocyanin production show increased susceptibility to host immune defenses in murine lung infection models. Given that individuals with cystic fibrosis often suffer from chronic colonization of the lungs by *P. aeruginosa*, which significantly reduces their life expectancy, targeting phenazine biosynthesis presents a promising strategy for therapeutic intervention.

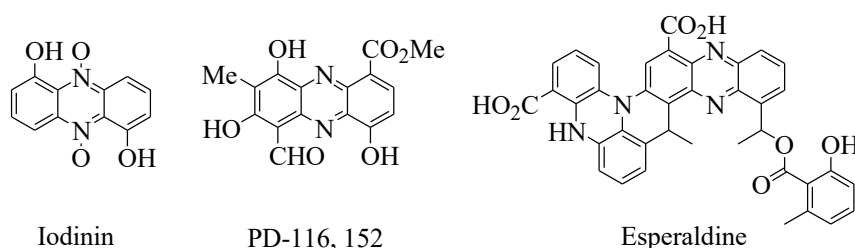
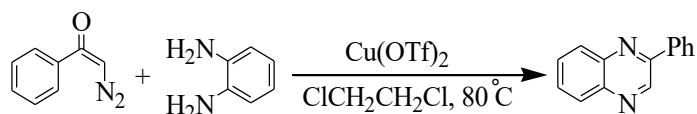


Figure 2.2: Biologically active phenazines

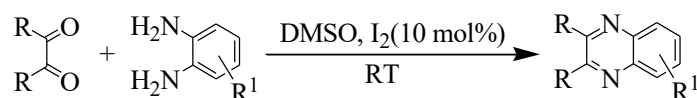
These types of heterocyclic ring systems are most frequently constructed through the annulation of a heterocyclic unit onto an already existing benzene core.¹⁰ Yadav and colleagues have reported a method for synthesizing quinoxaline derivatives by reacting α -diazoketones with aryl 1,2-diamines in the presence of 10 mol% copper(II) triflate, yielding the desired products with

excellent efficiency and selectivity. $\text{Rh}_2(\text{OAc})_4$ was also shown to be an equally competent catalyst for this transformation (Scheme 2.1).



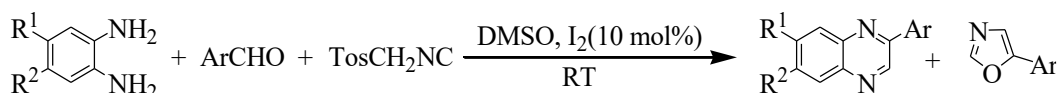
Scheme 2.1

The condensation of 1,2-dicarbonyl compounds with various substituted *o*-phenylenediamines proceeds smoothly at room temperature in DMSO, yielding functionalized quinoxalines in excellent yields when catalyzed by a small amount of molecular iodine, as demonstrated by co-workers (Scheme 2.2).¹¹



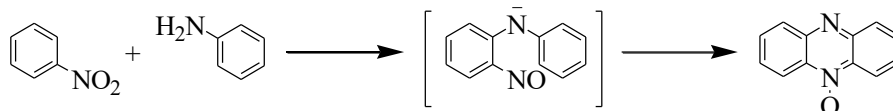
Scheme 2.2

Tsoleridis and co-workers reported a novel multicomponent reaction involving *o*-phenylenediamines, aldehydes, and *p*-toluenesulfonylmethyl isocyanide (TosMIC) in the presence of a base, which led to the efficient formation of quinoxaline derivatives in very good yields (Scheme 2.3).¹²



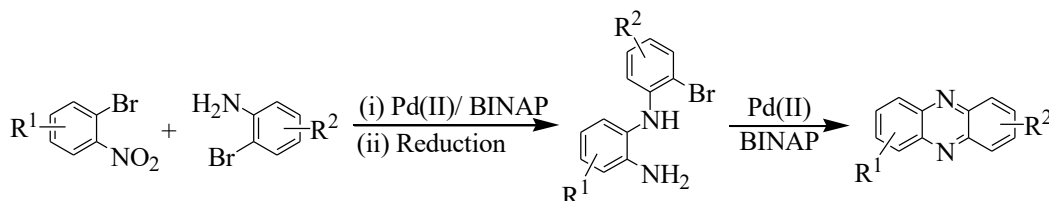
Scheme 2.3

Back in 1901, Wohl and Aue introduced an early method for synthesizing phenazines.¹³ Their procedure involved heating a mixture of anilines and nitrobenzenes to 200 °C in the presence of a strong base, resulting in the formation of phenazines or phenazine-N-oxides (Scheme 4). However, this approach suffered from certain limitations, including only moderate product yields and the generation of substantial quantities of byproducts—mainly various azacompounds—due to the harsh reaction conditions employed (Scheme 2.4).



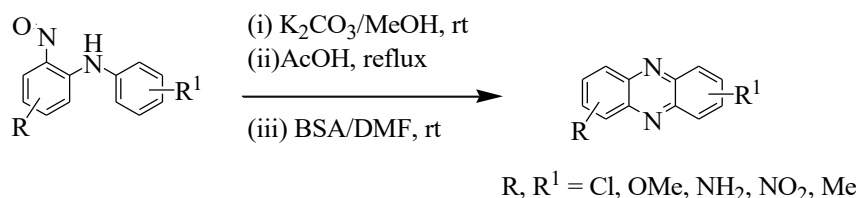
Scheme 2.4

Emoto and co-workers described the synthesis of phenazine derivatives via a sequential palladium(II)-catalyzed aryl amination process, employing BINAP as the ligand (Scheme 2.5).¹⁴



Scheme 2.5

Substituted phenazines can be synthesized through the cyclization of N-aryl-2-nitrosoanilines, which are generated by reacting nitroarenes with anilide anions. This transformation is effectively promoted using potassium carbonate in methanol, N,O-bis(trimethylsilyl)acetamide (BSA) in aprotic solvents, or acetic acid. The methodology is exemplified by the preparation of 1-methoxyphenazine—a key intermediate in the synthesis of pyocyanine—from suitable nitroarene–aniline combinations (Scheme 2.6).¹⁵

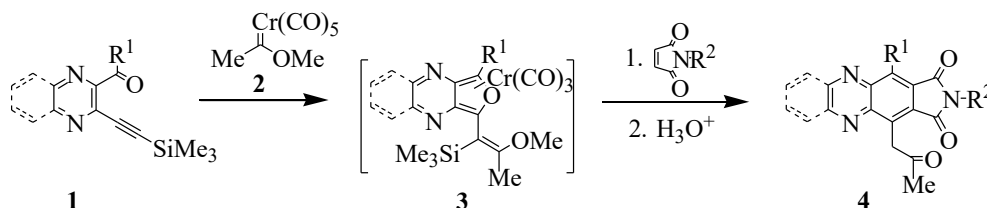


Scheme 2.6

Approaches Using Fischer Carbene Complexes

Multicomponent reactions (MCRs) are defined as chemical transformations where three or more reactants are combined under identical conditions in a single vessel to form a single product that incorporates elements of all starting materials. These reactions have gained immense popularity due to their efficiency, superior atom economy, and utility in the fields of diversity-oriented and combinatorial synthesis. Simultaneously, group VI Fischer carbene complexes (FCCs) have established themselves as versatile reagents in organic synthesis and have emerged as valuable partners in MCR strategies. Numerous reviews have highlighted the diverse reactivity and synthetic applications of FCCs in this context.¹⁶

In this chapter, we introduce a multicomponent synthetic route to generate quinoxaline and phenazine frameworks via the use of chromium-based Fischer carbene complexes. Our methodology draws inspiration from the seminal contributions of Herndon and colleagues.¹⁷ This synthetic protocol features a one-pot reaction wherein quinoxaline or phenazine scaffolds are assembled in tandem with the in situ formation and interception of an azaisobenzofuran intermediate. The transformation begins with the coupling of Fischer carbene complexes **2** with 2-alkynyl-3-pyrazine carbonyl precursors **1A**, leading to the generation of a novel intermediate—furo[3,4-b]pyrazine **3A**—which is then trapped by dienophiles. Similarly, phenazine derivatives **4** are synthesized from the corresponding 2-alkynyl-3-quinoxaline carbonyl compound **1C** via analogous formation and trapping of furo[3,4-b]quinoxaline intermediates **3C** (Scheme 2.7).



Scheme 2.7

Part 2: Focuses on the one-pot assembly of furo[2,3-*h*]quinoline and furo[2,3-*h*]isoquinoline derivatives.

Literature Review / Previous Work

The furoquinoline framework is found in a range of natural alkaloids, including compounds such as skimmianine and balfouridine.¹⁸ Derivatives of furo[2,3-*h*]quinoline have garnered particular interest for their potential in photochemotherapy, attributed to features like significant antiproliferative efficacy, minimal genotoxicity, and absence of skin phototoxic effects.¹⁹ Molecules capable of DNA intercalation, typically featuring linear or angular polyaromatic chromophores, can modulate both the structure and biological activity of DNA.²⁰ Several well-known intercalators—such as furocoumarins, acridines, anthraquinones, naphthalimides, and phenanthridines—have applications in cancer therapeutics. Angelicin (Figure 3.1), an angular variant of furocoumarin, has been traditionally employed to manage conditions like joint pain and skin ailments through phototherapy. Guiotto and collaborators developed a set of furoquinolinone analogues by replacing the oxygen atom in furocoumarin with nitrogen (NH); some members of this series demonstrated pronounced antiproliferative effects on tumor cells when exposed to UVA light.¹⁹ Nevertheless, these compounds were also found to exhibit considerable phototoxicity and clastogenic potential, attributed to their ability to form covalent monoadducts (MA) with DNA bases and to induce DNA–protein cross-linking (DPC) under UVA activation. When kept in the dark, their antiproliferative effects were minimal, likely resulting from topoisomerase II inhibition.²¹ Notably, elevated expression of topoisomerase II is a hallmark of many cancer cells, making it an attractive molecular target for anticancer drug development.²²

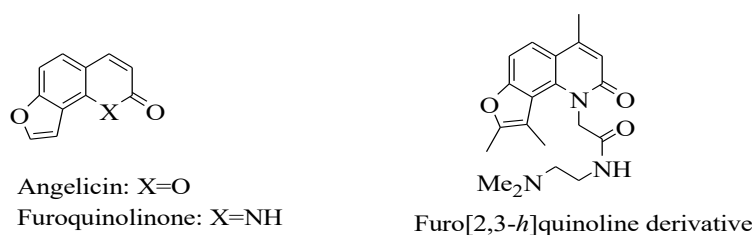


Figure 3.1

Eosinophils are recognized for their role in mediating proinflammatory responses, particularly in allergic conditions such as asthma.²³ Various cytokines—including hematopoietins, interleukin-5 (IL-5), IL-3, and GM-CSF—are known to stimulate eosinophil production in the bone marrow²⁴ and concurrently prevent apoptosis, thereby extending eosinophil lifespan during *in vitro* culture. In allergic individuals, eosinophils tend to accumulate in large numbers and discharge reactive oxygen species along with cytotoxic granule proteins like major basic protein and eosinophil cationic protein.²³ Therefore, targeting the mechanisms that sustain eosinophil survival may offer promising strategies for asthma therapy. Notably, in the search for such agents, the fungus

Aspergillus ustus (Bain.) Thorn & Church TC 1118 has been found to produce three novel isoquinoline alkaloids—TMC-120A, B, and C—which exhibit significant biological activity (Figure 3.2).

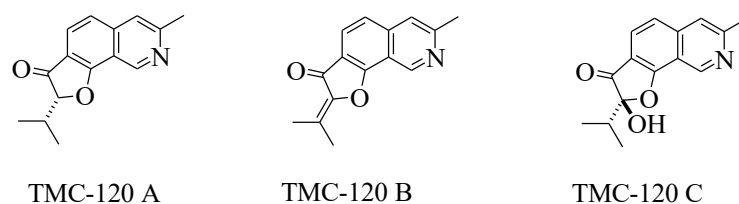
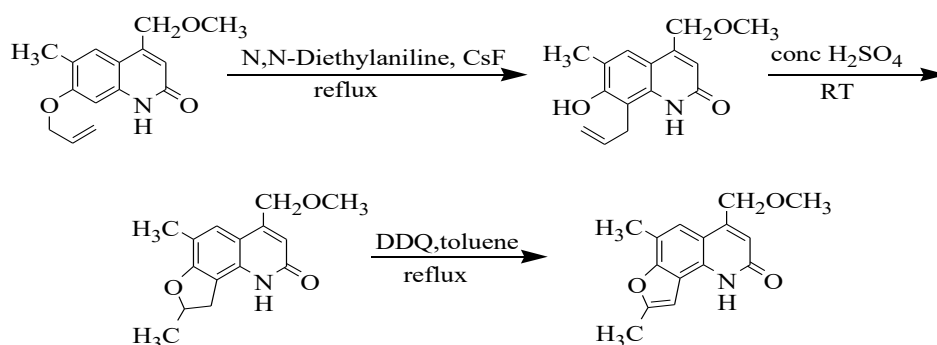


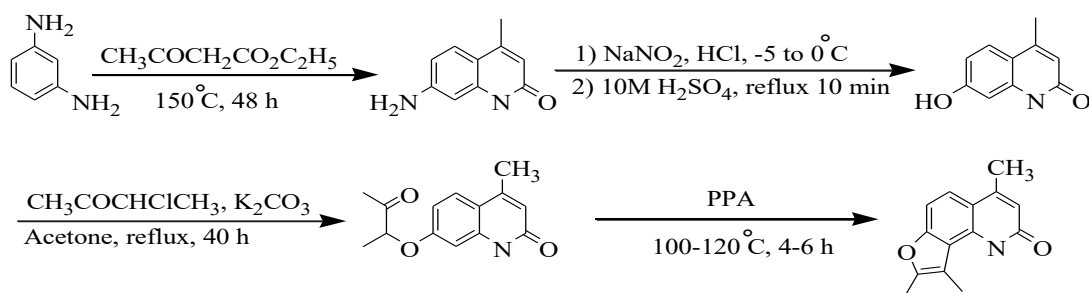
Figure 3.2

In recent decades, extensive research has focused on unveiling the biological relevance of these compounds. However, gentle and efficient methods for their synthesis remain relatively underexplored. Chilin and collaborators successfully developed a furo[2,3-h]quinoline derivative through the synthetic approach illustrated in Scheme 3.1.²⁵



Scheme 3.1

Xie and colleagues devised a stepwise synthetic pathway for angular furoquinolinones, initiating the process with *m*-phenylenediamine and ethyl acetoacetate as starting materials (Scheme 3.2).²⁶

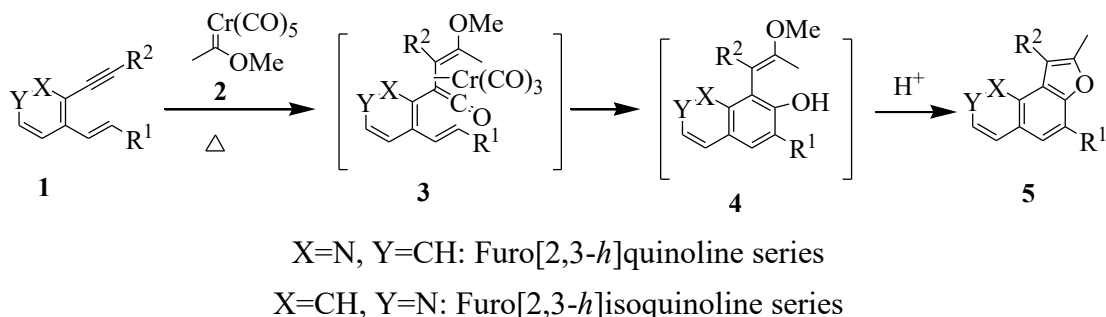


Scheme 3.2

Approaches Using Fischer Carbene Complexes²⁷

Fused furoquinoline and furoisoquinoline frameworks are typically synthesized by furan ring fusion onto existing quinoline or isoquinoline cores. However, annulation strategies involving the attachment of benzofuran motifs onto pyridine rings have, intriguingly, remained largely uninvestigated. In this chapter, we report the successful development of such a transformation, accomplished via a tandem sequence that builds both the furan and aromatic rings simultaneously. This is achieved through the coupling of Fischer carbene complex 2 with enyne

precursors featuring a pyridine bridge (1) as illustrated in Scheme 3.3. The mechanism mirrors the well-established Dötz benzannulation reaction, wherein a ketene intermediate (3), generated from a chromium carbene complex, undergoes cyclization to afford a phenolic intermediate (4), which upon acidic work-up yields the target furoquinoline or furoisoquinoline derivatives (5).

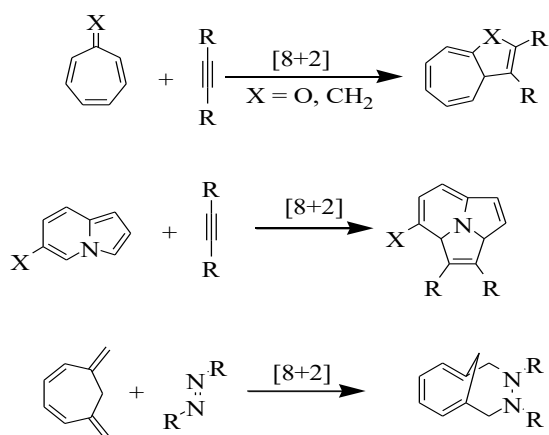


Scheme 3.3

Part 3: Delves into [8+2] cycloaddition reactions involving dienylazaisobenzofurans to access furan-bridged 10-membered aza-heterocycles.

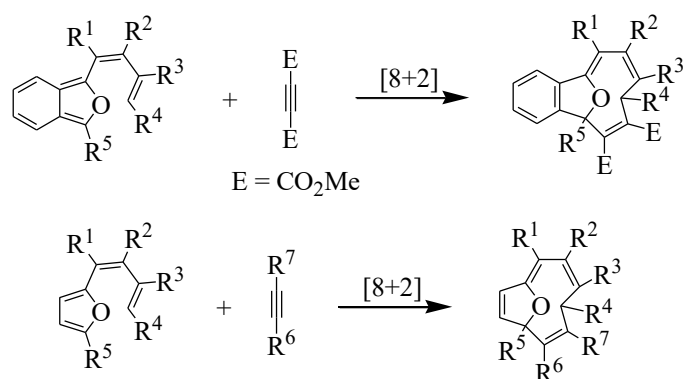
Literature Review / Previous Work

The [8+2] cycloaddition reaction, when allowed by orbital symmetry, represents a valuable tool for constructing 10-membered ring systems. Though promising, most examples to date have been limited to reactions involving structurally constrained tetraenes—such as tropones, heptafulvenes, or indolizine derivatives—where the termini (positions 1 and 8) are inherently positioned close enough to enable cyclization (Scheme 4.1, first and second reactions). In contrast, reactions utilizing geometrically flexible tetraenes have seen very limited exploration. A rare instance prior to 2003 involved the reaction of 1,6-dimethylene cyclohepta-2,4-diene with strong tetraenophiles like tetracyanoethylene or dimethyl azodicarboxylate, which demonstrated the feasibility of such systems (Scheme 4.1, third reaction).²⁸ Advancing this area by developing new [8+2] cycloaddition methodologies that incorporate flexible tetraenes and reactive tetraenophiles could open novel avenues for synthesizing 10-membered carbocycles.^{29, 30}



Scheme 4.1

Herndon and his team demonstrated in 2003 that dienyisobenzofuran undergoes a [8+2] cycloaddition with dimethyl acetylenedicarboxylate (DMAD), predominantly yielding products featuring the 11-oxabicyclo[6.2.1]undecane framework (Scheme 4.2, first reaction).³¹ In subsequent studies, they extended this approach to show that dienyifuran analogues also react similarly with DMAD to furnish analogous cycloadducts (Scheme 4.2, second reaction).³² Unlike typical [8+2] cycloadditions involving rigidly constrained tetraenes where reactive termini are pre-aligned, these reactions utilized geometrically flexible tetraenes where atoms at positions 1 and 8 are spatially distant. Yu and collaborators later conducted both experimental and theoretical investigations into the mechanistic nature of these transformations. Their study suggested that such [8+2] reactions might proceed via either a concerted pathway or a stepwise route involving sequential [4+2] cycloaddition followed by a [1,5]-vinyl shift.³³ Importantly, this methodology provides an efficient route to oxygen-bridged 10-membered ring systems through synthetically accessible intermediates.



Scheme 4.2

The 11-oxabicyclo[6.2.1]undecane framework serves as a crucial structural motif in a class of natural products referred to as 2,11-cyclized cembranoids or cladiellanes (Figure 4.1).

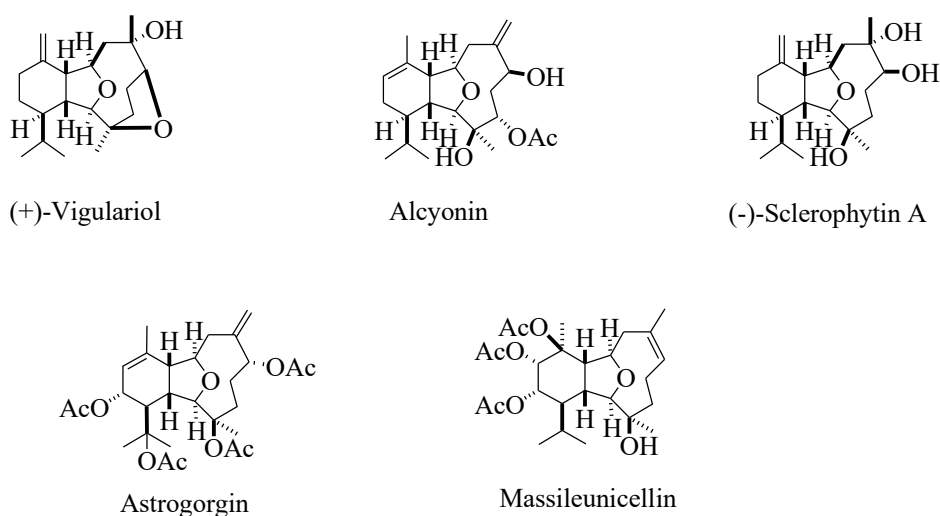
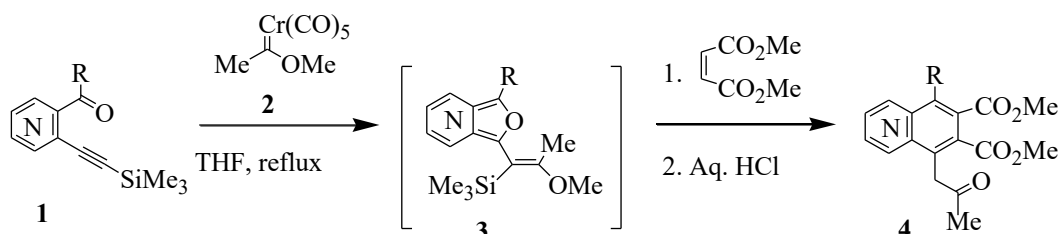


Figure 4.1: Representative eunicellin diterpenes

Numerous members of this family exhibit significant biological properties, particularly anti-inflammatory and anticancer effects. The transformation depicted in Scheme 4.2 offers a streamlined approach for constructing the full carbon skeleton characteristic of eunicellin-type diterpenes in a single synthetic operation.

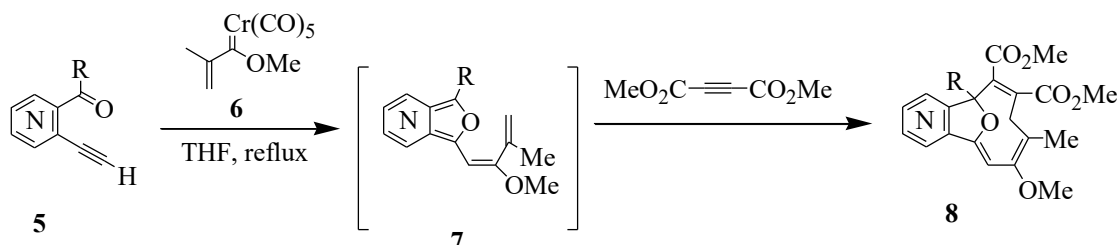
Approaches Using Fischer Carbene Complexes³⁴

A recent development from our laboratory demonstrated the synthesis of nitrogen-containing heterocycles via the coupling of *o*-alkynylheteroaryl carbonyl precursors **1** with Fischer carbene complexes **2** (Scheme 4.3). This transformation proceeds through the in situ formation of azaisobenzofuran intermediates **3**, which are subsequently intercepted using appropriate dienophiles. Although azaisobenzofurans are well-established as a fascinating class of reactive intermediates, their application has been largely confined to [4+2] cycloaddition pathways, limiting their broader synthetic potential in the construction of polycyclic N-heteroaromatic frameworks.



Scheme 4.3

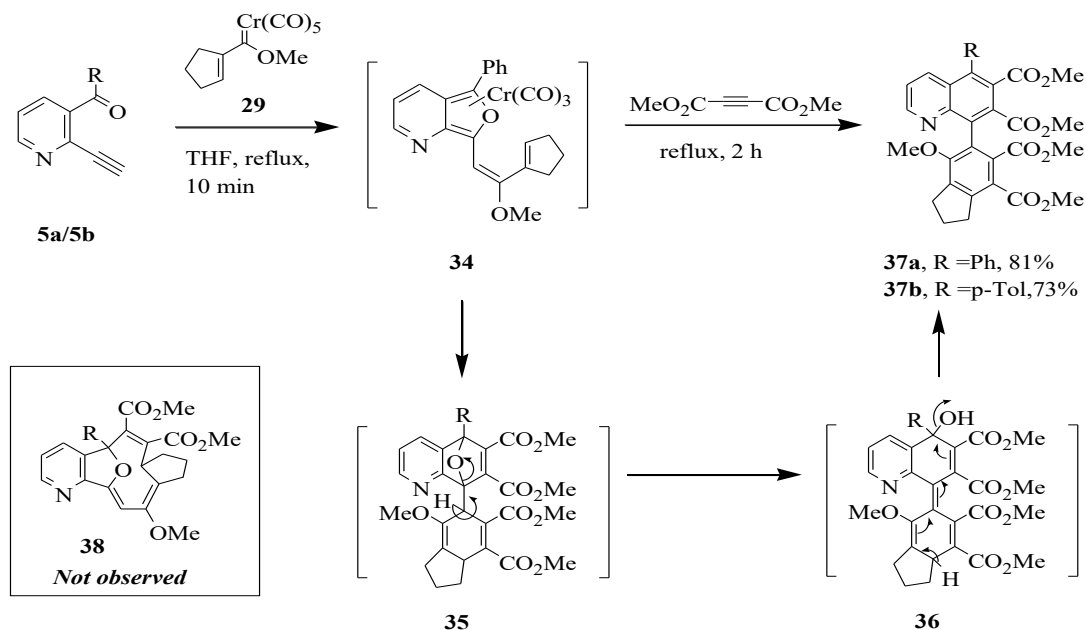
Motivated by the potential synthetic utility of these reactive intermediates, we turned our attention to exploring [8+2] cycloaddition strategies as a pathway to develop a more efficient and broadly applicable methodology. In this chapter, we present a three-component coupling approach involving *o*-alkynylheteroaryl carbonyl derivatives **5**, α,β -unsaturated Fischer carbene complexes **6**, and dimethyl acetylenedicarboxylate (DMAD), which leads to the formation of heterocyclic furanophane analogues. It is anticipated that the reaction between compounds **5** and **6** would proceed analogously to the coupling of ketone **1** with carbene complex **2**, generating the intermediate dienzylazaisobenzofuran **7** (Scheme 4.4). In this system, the tetraene moiety of intermediate **7** serves as the 8π -electron component in a [8+2] cycloaddition with DMAD.



Scheme 4.4

A distinctive benzannulation outcome was observed during the reaction of alkyne derivatives **5a/5b** with carbene complex **29**, where the alkene moiety is embedded within a five-membered

ring (Scheme 4.10). This transformation proceeds through the formation of dienyloxyisobenzofuran intermediate 34, which undergoes a sequential double Diels–Alder reaction with DMAD, yielding oxanorbornene intermediate 35. This intermediate further rearranges via ring opening and elimination of water to furnish the heterocyclic analogues of 1-arylnaphthalene lignan derivatives 37a/37b. Notably, the formation of the alternative [8+2] cycloadduct 38 was not detected in this case.



Scheme 4.10

Part 4: Describes an intramolecular [4+2] cycloaddition strategy involving azaisobenzofuran intermediates to achieve aza-homosteroid skeletons in a convergent one-step fashion.

Literature Review / Previous Work

Intramolecular cycloaddition reactions offer an efficient and stereoselective pathway for assembling structurally complex frameworks in organic synthesis.³⁵ Among these, the intramolecular Diels–Alder (IMDA) reaction, a subset of [4+2] cycloadditions, has proven especially valuable for constructing natural products and bioactive molecules when the diene and dienophile are properly positioned within the substrate.³⁶ The development of more accessible and reactive four-carbon synthons—such as azaisobenzofurans—holds promise for further expanding the utility of these methods. These intermediates, functioning as o-quinodimethane analogues, exhibit significant reactivity and can engage in both intra- and intermolecular cycloaddition processes.³⁷ Appropriately substituted azaisobenzofurans have thus become strategic intermediates for the efficient synthesis of polycyclic nitrogen-containing heteroaromatics with potential pharmacological relevance.

Despite the extensive research devoted to the structure, reactivity, and biological roles of the homosteroid ring system,³⁸ its nitrogen-containing counterpart—the azahomosteroid framework—has received comparatively limited attention.³⁹ However, recent developments in medicinal chemistry have highlighted the azahomosteroid scaffold (Figure 6.1) due to its notable pharmacological potential. For instance, azasteroid 2 exhibits biological activity on par with the anesthetic steroid 1. Furthermore, lactandrate (3), a representative of this structural class, has emerged as a promising lead compound in the search for effective treatments for breast cancer.

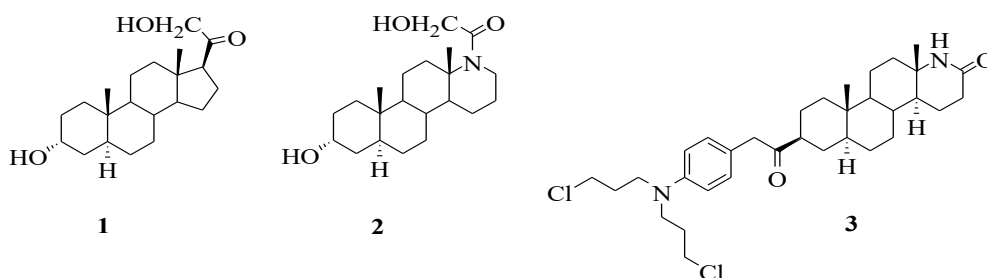
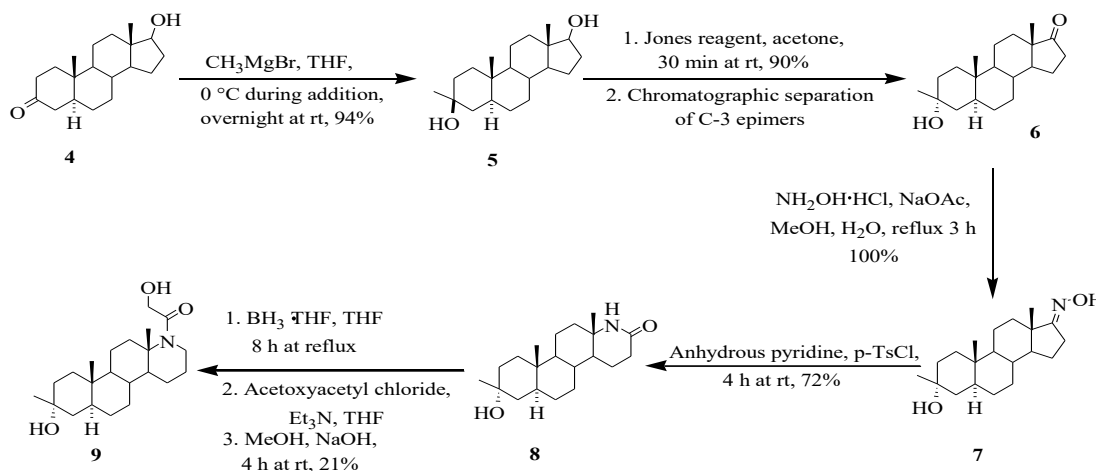


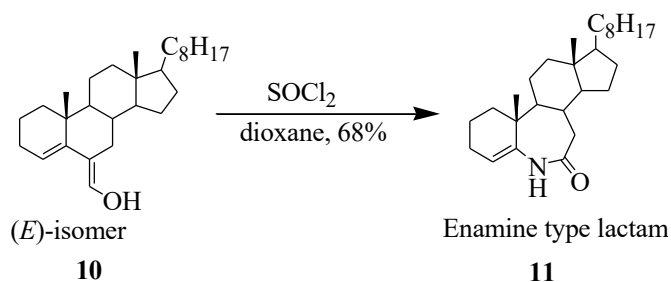
Figure 6.1: Biologically important steroid and their aza-analogues

Only a limited number of synthetic strategies for azahomosteroids have been documented in the literature. In 2000, Covey and his team outlined a method for preparing 17a-aza-D-homosteroids 9, as depicted in Scheme 6.1.⁴⁰ Their approach utilized the classic Beckmann rearrangement of oximes derived from 17-ketosteroids 7, leading to the formation of 17a-aza-17-oxo-D-homosteroids 8. Subsequent steps followed conventional synthetic methodologies.



Scheme 6.1

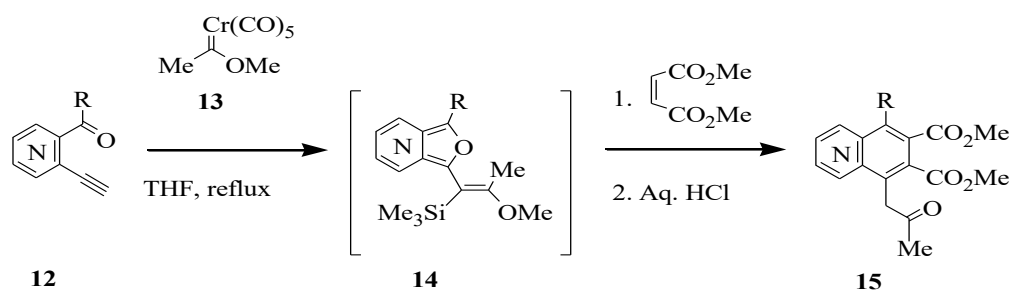
Krstić and co-workers reported that the enamine-type lactam 6-aza-B-homocholest-4-en-7-one (11) could be synthesized from (E)-oxime 10 through a Beckmann rearrangement reaction (Scheme 6.2).⁴¹



Scheme 6.2

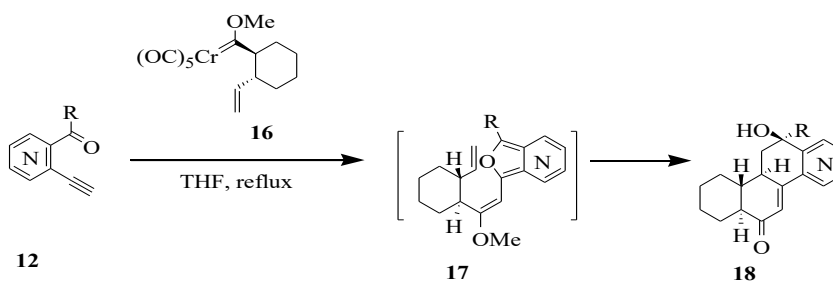
Approaches Using Fischer Carbene Complexes⁴²

Synthetic approaches toward azahomosteroids are relatively scarce and generally require multiple steps. Our review of the existing literature revealed a surprising reliance on preformed steroid frameworks for such syntheses. In a recent study, we demonstrated that azaisobenzofuran intermediates **14** (Scheme 6.3) could be effectively produced via the reaction of Fischer carbene complexes **13** with *o*-alkynylheteroaryl carbonyl compounds **12**. These reactive species were then moderately successfully intercepted in intermolecular Diels–Alder cycloadditions with electron-deficient alkenes, affording six-membered benzofused azaheterocyclic products **15**.



Scheme 6.3

This chapter presents a strategy involving the coupling of *o*-alkynylheteroaryl carbonyl derivative **12** with a carbene complex that incorporates a built-in dienophile, specifically 2-alkenylcyclohexylcarbene complexes **16**, as outlined in the synthetic scheme (Scheme 6.4). This transformation enables the formation of a compound bearing the azahomosteroid core **18** in a single step, starting from two key components that retain only the A and D rings of the azahomosteroid framework. Notably, the same reaction responsible for connecting the A and D rings also generates the reactive intermediate azaisobenzofuran **17**, which facilitates the construction of the B and C rings.



Scheme 6.4

Conclusion:

In this chapter, we have highlighted a series of synthetic strategies that employ Fischer carbene complexes as powerful intermediates for the construction of diverse fused aza-heterocycles. Through a combination of multicomponent, one-pot, and cascade reactions, these methodologies offer efficient, selective, and environmentally friendly routes to structurally complex heterocyclic frameworks that are of great importance in the fields of medicinal and agrochemical chemistry.

We began by discussing the synthesis of quinoxaline and phenazine derivatives using a three-component annulation strategy, where the in situ generation and trapping of azaisobenzofuran intermediates played a crucial role. We then demonstrated the successful construction of furo[2,3-h]quinoline and furo[2,3-h]isoquinoline skeletons through a benzannulation-type reaction, which represents a novel approach in the domain of furan annulation onto pre-existing nitrogen-containing heterocycles.

Moving forward, we presented a unique application of [8+2] cycloaddition involving dienzylazaisobenzofurans and dimethyl acetylenedicarboxylate (DMAD) to access 10-membered furan-bridged aza-heterocycles—structurally related to naturally occurring bioactive macrocycles. Furthermore, the chapter described an intramolecular [4+2] cycloaddition route to azahomosteroid skeletons, offering a concise and convergent strategy for accessing these biologically relevant frameworks.

The utility of Fischer carbene complexes in these annulation strategies lies in their unique ability to generate highly reactive intermediates such as ketenes and azaisobenzofurans under mild conditions, enabling the rapid assembly of complex polycyclic structures in a single operation. These approaches not only enhance synthetic efficiency but also expand the scope of accessible nitrogen-rich heterocyclic architectures.

Overall, the methodologies discussed in this chapter provide valuable insights into the application of Fischer carbene complexes in modern heterocyclic chemistry. They open up new avenues for designing novel aza-heterocycles with potential pharmaceutical relevance and contribute to the growing interest in one-pot, atom-economical synthesis. Future research in this direction may involve the development of asymmetric variants, catalytic versions, and exploration of greener reaction conditions to further broaden the utility of this powerful strategy.

References:

1. Sakata, G., Makino, K., & Kuraswa, Y. (1988). *Heterocycles*, 27, 2481; He, W., Meyers, M. R., Hanney, B., Sapada, A., Blider, G., Galzeinski, H., Amin, D., Needle, S., Page, K., Jayyosi, Z., & Perrone, H. (2003). *Bioorganic & Medicinal Chemistry Letters*, 13, 3097; Kim, Y. B., Kim, Y. H., Park, J. Y., & Kim, S. K. (2004). *Bioorganic & Medicinal Chemistry Letters*, 14, 541.

2. Katoh, A., Yoshida, T., & Ohkanda, J. (2000). *Heterocycles*, 52, 911; Thomas, K. R. J., Velusamy, M., Lin, J. T., Chuen, C. H., & Tao, Y. T. (2005). *Chemistry of Materials*, 17, 1860; Dailey, S., Feast, W. J., Peace, R. J., Sage, I. C., Till, S., & Wood, E. L. (2001). *Journal of Materials Chemistry*, 11, 2238.
3. Vitaku, E., Smith, D. T., & Njardarson, J. T. (2014). Analysis of the structural diversity, substitution patterns, and frequency of nitrogen heterocycles among U.S. FDA approved pharmaceuticals. *Journal of Medicinal Chemistry*, 57(24), 10257–10274.
4. Dömling, A., Wang, W., & Wang, K. (2012). Chemistry and biology of multicomponent reactions. *Chemical Reviews*, 112(6), 3083–3135.
5. Herndon, J. W. (2000). Fischer carbene complexes in organic synthesis. *Tetrahedron*, 56, 1257–1276.
6. Allen, C. L., & Williams, J. M. J. (2011). *Chemical Society Reviews*, 40, 3405–3415.
7. Rauf, M. K., Ihsan, A., Badshah, A., et al. (2014). *European Journal of Medicinal Chemistry*, 80, 243–252.
8. Mavrodi, D. V., Blankenfeldt, W., & Thomashow, L. S. (2006). *Annual Review of Phytopathology*, 44, 417–445.
9. Price-Whelan, A., Dietrich, L. E., & Newman, D. K. (2006). *Nature Chemical Biology*, 2, 71–78.
10. Yadav, J. S., Reddy, B. V. S., Rao, Y. G., & Narsaiah, A. V. (2008). *Chemistry Letters*, 37, 348; Brown, D. J. (2004). *Quinoxalines: Supplement II. The Chemistry of Heterocyclic Compounds* (Vol. 61, E. C. Taylor & P. Wipf, Eds.). John Wiley & Sons; Huang, T. K., Shi, L., Wang, R., Guo, X. Z., & Lu, X. X. (2009). *Chinese Chemical Letters*, 20, 161; Zhao, Z., Wisnoski, D. D., Wolkenberg, S. E., Leister, W. H., Wang, Y., & Lindsley, C. W. (2004). *Tetrahedron Letters*, 45, 4873; Bhosale, R. S., Sarda, S. R., Ardhapure, S. S., Jadhav, W. N., Bhusare, S. R., & Pawar, R. P. (2005). *Tetrahedron Letters*, 46, 7183; Bouilly, L., Darabantu, M., Turck, A., & Ple, N. (2005). *Journal of Heterocyclic Chemistry*, 42, 1423; Neochoritis, C., Stephanidou-Stephanatou, J., & Tsoleridis, C. A. (2009). *Synlett*, 2, 302; Beifuss, U., & Tietze, M. (2005). Methanophenazine and other natural biologically active phenazines. In J. Mulzer (Ed.), *Topics in Current Chemistry* (Vol. 244, pp. 77). Springer; Davarani, S. S. H., Fakhari, A. R., Shaabani, A., Ahmar, H., Maleki, A., & Fumani, N. S. (2008). *Tetrahedron Letters*, 49, 5622; Pachter, J., & Kloetzel, M. C. (1951). *Journal of the American Chemical Society*, 73, 4958–4961.
11. Pal, S., Basak, S., Jana, A. D., & Maiti, D. K. (2009). *Tetrahedron Letters*, 50, 1215–1218.
12. Tsoleridis, C. A., Aliev, A. E., & Philp, D. (2008). *Tetrahedron Letters*, 49, 4193–4197.
13. Wohl, A., & Aue, W. (1901). *Berichte der Deutschen Chemischen Gesellschaft*, 34, 2430–2434.

14. Emoto, K., Inoue, S., & Ishibashi, H. (1996). *Chemical & Pharmaceutical Bulletin*, 44(2), 380–385.
15. Wang, L., Jiang, Y., Zhang, Y., & Wang, Y. (2006). *Journal of Organic Chemistry*, 71(9), 3642–3645.
16. Barluenga, J., Fernández-Rodríguez, M. A., & Aguilar, E. (2005). *Journal of Organometallic Chemistry*, 690, 539; Fernández-Rodríguez, M. A., García-García, P., & Aguilar, E. (2010). *Chemical Communications*, 46, 7670; Herndon, J. W. (2010). *Coordination Chemistry Reviews*, 254, 103; Dötz, K. H., & Stendel, J. (2009). *Chemical Reviews*, 109, 3227; Santamaría, J. (2009). *Current Organic Chemistry*, 13, 31; Waters, M. L., & Wulff, W. D. (2008). *Organic Reactions*, 70, 121; Sierra, M. A., Fernández, I., & Cossío, F. P. (2008). *Chemical Communications*, 4671; Sierra, M. A., Gómez-Gallego, M., & Martínez-Álvarez, R. (2007). *Chemistry – A European Journal*, 13, 736.
17. Herndon, J. W. (2000). *Coordination Chemistry Reviews*, 209, 387–451; Herndon, J. W., Zhang, Y., Wang, H., & Wang, K. (2000). *Tetrahedron Letters*, 41(45), 8687–8690; Li, R., Zhang, L., Camacho Davila, A., & Herndon, J. W. (2005). *Tetrahedron Letters*, 46(31), 5117–5120.
18. Benassi, R., Zanirato, V., & Uccello-Barretta, G. (2001). Furoquinoline alkaloids: Isolation and synthesis. *Natural Product Reports*, 18, 444–457. <https://doi.org/10.1039/B100638N>
19. Rodighiero, P., Guiotto, A., Chilin, A., Bordin, F., Baccichetti, F., Carllassare, F., Vedaldi, D., Caffieri, S., Pozzan, A., & Dall'Acqua, F. (1996). *Journal of Medicinal Chemistry*, 39, 1293; Marzano, C., Chilin, A., Guiotto, A., Baccichetti, F., & Carllassare, F. (2000). *Il Farmaco*, 55, 650; Chilin, A., Marzano, C., Guiotto, A., Baccichetti, F., & Carllassare, F. (2002). *Journal of Medicinal Chemistry*, 45, 1146; Marzano, C., Chilin, A., Bordin, F., Baccichetti, F., & Guiotto, A. (2002). *Bioorganic & Medicinal Chemistry*, 10, 2835; Chilin, A., Marzano, C., Baccichetti, F., Simonato, M., & Guiotto, A. (2003). *Bioorganic & Medicinal Chemistry*, 11, 1311; Marzano, C., Chilin, A., Baccichetti, F., Bettio, F., Guiotto, A., Miolo, G., & Bordin, F. (2004). *European Journal of Medicinal Chemistry*, 39, 411.
20. Hurley, L. H. (2002). DNA and its associated processes as targets for cancer therapy. *Nature Reviews Cancer*, 2, 188–200. <https://doi.org/10.1038/nrc749>
21. Pommier, Y., Leo, E., Zhang, H., & Marchand, C. (2010). DNA topoisomerases and their poisoning by anticancer and antibacterial drugs. *Chemistry & Biology*, 17, 421–433. <https://doi.org/10.1016/j.chembiol.2010.04.012>
22. Vignoni, M., Giannini, G., Vesci, L., Milazzo, F. M., Finotto, A., Fravolini, A., & Mattioli, F. (2006). Synthesis and biological evaluation of new furo[2,3-h]quinolin-2(1H)-ones as

- topoisomerase II inhibitors. *Bioorganic & Medicinal Chemistry*, 14, 164–172. <https://doi.org/10.1016/j.bmc.2005.08.014>
23. Kroegel, C., Dent, G., Meyer, A., Wiesner, O., & Vancheri, C. (1994). Role of eosinophils in bronchial asthma and airway hyperresponsiveness. *Clinical & Experimental Allergy*, 24(8), 539–550. <https://doi.org/10.1111/j.1365-2222.1994.tb00335.x>
24. Rothenberg, M. E., & Hogan, S. P. (2006). The eosinophil. *Annual Review of Immunology*, 24, 147–174. <https://doi.org/10.1146/annurev.immunol.24.021605.090720>
25. Chilin, A., Guiotto, A., Rodighiero, G., Bordin, F., & Ferrazzi, E. (1996). Photochemotherapeutic agents. 1. Synthesis of angular and linear furoquinoline and furoquinolinone derivatives. *Journal of Medicinal Chemistry*, 39(19), 3854–3861. <https://doi.org/10.1021/jm950908g>
26. Xie, J., Bai, X., Wang, Z., Xu, Y., Liu, Y., & Zhao, Q. (2004). A convenient synthesis of furo[2,3-h]quinolin-2-ones via cyclization of m-phenylenediamine and ethyl acetoacetate. *Tetrahedron*, 60(31), 6607–6611. <https://doi.org/10.1016/j.tet.2004.04.098>
27. Roy, P., & Ghorai, B. K. (2011). *Tetrahedron Letters*, 52, 251–253.
28. Ghosh, S., & Herndon, J. W. (2003). *Journal of Organic Chemistry*, 68, 8599–8603. <https://doi.org/10.1021/jo034867s>
29. Liu, C. Y., Mareda, J., Houk, K. N., & Fronczek, F. R. (1983). *Journal of the American Chemical Society*, 105, 6714; Liu, C. Y., & Ding, S. T. (1992). *Journal of Organic Chemistry*, 57, 4539; Liu, C. Y., & Houk, K. N. (1987). *Tetrahedron Letters*, 28, 1371; Daub, J., Hirmer, G., Kakob, L., Maas, G., Pickl, W., & Pirzer, E. (1985). *Chemische Berichte*, 118, 1836; Bäumlner, A., Daub, J., Pickl, W., & Rieger, W. (1985). *Chemische Berichte*, 118, 1857; Hayakawa, K., Nishiyama, H., & Kanematsu, K. (1985). *Journal of Organic Chemistry*, 50, 512; Kumar, K., Kapur, A., & Ishar, M. P. S. (2000). *Organic Letters*, 2, 787; Farrant, G. C., & Feldmann, R. (1970). *Tetrahedron Letters*, 11, 4979; Komatsu, K., Fujimori, M., & Okamoto, K. (1977). *Tetrahedron*, 33, 2791; Pham, W., Weissleder, R., & Tung, C. H. (2002). *Tetrahedron Letters*, 43, 19; Nair, V., Anikumar, G., Nandakumar, M. V., Mathew, B., & Rath, N. P. (1997). *Tetrahedron Letters*, 38, 6441; Babaev, E. V., Simonyan, V. V., Pasichnichenko, K. Y., Nosova, V. M., Kisin, A. V., & Jug, K. (1999). *Journal of Organic Chemistry*, 64, 9057.
30. Bernardelli, P., & Paquette, L. (1998). *Heterocycles*, 49, 531; Lindel, T., Jensen, P. R., Fenical, W., Long, B. H., Casazza, A. M., Carboni, J., & Fairchild, C. R. (1997). *Journal of the American Chemical Society*, 119, 8744; Lindel, T. (1998). *Angewandte Chemie International Edition*, 37, 774.
31. Herndon, J. W., & Ghosh, S. (2003). *Journal of Organic Chemistry*, 68, 8599–8603. <https://doi.org/10.1021/jo034867s>

32. Ghosh, S., & Herndon, J. W. (2004). *Tetrahedron Letters*, 45, 3517–3520.
<https://doi.org/10.1016/j.tetlet.2004.03.007>
33. Yu, P., Lu, Z., Shen, Z., & Ma, S. (2009). *Journal of Organic Chemistry*, 74, 1386–1394.
<https://doi.org/10.1021/jo802382m>
34. Roy, P., & Ghorai, B. K. (2011). *Tetrahedron Letters*, 52(9), 5668–5671.
35. Sauer, J., & Sustmann, R. (1980). *Angewandte Chemie International Edition*, 19, 779–807.
36. Mehta, G., & Srikrishna, A. (1997). *Chemical Reviews*, 97, 671–720.
37. Herndon, J. W. (2000). *Tetrahedron*, 56, 1257–1280.
38. Kumar, N., Kaur, P., & Bansal, G. (2014). *Steroids*, 79, 36–45.
39. Köhler, G., Peters, M., & Muller, M. (2007). *Journal of Medicinal Chemistry*, 50, 5865–5870.
40. Covey, D. F., Keenan, S. M., & Mattson, M. V. (2000). *Journal of Organic Chemistry*, 65, 731–738.
41. Krstić, N. M., Bjelaković, M. S., Zizak, Z., Pavlović, M. D., Juranić, Z. D., & Pavlović, V. D. (2007). *Steroids*, 72, 406.
42. P. Roy, P. Mitra, B. K. Ghorai, *Tetrahedron Lett.*, **2013**, 54(7), 1440–1443.

NEXT-GENERATION SCIENCE: SHAPING SOCIETY, OVERCOMING HURDLES, AND SHAPING FUTURE FRONTIERS

K Janani*¹ and P Sivakami²

¹Department of Science and Humanities,
Nehru Institute of Technology, Kaliyapuram, Coimbatore 641 105

²Department of Physics,
S. T. Hindu College, Nagercoil – 629 002.

*Corresponding author E-mail: nitdrkjanani@nehrucolleges.com

Abstract:

Next-generation science covers fields like artificial intelligence, biotechnology, nanotechnology, quantum computing, and renewable energy. These areas are transforming the way society functions. Technological developments like telemedicine and precision medicine are enhancing access and customisation in the healthcare industry. AI-powered platforms and immersive tools are bringing new learning experiences to the classroom. Smart infrastructure and green technologies are promoting sustainable growth. Digital marketplaces, worldwide connectivity, and automation are transforming industry. These developments collectively show how science can enhance human welfare. They also emphasize the importance of research in tackling pressing worldwide issues including inequality, health crises, and climate change.

Next-generation science has a lot of obstacles to overcome, despite its potential. Concerns about data privacy and cybersecurity, ethical conundrums in genetic modification and artificial intelligence, and growing inequities in technology access highlight the difficulties in advancing science. The necessity of responsible innovation is further underscored by environmental hazards including resource scarcity and electronic waste. On the horizon, emerging fields like space exploration, human-AI collaboration, quantum innovations, and citizen science offer chances to create a more sustainable and inclusive future. This chapter highlights the need for interdisciplinary cooperation, strong governance, and an ethical commitment to ensure that advancement benefits all people in order to fully utilize next-generation science.

Keywords: Next-generation Science, Artificial Intelligence, Sustainable Development, Society.

Introduction:

Science and technology have long served as the cornerstones of human progress, shaping societies and transforming the way people live, work, and interact. From the industrial revolution to the digital age, each wave of scientific advancement has generated profound social, economic, and cultural impacts. In the 21st century, the rapid growth of fields such as artificial intelligence (AI), biotechnology, nanotechnology, and quantum science has given rise to what is often

referred to as next-generation science. These cutting-edge innovations are not only enhancing human capabilities but also addressing pressing global challenges, including climate change, public health crises, and sustainable development (Schwab, 2017; UNESCO, 2021).

At the same time, the integration of science and technology into everyday life raises complex questions about equity, ethics, and responsibility. While advances such as gene editing and autonomous systems offer transformative benefits, they also provoke debates about privacy, social justice, and the boundaries of human intervention in nature. The Science, Technology, and Society (STS) framework highlights that scientific progress is never isolated but is deeply embedded in political, cultural, and social contexts (Bijker, Hughes, & Pinch, 2012; Jasanoff, 2004). Thus, examining next-generation science requires a holistic perspective that considers not only innovation but also its wider implications for humanity.

This chapter explores the transformative power of next-generation science in shaping society, identifies the hurdles that must be addressed to ensure equitable progress, and highlights the emerging frontiers that could redefine the future of human civilization. By analyzing the interplay between innovation, societal needs, and ethical responsibility, the discussion aims to provide a comprehensive understanding of how science can serve as a tool for sustainable and inclusive development in the decades to come.

Shaping Society Through Next-Generation Science:

1. Healthcare Revolution

Next-generation science is redefining healthcare. Precision medicine, powered by genomics and big data, allows for treatments tailored to individual patients. Telemedicine, accelerated by the COVID-19 pandemic, has transformed healthcare access, reducing geographical barriers. Technologies such as CRISPR-Cas9 gene editing open new possibilities for curing genetic diseases but also raise ethical dilemmas (Collins & Varmus, 2015; National Academies of Sciences, 2022).

2. Education and Knowledge Systems

Digital learning platforms, AI-driven tutors, and immersive technologies such as virtual and augmented reality are reshaping education. These tools democratize access to high-quality education but also risk reinforcing digital divides if access to technology is unequal. The integration of interdisciplinary learning prepares students for complex problem-solving in a technology-driven world (UNESCO, 2021; Selwyn, 2016).

3. Sustainable Development and Environment:

Addressing climate change requires scientific innovation. Solar photovoltaics, wind turbines, biofuels, and green hydrogen are transforming the global energy landscape. Smart cities, enabled by IoT (Internet of Things) and AI, optimize resource use, reduce emissions, and promote

sustainable urban living. Science thus plays a pivotal role in achieving the United Nations Sustainable Development Goals (SDGs) (Rockström *et al.*, 2009).

4. Economy and Industry:

Industry 4.0 integrates automation, robotics, and AI into production lines, boosting efficiency but also raising concerns about job displacement. The gig economy and digital marketplaces reshape labour markets, offering flexibility while challenging traditional labour rights frameworks. Emerging sciences are also redefining entrepreneurship, fostering global startup ecosystems (Schwab, 2017; Brynjolfsson & McAfee, 2014).

Overcoming Hurdles

1. Ethical and Social Challenges

Rapid advances raise ethical dilemmas. AI algorithms can perpetuate bias; genetic editing can be misused; and autonomous weapons pose threats to human security. Ethical frameworks and global governance mechanisms are urgently needed (Jasanoff, 2004; Floridi, 2014).

2. Inequality and Digital Divide

Not all regions have equal access to next-generation technologies. The digital divide risks reinforcing existing inequalities, as developing nations may lag behind in adopting and benefiting from innovations. Equitable technology transfer and inclusive policies are vital (Hilbert, 2011; UNESCO, 2021).

3. Privacy and Security Concerns

The increasing reliance on digital systems raises concerns about data privacy, cybersecurity, and surveillance. Balancing innovation with protection of fundamental rights is one of the foremost challenges of the digital era (Floridi, 2014; Zuboff, 2019).

4. Environmental Risks:

Technology can help fight climate change, but it also brings concerns including energy-intensive data centers, resource exploitation for rare-earth elements, and electronic waste. Sustainable design and circular economy principles are essential to mitigate these impacts.

Shaping Future Frontiers

1. Artificial Intelligence and Human Collaboration

The future will see greater collaboration between humans and intelligent systems. AI can boost scientific research, increase human creativity, and help with global issues like pandemics and climate modeling. (Schwab, 2017; Brynjolfsson & McAfee, 2014).

2. Quantum and Space Frontiers

Quantum technologies promise breakthroughs in computation, secure communication, and materials science. Simultaneously, space science and exploration such as Mars missions, asteroid mining, and satellite-based internet—are redefining humanity’s relationship with the cosmos (National Academies of Sciences, 2022; Davenport, 2021).

3. Biotechnology and Human Enhancement

The intersection of information science, neurology, and biotechnology creates new opportunities in regenerative medicine, brain-machine interfaces, and human enhancement. These developments raise serious ethical concerns about what it means to be human, even while they may increase human lifespans and capabilities. (Collins & Varmus, 2015; Jasanoff, 2004).

4. Global Collaboration and Citizen Science

International cooperation is vital to next-generation science. In order to bridge the gap between professionals and society, international research networks, open-access platforms, and citizen science programs enable communities to participate to scientific discoveries. (UNESCO, 2021; Bonney *et al.*, 2014).

Conclusion:

Next-generation science is reshaping the fabric of society, offering transformative solutions in healthcare, education, sustainability, and industry. Its promise lies in advancing human well-being, addressing global crises, and opening unprecedented opportunities in fields such as artificial intelligence, quantum computing, and biotechnology. Yet, these benefits are accompanied by challenges that demand critical attention, including ethical dilemmas, widening digital divides, privacy concerns, and environmental risks. The future of science cannot be measured solely by technological breakthroughs, but by how inclusively and responsibly those breakthroughs are implemented. By fostering interdisciplinary collaboration, strengthening global governance, and prioritizing sustainability, humanity can ensure that innovation serves as a catalyst for equitable progress. Ultimately, next-generation science is not only about pushing the boundaries of knowledge but about forging a future where scientific discovery and societal good are inseparable, paving the way for a just and sustainable world.

References

1. Bonney, R., Shirk, J. L., Phillips, T. B., Wiggins, A., Ballard, H. L., Miller-Rushing, A. J., & Parrish, J. K. (2014). Next steps for citizen science. *Science*, 343(6178), 1436–1437.
2. Brynjolfsson, E., & McAfee, A. (2014). *The second machine age: Work, progress, and prosperity in a time of brilliant technologies*. W.W. Norton.
3. Collins, F. S., & Varmus, H. (2015). A new initiative on precision medicine. *New England Journal of Medicine*, 372(9), 793–795.
4. Davenport, C. (2021). *The space barons: Elon Musk, Jeff Bezos, and the quest to colonize the cosmos*. PublicAffairs.
5. Floridi, L. (2014). *The ethics of information*. Oxford University Press.
6. Hilbert, M. (2011). Digital gender divide or technologically empowered women in developing countries? *Women's Studies International Forum*, 34(6), 479–489.

7. Jasanoff, S. (2004). *States of knowledge: The co-production of science and the social order*. Routledge.
8. National Academies of Sciences, Engineering, and Medicine. (2022). *The future of science, technology, and innovation: Driving discovery and sustainability*. National Academies Press.
9. Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F. S., Lambin, E., ... Foley, J. (2009). A safe operating space for humanity. *Nature*, 461(7263), 472–475.
10. Schwab, K. (2017). *The fourth industrial revolution*. World Economic Forum.
11. Selwyn, N. (2016). *Education and technology: Key issues and debates*. Bloomsbury.
12. UNESCO. (2021). *Science report: The race against time for smarter development*. UNESCO Publishing.
13. Zuboff, S. (2019). *The age of surveillance capitalism: The fight for a human future at the new frontier of power*. PublicAffairs.

THE NUTRITIONAL ADEQUACY OF PLANT BASED DIETS

Prachi Chaturvedi

Faculty of Food Science and Quality Control,
Institute for Excellence in Higher Education (IEHE), Bhopal

Introduction:

Plant-based diets have gained significant attention in recent years due to their potential health benefits, environmental sustainability, and ethical considerations. The term "plant-based diet" encompasses a spectrum of eating patterns that emphasize foods derived from plants, including vegetables, fruits, whole grains, legumes, nuts, and seeds, while minimizing or eliminating animal products (McMacken & Shah, 2017). This chapter examines the nutritional adequacy of plant-based diets, addressing both their benefits and potential challenges in meeting human nutritional needs across different life stages. The growing body of scientific evidence suggests that well-planned plant-based diets can provide all essential nutrients required for optimal health and may offer protection against various chronic diseases (Craig & Mangels, 2009). However, certain nutrients require careful attention to ensure adequacy, particularly in populations following strict vegan diets. Understanding these nutritional considerations is crucial for healthcare professionals, dietitians, and individuals considering or following plant-based eating patterns.

Macronutrient Adequacy in Plant-Based Diets

Protein Requirements and Quality

One of the most common concerns regarding plant-based diets is protein adequacy. Contrary to popular belief, plant-based diets can easily meet protein requirements when caloric needs are satisfied and a variety of plant foods are consumed (Young & Pellett, 1994). The concept of protein combining, once thought necessary for vegetarians, has been largely debunked, as the human body maintains amino acid pools that can complement proteins consumed throughout the day (American Dietetic Association, 2016). Plant proteins from legumes, nuts, seeds, and whole grains provide all essential amino acids, though the proportions may differ from animal proteins. Soy products, quinoa, and hemp seeds are considered complete proteins, containing all essential amino acids in optimal ratios (Messina *et al.*, 2004). Research demonstrates that plant protein can support muscle protein synthesis and athletic performance when consumed in adequate amounts (Lynch *et al.*, 2018).

Carbohydrates and Fiber

Plant-based diets naturally provide abundant complex carbohydrates and dietary fiber, which are associated with numerous health benefits. The high fiber content of plant foods supports digestive health, helps maintain healthy blood glucose levels, and may reduce the risk of

cardiovascular disease and certain cancers (Anderson *et al.*, 2009). Most plant-based eaters consume 25-50 grams of fiber daily, significantly exceeding the recommended intake of 25-35 grams per day.

Fats and Essential Fatty Acids

Plant-based diets can provide adequate amounts of essential fatty acids, though attention must be paid to omega-3 fatty acid intake. While plant foods contain alpha-linolenic acid (ALA), the conversion to EPA and DHA is limited in humans (Saunders *et al.*, 2013). Plant-based sources of omega-3 fatty acids include flaxseeds, chia seeds, walnuts, and algae-based supplements, which can provide EPA and DHA directly.

Micronutrient Considerations

Vitamin B12

Vitamin B12 is perhaps the most critical nutrient of concern for those following plant-based diets, as it is primarily found in animal products. B12 deficiency can lead to megaloblastic anemia and neurological complications (Pawlak *et al.*, 2013). All individuals following plant-based diets should supplement with vitamin B12 or consume fortified foods regularly. The recommended approach includes either a daily supplement of 25-100 mcg or a weekly supplement of 2000 mcg (Norris & Messina, 2011).

Iron

Plant foods contain non-heme iron, which has lower bioavailability compared to heme iron from animal products. However, vitamin C and other organic acids can significantly enhance non-heme iron absorption (Hunt, 2003). Plant-based eaters should consume iron-rich foods such as legumes, fortified cereals, spinach, and pumpkin seeds alongside vitamin C-rich foods. Interestingly, studies show that vegetarians often have similar iron status to omnivores, likely due to adaptive mechanisms (Craig, 2010).

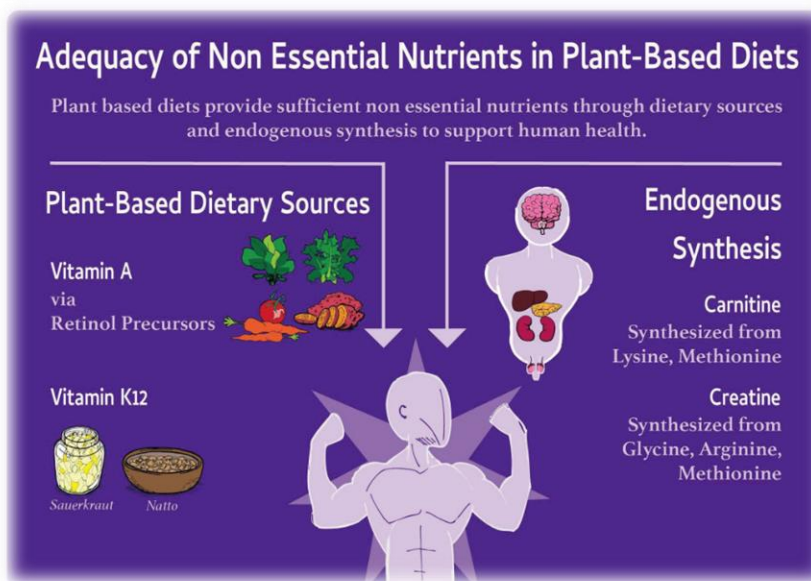
Zinc

Zinc bioavailability from plant foods may be reduced due to phytates, but adequate intake can be achieved through consumption of legumes, nuts, seeds, and whole grains. Soaking, sprouting, and fermenting can improve zinc bioavailability from plant sources (Gibson *et al.*, 2018).

Calcium

Plant-based diets can provide adequate calcium through fortified plant milks, tofu made with calcium sulfate, tahini, almonds, and leafy green vegetables such as kale and bok choy. Some studies suggest that calcium absorption from certain plant sources may be superior to that from dairy products (Weaver *et al.*, 1999).

Vitamin D Vitamin D status depends primarily on sun exposure and supplementation rather than dietary sources. Plant-based eaters should monitor their vitamin D status and supplement as needed, particularly in higher latitudes or during winter months (Crowe *et al.*, 2011).



Omega-3 Fatty Acids

As mentioned earlier, EPA and DHA are limited in plant foods. Algae-based supplements provide a plant-based source of these important fatty acids and may be beneficial for cardiovascular and cognitive health (Geppert *et al.*, 2005).

Health Outcomes of Plant-Based Diets

Cardiovascular Disease

Extensive research demonstrates that plant-based diets are associated with reduced risk of cardiovascular disease. The EPIC-Oxford study found that vegetarians had a 32% lower risk of heart disease compared to omnivores (Crowe *et al.*, 2013). Plant-based diets typically result in lower LDL cholesterol, blood pressure, and inflammatory markers (Yokoyama *et al.*, 2017).

Diabetes Prevention and Management

Plant-based diets show particular promise for diabetes prevention and management. A meta-analysis by Qian *et al.* (2019) found that plant-based diets were associated with a 23% lower risk of type 2 diabetes. The high fiber content and lower caloric density of plant foods contribute to improved insulin sensitivity and glucose control.

Cancer Prevention

The World Cancer Research Fund recommends a diet rich in plant foods for cancer prevention (World Cancer Research Fund, 2018). Plant foods provide protective compounds such as antioxidants, phytochemicals, and fiber while being free from potential carcinogens found in processed meats.

Weight Management

Plant-based diets are often associated with lower body mass index and may facilitate weight loss due to their lower caloric density and higher fiber content (Turner-McGrievy *et al.*, 2015). The thermic effect of plant proteins may also contribute to improved weight management.

Special Populations and Life Stages

Pregnancy and Lactation

Well-planned plant-based diets can support healthy pregnancy and lactation outcomes. Key considerations include adequate intake of protein, iron, calcium, vitamin B12, vitamin D, and omega-3 fatty acids. Prenatal supplements designed for plant-based diets are recommended (Sebastiani *et al.*, 2019).

Infants and Children

Plant-based diets can support normal growth and development in children when properly planned. Breast milk or fortified plant-based infant formulas are appropriate for infants. Attention to energy density, protein quality, and key micronutrients is essential during periods of rapid growth (Mangels & Messina, 2001).

Older Adults

Plant-based diets may offer particular benefits for older adults, including reduced risk of chronic diseases and maintenance of cognitive function. However, attention to vitamin B12, vitamin D, calcium, and protein intake becomes increasingly important with age (Dinu *et al.*, 2017).

Athletes

Plant-based diets can support athletic performance across all levels of competition. Adequate energy and protein intake, along with proper meal timing, are key considerations for plant-based athletes (Rogerson, 2017). Several elite athletes have demonstrated that plant-based diets are compatible with high-level athletic performance.

Practical Guidelines for Nutritional Adequacy

Meal Planning Principles

Successful plant-based nutrition relies on variety, balance, and adequate caloric intake. The plate method can be adapted for plant-based eating: half the plate with vegetables and fruits, one-quarter with whole grains, and one-quarter with protein-rich foods such as legumes, nuts, or seeds.

Supplementation Recommendations

While plant-based diets can provide most nutrients, certain supplements are recommended:

- Vitamin B12: Essential for all plant-based eaters
- Vitamin D: Based on blood levels and sun exposure
- EPA/DHA: Algae-based supplements for optimal omega-3 status
- Iron: Only if deficiency is documented

Food Safety and Preparation

Proper food handling and preparation techniques can maximize nutrient availability and safety. Soaking legumes, sprouting grains, and fermenting foods can improve nutrient bioavailability and digestibility.

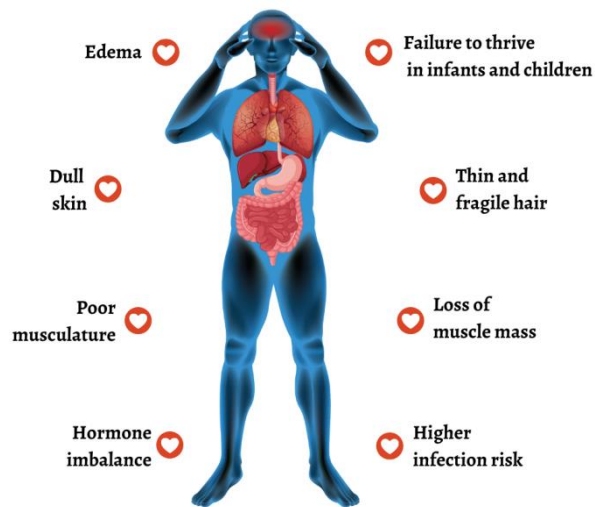
Addressing Common Nutritional Myths

Protein Deficiency Concerns

The myth that plant-based diets cannot provide adequate protein has been thoroughly debunked by scientific research. Plant proteins, when consumed in variety and adequate amounts, can meet all amino acid requirements (Rand *et al.*, 2003).

Bone Health Misconceptions

Contrary to popular belief, countries with the highest dairy consumption do not have the lowest rates of osteoporosis. Plant-based diets can support bone health through adequate calcium intake, vitamin D status, and reduced acid load (Lanou, 2009).



Future Directions and Research Needs

Ongoing research continues to refine our understanding of plant-based nutrition. Areas of active investigation include:

- Optimal protein requirements for different populations
- Long-term effects of various plant-based eating patterns
- Personalized nutrition approaches based on genetic factors
- Environmental impact of different protein sources

Conclusion:

The scientific evidence strongly supports the nutritional adequacy of well-planned plant-based diets across all life stages. These dietary patterns can provide all essential nutrients while offering significant health benefits, including reduced risk of chronic diseases such as cardiovascular disease, type 2 diabetes, and certain cancers. Key considerations include ensuring adequate intake of vitamin B12, monitoring iron and zinc status, and paying attention to omega-3 fatty acids. Healthcare professionals should be equipped to support patients choosing plant-based diets by providing evidence-based guidance on meal planning, supplementation, and monitoring. As the popularity of plant-based eating continues to grow, it is essential that both practitioners

and consumers understand how to optimize these dietary patterns for health and longevity. The transition to plant-based eating represents not only a personal health choice but also a sustainable approach to feeding the growing global population. With proper planning and knowledge, plant-based diets can serve as a foundation for optimal health throughout the human lifespan.

References:

1. American Dietetic Association. (2016). Position of the American Dietetic Association: Vegetarian diets. *Journal of the American Dietetic Association*, 116(12), 1970-1980.
2. Anderson, J. W., Baird, P., Davis, R. H., Ferreri, S., Knudtson, M., Koraym, A., ... & Williams, C. L. (2009). Health benefits of dietary fiber. *Nutrition Reviews*, 67(4), 188-205.
3. Craig, W. J. (2010). Nutrition concerns and health effects of vegetarian diets. *Nutrition in Clinical Practice*, 25(6), 613-620.
4. Craig, W. J., & Mangels, A. R. (2009). Position of the American Dietetic Association: Vegetarian diets. *Journal of the American Dietetic Association*, 109(7), 1266-1282.
5. Crowe, F. L., Appleby, P. N., Travis, R. C., & Key, T. J. (2013). Risk of hospitalization or death from ischemic heart disease among British vegetarians and nonvegetarians: Results from the EPIC-Oxford cohort study. *American Journal of Clinical Nutrition*, 97(3), 597-603.
6. Crowe, F. L., Steur, M., Allen, N. E., Appleby, P. N., Travis, R. C., & Key, T. J. (2011). Plasma concentrations of 25-hydroxyvitamin D in meat eaters, fish eaters, vegetarians and vegans: Results from the EPIC-Oxford study. *Public Health Nutrition*, 14(2), 340-346.
7. Dinu, M., Abbate, R., Gensini, G. F., Casini, A., & Sofi, F. (2017). Vegetarian, vegan diets and multiple health outcomes: A systematic review with meta-analysis of observational studies. *Critical Reviews in Food Science and Nutrition*, 57(17), 3640-3649.
8. Geppert, J., Kraft, V., Demmelmair, H., & Koletzko, B. (2005). Docosahexaenoic acid supplementation in vegetarians effectively increases omega-3 index: A randomized trial. *Lipids*, 40(8), 807-814.
9. Gibson, R. S., Raboy, V., & King, J. C. (2018). Implications of phytate in plant-based foods for iron and zinc bioavailability, setting dietary requirements, and formulating programs and policies. *Nutrition Reviews*, 76(11), 793-804.
10. Hunt, J. R. (2003). Bioavailability of iron, zinc, and other trace minerals from vegetarian diets. *American Journal of Clinical Nutrition*, 78(3), 633S-639S.
11. Lanou, A. J. (2009). Should dairy be recommended as part of a healthy vegetarian diet? Counterpoint. *American Journal of Clinical Nutrition*, 89(5), 1638S-1642S.
12. Lynch, H., Johnston, C., & Wharton, C. (2018). Plant-based diets: Considerations for environmental impact, protein quality, and exercise performance. *Nutrients*, 10(12), 1841.

13. Mangels, A. R., & Messina, V. (2001). Considerations in planning vegan diets: Infants. *Journal of the American Dietetic Association*, 101(6), 670-677.
14. McMacken, M., & Shah, S. (2017). A plant-based diet for the prevention and treatment of type 2 diabetes. *Journal of Geriatric Cardiology*, 14(5), 342-354.
15. Messina, V., Melina, V., & Mangels, A. R. (2004). A new food guide for North American vegetarians. *Journal of the American Dietetic Association*, 103(6), 771-775.
16. Norris, J., & Messina, V. (2011). *Vegan for life: Everything you need to know to be healthy and fit on a plant-based diet*. Da Capo Lifelong Books.
17. Pawlak, R., Parrott, S. J., Raj, S., Cullum-Dugan, D., & Lucas, D. (2013). How prevalent is vitamin B12 deficiency among vegetarians? *Nutrition Reviews*, 71(2), 110-117.
18. Qian, F., Liu, G., Hu, F. B., Bhupathiraju, S. N., & Sun, Q. (2019). Association between plant-based dietary patterns and risk of type 2 diabetes: A systematic review and meta-analysis. *JAMA Internal Medicine*, 179(10), 1335-1344.
19. Rand, W. M., Pellett, P. L., & Young, V. R. (2003). Meta-analysis of nitrogen balance studies for estimating protein requirements in healthy adults. *American Journal of Clinical Nutrition*, 77(1), 109-127.
20. Rogerson, D. (2017). Vegan diets: Practical advice for athletes and exercisers. *Journal of the International Society of Sports Nutrition*, 14(1), 36.
21. Saunders, A. V., Davis, B. C., & Garg, M. L. (2013). Omega-3 polyunsaturated fatty acids and vegetarian diets. *Medical Journal of Australia*, 199(4), S22-S26.
22. Sebastiani, G., Herranz Barbero, A., Borrás-Novell, C., Alsina Casanova, M., Aldecoa-Bilbao, V., Andreu-Fernández, V., & García-Algar, Ó. (2019). The effects of vegetarian and vegan diet during pregnancy on health of mothers and offspring. *Nutrients*, 11(3), 557.
23. Turner-McGrievy, G. M., Davidson, C. R., Wingard, E. E., Wilcox, S., & Frongillo, E. A. (2015). Comparative effectiveness of plant-based diets for weight loss: A randomized controlled trial of five different diets. *Nutrition*, 31(2), 350-358.
24. Weaver, C. M., Proulx, W. R., & Heaney, R. (1999). Choices for achieving adequate dietary calcium with a vegetarian diet. *American Journal of Clinical Nutrition*, 70(3), 543S-548S.
25. World Cancer Research Fund. (2018). *Diet, nutrition, physical activity and cancer: A global perspective*. World Cancer Research Fund International.
26. Yokoyama, Y., Nishimura, K., Barnard, N. D., Takegami, M., Watanabe, M., Sekikawa, A., ... & Miyamoto, Y. (2017). Vegetarian diets and blood pressure: A meta-analysis. *JAMA Internal Medicine*, 174(4), 577-587.
27. Young, V. R., & Pellett, P. L. (1994). Plant proteins in relation to human protein and amino acid nutrition. *American Journal of Clinical Nutrition*, 59(5), 1203S-1212S.

METAL-BASED ANTICANCER AGENTS: EXPLORING THE PROMISE OF TRANSITION COMPLEXES IN CANCER THERAPY

Pawanjeet Kaur

School of Mechatronics Engineering,

Symbiosis Skills and Professional University, Pune, Maharashtra, India- 412101

Corresponding author E-mail: pawanjeet514@gmail.com

Abstract:

Cancer is nowadays becoming the most common death issue among people due to environmental factors and unhealthy eating habits. Multiple cancer treatments have been perceived in past few decades but still few tumours are considered non-treatable via conventional chemotherapies which emphasises the requirement of new effective treatment methodologies. In such scenario, the transition metal based anticancer complexes has gain attention because of their exclusive physicochemical properties like variable oxidation states, redox activity, specificity towards target molecules, tailoring according to the desired target tumour cells, etc. They work via numerous mechanisms like DNA binding and cross-linking in proteins, enzyme inhibition, creating oxidative stress, and programmed death of cancer cells. Multiple transition metal based anticancer complexes of ruthenium, copper, gold, platinum, titanium, etc. are tailored till now that have proven the selective action towards the tumour cells, however there have been few challenges like drug resistance, body-specific side effects like loss of healthy cells due to toxicity which need further research for providing personalized cancer treatments with better selectivity towards the tumour cells, better solubility and bioavailability along with their imitation.

Keywords: Transition Metal Complexes; Anticancer Agents; Coordination Chemistry; Cytotoxicity; Platinum Drugs; Bioinorganic Chemistry; Drug Design.

Introduction:

Cancer, being an acquiescent health disease, the world is suffering from, causes anomalous and uncontrolled cell damage to tissues and organs. As per WHO reports, cancer is the second leading cause of death globally, with millions of cases reported every year. In 2022, there were an estimated 20 million new cases and 9.7million deaths, projections that may reach nearly 30million new cases and 15million deaths annually by 2040. Changing lifestyles, eating habits, pollution, and longer life expectancies have all led to a steady rise in cancer cases in India, specifically breast cancer, cervical cancer, lung cancer, and oral cancer cases are commonly reported. Even though medical technology has come a long way, many distortions still have a dismal survival probability, especially when they are found at an advanced stage, so, we need to

find and create better, safer, and more specific ways to cure cancer as soon as possible to lessen its effects on society.

Chemotherapeutic agents are chemical compounds that are often used in traditional cancer therapies. They work by killing cells that are dividing quickly, which is a significant sign of cancer. But a lot of healthy cells in the body, like those in the bone marrow, digestive tract, and hair follicles, also divide quickly. This means that normal cells can also be harmed by chemotherapy, which can cause serious side effects like nausea, hair loss, fatigue, and immune suppression. Many cancer cells get used to these drugs over time (drug resistance) making the treatment less effective. Also, these drugs are not always able to identify the difference between healthy and cancerous tissues, which limits their ability to help. As a result, there is a critical need to produce agents that are more selective, less toxic, and capable of overcoming drug resistance.

The researchers are working on designing metal-based targeted therapies as they have shown promising results. In comparison with organic molecules, the transition metals can form stable and wide-ranging complexes with various ligands due to their discrete chemical and biological properties. Due to their adaptability and tendency to exhibit various oxidation states, the compounds can be formulated with specific sizes, geometries, charges, and reactivities that are targeted to specific cancer cells by causing oxidative stress. Metal ions can mimic biological functions or interfere with important cellular processes, making them extremely effective at disrupting cancer cell metabolism. The complexes show different geometries like square planar, octahedral, or tetrahedral and accordingly they interact with DNA, proteins, and enzymes in the body. For instance, the square planar cisplatin binds effectively to DNA, leading to programmed cancer cell death.

Table 1 provides an overview of existing metal-based anticancer drugs along with their mechanism of action, limitations, and scope for innovation.

Table 1: Existing Metal-Based Anticancer Drugs

Metal Complex	Drug Name	Clinical Status	Mechanism of Action	Limitations	Scope for Innovation
Platinum (II)	Cisplatin	FDA approved	Binds to DNA, causes crosslinking, triggers apoptosis	Nephrotoxicity, drug resistance, low selectivity	Ligand modifications to reduce toxicity and enhance targeting
Platinum (II)	Carboplatin	FDA approved	Similar to cisplatin, slower activation	Less potent, still causes side effects	Development of prodrugs and delivery systems

Platinum (II)	Oxaliplatin	FDA approved (colorectal)	DNA binding, inhibits DNA synthesis	Peripheral neuropathy, resistance	Use in combination therapy to improve outcomes
Ruthenium (III)	NAMI-A	Phase I/II clinical trials	Anti-metastatic, affects angiogenesis	Limited cytotoxicity against primary tumors	Dual-targeting with photosensitizers or nanocarriers
Ruthenium (III)	KP1019 (NKP1339)	Phase I/II clinical trials	Induces oxidative stress, binds transferrin	Poor water solubility, short half-life	Improved solubility and bioavailability via formulation
Gold(I/III)	Auranofin (repurposed)	In clinical trials (various)	Inhibits thioredoxin reductase, induces ROS	Systemic toxicity, instability in vivo	Ligand engineering for tumor selectivity
Copper (II)	Various experimental	Preclinical stage	Generates ROS, disrupts mitochondrial functions	Redox cycling may damage healthy tissues	Development of tumor-targeted copper carriers
Titanium (IV)	Titanocene dichloride	Discontinued (Phase II)	DNA interaction, cell cycle arrest	Hydrolysis in aqueous media	Stabilized analogues with better pharmacokinetics

This chapter emphasizes the evolving field of metal-based anticancer agents, specifically the therapeutic drugs derived from transition metal complexes, their tailoring capacity, action mechanisms, current developments along with the challenges observed and future research directions, which is highly required as an alternative to conventional therapies.

Chemical Basis of Metal-Based Drug Design

Transition metals possess a unique set of physicochemical properties that make them suitable for drug design and therapeutic applications as shown in figure 1. They form active but stable coordination complexes with a variety of ligands that are tailored for interactions with biological targets. The following characteristics play a crucial role in their anticancer potential:

- 1. Variable Oxidation States:** Transition metals exist in multiple oxidation states, which is required for feasible redox reactions with targets due to selective oxidative stress in cancer cells. For example, Ru (II)/Ru (III), Cu (I)/Cu (II) complexes can switch oxidation states and

generate reactive oxygen species (ROS), are activated only within the tumor microenvironment.

- 2. Ligand Exchange Kinetics:** Transition metals when reaches the target site, it can effectively release or exchange ligands, interact with biomolecules such as DNA or proteins, and enact its therapeutic action. For example, cisplatin undergoes hydration by replacing chloride in the cytoplasm, which activates it for DNA binding. The control of ligand lability is required for tailoring the reactivity and selectivity of the drug.
- 3. Versatile Geometries:** Transition metal complexes can adopt a range of coordination geometries such as square planar, octahedral, tetrahedral, and trigonal bipyramidal, depending on the central metal ion and ligands used. This geometric flexibility provides diverse options for designing complexes that can mimic biological structures, fit into enzyme active sites, or interact with specific DNA grooves. For instance, the square planar geometry of Pt (II) complexes allows for optimal crosslinking of DNA bases, which disrupts DNA replication in cancer cells. On the other hand, octahedral ruthenium complexes are known to exhibit better three-dimensional selectivity for certain cellular targets.
- 4. Biological Availability and Cellular Transport:** For any therapeutic agent to be effective, it must reach its site of action in adequate concentrations. However, many transition metals exhibit high affinity for biomolecular carriers such as transferrin, albumin, and glutathione, which can assist in their cellular uptake and systemic transport. Ruthenium (III) complexes, for instance, can bind to transferrin and enter cells via receptor-mediated endocytosis, enhancing their tumor-selective accumulation. The physicochemical properties of metal complexes like lipophilicity, charge, and size can be optimized to improve cell membrane permeability and bioavailability.
- 5. Ligand Design and Stability:** The ligands surrounding the transition metal ion play a critical role in modifying the biological activity, selectivity, stability, and solubility of metal-based anticancer drugs. Proper ligand designing is required for stability and attacking the target site for therapies. Chelating ligands form more stable complexes than monodentate ligands due to the chelate effect, multidentate ligands also helps control the geometry of the complex, which is vital for cellular interactions.
- 6. Targeting and Functional Groups:** Secondary ligands can be tailored with bioactive molecules that can detect the tumor specific receptors and improve the drug selectivity for specific sites. They can also respond to specific pH, enzymatic and redox conditions.

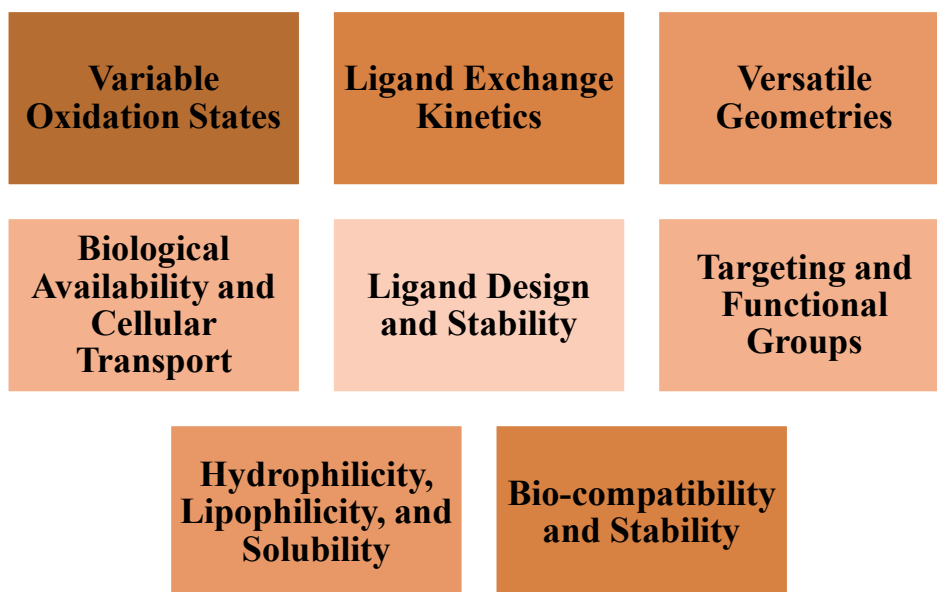


Figure 1: Chemical Basis of Metal-Based Drug Design

- 7. Hydrophilicity, Lipophilicity, and Solubility:** Hydrophilic ligands increase aqueous solubility, while lipophilic ligands can enhance membrane permeability. A proper metal complex ensures the solubility for transport and enough lipophilicity for cellular entry. Poorly soluble metal complexes can aggregate in blood plasma, reducing their bioavailability and potentially causing toxicity. Therefore, solubility-enhancing ligands such as sulfonates, carboxylates, or polyethylene glycol (PEG) are performed.
- 8. Bio-compatibility and Stability:** Ligands must also be non-toxic, biodegradable, and non-immunogenic to avoid adverse reactions. The bioinspired ligands, such as amino acids, nucleobases, or small peptides, are preferred for their better biocompatibility and ease of metabolism. A highly stable complex resists hydrolysis, oxidation, and ligand substitution but controlled lability is essential for activation at the tumor site. For example, cisplatin remains relatively stable in blood but becomes active upon hydration.

Mechanisms of Anticancer Action

Transition metal complexes can combat cancer through multiple mechanisms that enhance their efficacy, making them highly versatile in their mode of action and also help in overcoming drug resistance. The traditional drugs often target a single biological process, but the transition metal complexes routes via following mechanisms:

- 1. Protein and Enzyme Inhibition:** Many metal complexes interact with enzymes and proteins, interfering with key cellular processes. Au (I) and Au (III) complexes, are strong inhibitors of thiol-containing enzymes like thioredoxin reductase, which is crucial for maintaining redox balance in cancer cells. Transition metals may also bind to proteasomes, kinases, or topoisomerases, leading to disruption of signaling pathways and cellular stress responses which cause misfolding of proteins and initiate apoptosis.

2. **DNA Interaction:** The most established mechanism is direct interaction with DNA. Platinum-based drugs such as cisplatin bind to the N7 position of guanine bases, forming intra- and inter-strand DNA crosslinks which distort the DNA structure, blocks replication and activates cell repairing. Ruthenium or copper complexes, can cleave DNA strands, leading to cytotoxic effects. The table 2 shows the types of DNA interactions by metal complexes.

Table 2: Types of DNA Interactions by Metal Complexes

Type of Interaction	Example Metals	Effect on DNA
Covalent binding	Platinum(II), Gold(III)	Crosslinking, helix distortion
Intercalation	Ruthenium(II), Copper(II)	Insertion between base pairs
Groove binding	Titanium(IV), Zinc(II)	Non-covalent interaction with DNA grooves
Strand cleavage	Copper(II), Iron(III)	Oxidative damage, fragmentation

3. **Initiation of reactive oxygen species:** many transition metal complexes catalyse the production of reactive oxygen species (ros) inside cancer cells, leading to oxidative stress. Since cancer cells are already under higher oxidative pressure than normal cells, additional ros can push them over the threshold, resulting in mitochondrial dysfunction, lipid peroxidation, and cell death. Cu (ii), fe (iii), and manganese-based complexes are known to generate ros.

Table 3: Metal Complexes and Their Role in ROS Generation

Metal	Oxidation State	Mechanism	Effects
Copper(II)	+2	Redox cycling, Fenton reaction	DNA/protein oxidation, apoptosis
Iron(III)	+3	Fenton chemistry	Mitochondrial damage
Ruthenium(III)	+3	Ligand-mediated ROS generation	Cell stress, apoptosis
Manganese(II)	+2	Catalytic ROS release	Lipid peroxidation, necrosis

4. **Targeted Action and Selectivity:** Modern metal-based drugs emphasize selective toxicity i.e. maximizing damage to cancer cells while sparing healthy ones. These are activated only under tumor-specific conditions. The ligand-conjugated complexes or nanocarriers can enhance specificity. For example, Ru (III) complexes are relatively inactive in blood but are reduced to Ru(II) in the hypoxic environment of tumors, where they become pharmacologically active. They inhibit the formation of new blood vessels

required for tumor growth. For example, NAMI-A, a Ru(III) complex, reduces tumor spread without severely affecting primary tumor size.

Analytical Techniques for Characterizing Metal-Based Anticancer Complexes

Table 4: Analytical Techniques for Characterizing Metal-Based Anticancer Complexes

Technique	Parameter Studied	Key Insights for Drug Design
Elemental Analysis	Composition (C, H, N, metal content)	Confirms empirical formula and stoichiometry of complex.
X-ray Crystallography	3D molecular structure and geometry	Reveals coordination environment, ligand orientation, and bond lengths; essential for structure-activity relationship (SAR) studies.
UV-Visible Spectroscopy	Electronic transitions (d–d, LMCT)	Indicates changes in metal oxidation state and interactions with biomolecules like DNA.
IR Spectroscopy	Functional groups, metal–ligand bonding	Confirms coordination through shifts in ligand vibrational bands.
NMR Spectroscopy	Proton and carbon environment in ligands	Helps identify ligand binding mode (for diamagnetic complexes); detects dynamic behaviour.
EPR Spectroscopy	Unpaired electrons, oxidation states	Useful for paramagnetic metals; gives information on metal oxidation state and ligand field.
Mass Spectrometry (MS)	Molecular weight, fragmentation pattern	Confirms integrity and stability of complex under physiological-like conditions.
Cyclic Voltammetry (CV)	Redox behaviour, electrochemical potential	Evaluates ability of complex to undergo redox changes; important for ROS-mediated activity.
TGA / DSC	Thermal stability, decomposition temperature	Predicts shelf life, formulation parameters, and suitability for pharmaceutical processing.
DNA Binding Assays	DNA intercalation, cleavage, affinity	Correlates drug–DNA interaction with mechanism of cytotoxicity.
ICP-MS / Fluorescence	Cellular uptake, metal quantification	Measures drug internalization and localization in cells.
Cytotoxicity Assays	Cell viability (e.g., MTT, SRB)	Determines anticancer potency and therapeutic window.

The characterization of metal-based anticancer agents is performed to evaluate both the chemical integrity and biological relevance of transition metal complexes. Each technique contributes to understand how these compounds function as therapeutic agents. For instance, X-ray crystallography offers precise structural data that inform ligand design, while UV-Visible and IR spectroscopy detect subtle shifts in coordination environment upon biomolecular interaction. Techniques like EPR and CV help decode redox-mediated mechanisms, critical for drugs that induce oxidative stress. Additionally, DNA binding studies and cytotoxicity analysis investigates the pharmacological applications. Table 4 summarizing key analytical and spectroscopic techniques used in the characterization of metal-based anticancer agents.

Notable Metal-Based Anticancer Drugs

Transition metal-based chemotherapeutics have gained considerable consideration due to their unique chemical reactivity and ability to interact with biological macromolecules. Several metal complexes have either been approved for clinical use or are undergoing preclinical and clinical trials. Platinum-based drugs form crosslinks to DNA that leads to disruption in cancer cell replication for example, Cisplatin is used for testicular, ovarian, bladder, and lung cancers, Carboplatin is toxic to cancer cells but having less effectiveness, Oxaliplatin is effective against colorectal cancer but induces neurotoxicity. Ruthenium complexes offer advantages over platinum drugs due to their lower toxicity, variable oxidation states, and better tumour selectivity. For example, NAMI-A exhibits anti-metastatic properties but limited activity against primary tumours, whereas KP1019 (NKP1339) shows cytotoxicity in colon and lung cancers is under Phase I/II trials. Gold complexes are gaining attention for their enzyme inhibition capabilities, especially thioredoxin reductase, which plays a key role in maintaining redox balance in cancer cells. Gold(I) phosphine complexes have shown promising results in mitochondrial targeting and ROS production. Copper is an essential trace element and its complexes exhibit potent redox cycling ability, leading to ROS-mediated cytotoxicity and act as enzyme inhibitors. Titanocene Dichloride is failed in clinical trials due to hydrolytic instability, whereas Gallium (III) complexes are disrupting tumour proliferation and Iridium complexes are reputable for photo-activated therapies and redox activity. Table 4. outlines the most significant examples of the metal complexes have either been approved for clinical use.

Table 5. Comparative Overview of reported Metal-Based Anticancer Agents

Metal	Drug/ Complex	Oxidation State	Primary Mechanism	Cancer Type	Clinical Status	Limitations
Platinum	Cisplatin	+2	DNA crosslinking, apoptosis	Testicular, ovarian, lung, etc.	FDA Approved	Nephrotoxicity, resistance

Platinum	Oxaliplatin	+2	DNA adduct formation	Colorectal	FDA Approved	Neurotoxicity
Ruthenium	NAMI-A	+3	Anti-metastatic, non-DNA targets	Lung, colon (metastasis)	Phase I/II Clinical Trials	Weak activity on primary tumors
Ruthenium	KP1019	+3	DNA binding, ROS induction	Colon, lung	Phase I/II Clinical Trials	Solubility and pharmacokinetics issues
Gold	Auranofin	+1	TrxR inhibition, ROS generation	Various (repurposed)	Clinical Trials	Toxicity, in vivo instability
Copper	Experimental complexes	+2	ROS production, DNA cleavage	Breast, colon, leukemia	Preclinical	Redox imbalance in healthy cells
Titanium	Titanocene Dichloride	+4	DNA interaction	Various	Discontinued (Phase II)	Hydrolytic instability
Gallium	Gallium nitrate	+3	Iron metabolism interference	Non-Hodgkin's lymphoma, bladder	Limited Clinical Use	Weak cytotoxicity

Challenges and Limitations of Metal-Based Anticancer Agents

Despite the promising advancements in metal-based drug design, several scientific and clinical challenges continue to hinder their widespread adoption in cancer therapy. A major limitation of many metal-based drugs, including cisplatin, is their lack of selectivity toward cancer cells. While these agents effectively kill rapidly dividing cells, they may also damage healthy tissues, leading to severe side effects such as nephrotoxicity, neurotoxicity, and gastrointestinal disturbances. Figure 2. Represents the challenges and limitations of metal-based anticancer agents.

Many transition metal complexes are sensitive to aqueous environments and may undergo hydrolysis, ligand exchange, or redox changes before reaching the tumour site. This instability reduces their bioavailability and therapeutic action. For example, premature hydration of cisplatin in the bloodstream can lead to unintended interactions and reduced efficacy.

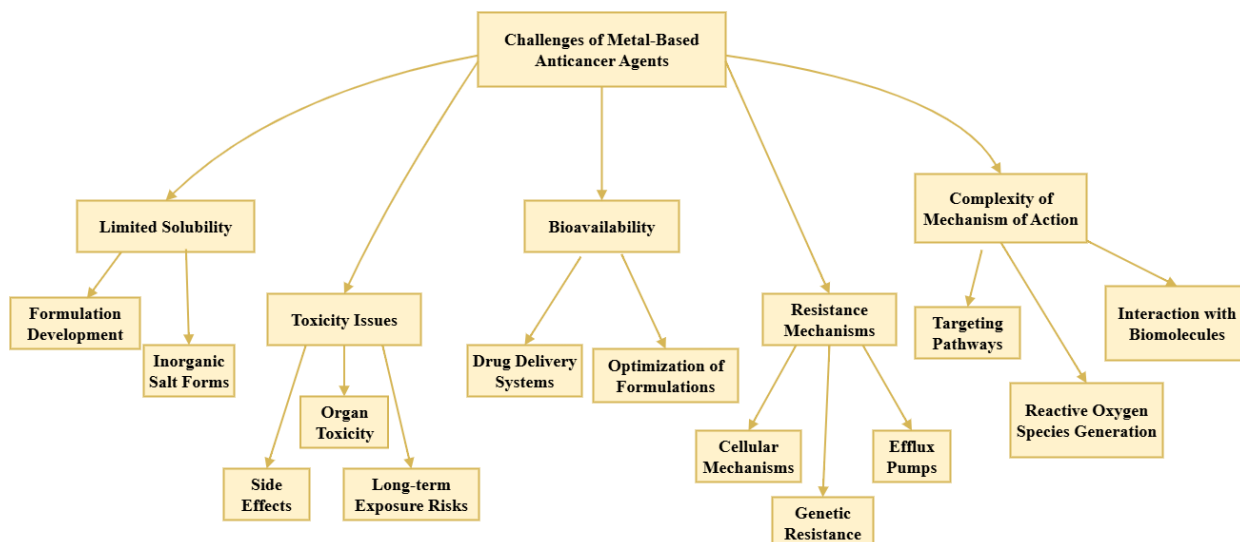


Figure 2: Challenges of Metal-Based Anticancer Agents

Few complexes have shown interaction with serum proteins (e.g., albumin, transferrin) can affect biodistribution and circulation time, complicating dosage design. Moreover, accumulation in non-target tissues can cause long-term toxicity. Compared to organic drugs, metal-based agents face additional scrutiny during regulatory approval due to concerns about long-term metal accumulation and difficulties in standardizing synthesis and formulation.

The synthesis and purification of metal complexes often require expensive reagents, high-purity solvents, and sophisticated instrumentation, contributing to high production costs. Unused or excreted metal-based drugs may persist in the environment, raising concerns about bioaccumulation and ecosystem toxicity.

Conclusion:

In conclusion, while the journey of metal-based anticancer agents has come a long way—from serendipitous discoveries to sophisticated molecular design—the path ahead is both exciting and demanding. These compounds hold extraordinary potential, but realizing their full clinical value will require persistent innovation, thoughtful collaboration, and a patient-centred approach. As science and technology converge, the hope is not just to create better drugs, but to offer renewed hope to patients and families facing the realities of cancer. With sustained research efforts, especially in countries like India where the scientific talent is vast, metal-based therapeutics could play a transformative role in making cancer treatment more targeted, effective, and humane.

References:

1. Rubner, G., Bendorf, K., Wellner, A., Kircher, B., Bergemann, S., Ott, I., & Gust, R. (2010). Synthesis and Biological Activities of Transition Metal Complexes Based on Acetylsalicylic Acid as Neo-Anticancer Agents. *Journal of Medicinal Chemistry*, 53(19), 6889–6898. <https://doi.org/10.1021/jm101019j>

- Damercheli, M., Mahdi, M., Bita Mehravi, & Mehdi Shafiee Ardestani. (2019). Bioactive Salen-type Schiff Base Transition Metal Complexes as Possible Anticancer Agents. *PubMed*, 18(4), 2055–2066. <https://doi.org/10.22037/ijpr.2019.12792.11151>
- Komeda, S., & Casini, A. (2012). Next-Generation Anticancer Metallodrugs. *Current Topics in Medicinal Chemistry*, 12(3), 219–235. <https://doi.org/10.2174/156802612799078964>
- Ruiz-Azuara, L., & E. Bravo-Gomez, M. (2010). Copper Compounds in Cancer Chemotherapy. *Current Medicinal Chemistry*, 17(31), 3606–3615. <https://doi.org/10.2174/092986710793213751>
- Kostova, I., & Bentham Science Publishers, B. S. P. (2006). Gold Coordination Complexes as Anticancer Agents. *Anti-Cancer Agents in Medicinal Chemistry*, 6(1), 19–32. <https://doi.org/10.2174/187152006774755500>
- Manik Lal Saha, Yan, X., & Stang, P. J. (2016). Photophysical Properties of Organoplatinum(II) Compounds and Derived Self-Assembled Metallacycles and Metallacages: Fluorescence and its Applications. *Accounts of Chemical Research*, 49(11), 2527–2539. <https://doi.org/10.1021/acs.accounts.6b00416>
- Hadjiliadis, N. D., & Sletten, E. (2009). Metal Complex–DNA Interactions. In *Wiley eBooks*. Wiley. <https://doi.org/10.1002/9781444312089>
- Gil-Rubio, J., & Vicente, J. (2017). The Coordination and Supramolecular Chemistry of Gold Metalloligands. *LA Referencia* (Red Federada de Repositorios Institucionales de Publicaciones Científicas), 24(1), 32–46. <https://doi.org/10.1002/chem.201703574>
- Shaili, E. (2014). Platinum Anticancer Drugs and Photochemotherapeutic Agents: *Recent Advances and Future Developments*. *Science Progress*, 97(1), 20–40. <https://doi.org/10.3184/003685014x13904811808460>
- Leon, I., Cadavid-Vargas, J., Di Virgilio, A., & Etcheverry, S. (2017). Vanadium, Ruthenium and Copper Compounds: A New Class of Nonplatinum Metallodrugs with Anticancer Activity. *Current Medicinal Chemistry*, 24(2), 112–148. <https://doi.org/10.2174/0929867323666160824162546>
- Poursharifi, M., Wlodarczyk, M. T., & Mieszawska, A. J. (2018). Nano-Based Systems and Biomacromolecules as Carriers for Metallodrugs in Anticancer Therapy. *Inorganics*, 7(1), 2. <https://doi.org/10.3390/inorganics7010002>
- Kashyap, S., Kumar, S., Ramasamy, K., Lim, S. M., Shah, S. A. A., Om, H., & Narasimhan, B. (2018). Synthesis, biological evaluation and corrosion inhibition studies of transition metal complexes of Schiff base. *Chemistry Central Journal*, 12(1). <https://doi.org/10.1186/s13065-018-0487-1>

13. Dasari, S., & Tchounwou, P. B. (2014). Cisplatin in Cancer therapy: Molecular Mechanisms of Action. *European Journal of Pharmacology*, 740(1), 364–378. <https://doi.org/10.1016/j.ejphar.2014.07.025>
14. Ruiz-Azuara, L., & E. Bravo-Gomez, M. (2010). Copper Compounds in Cancer Chemotherapy. *Current Medicinal Chemistry*, 17(31), 3606–3615. <https://doi.org/10.2174/092986710793213751>
15. Jiao, Z., Chen, Y., Wan, Y., & Zhang, H. (2011). Anticancer efficacy enhancement and attenuation of side effects of doxorubicin with titanium dioxide nanoparticles. *International Journal of Nanomedicine*, 2321. <https://doi.org/10.2147/ijn.s25460>
16. Deo, K., Pages, B., Ang, D., Gordon, C., & Aldrich-Wright, J. (2016). Transition Metal Intercalators as Anticancer Agents—Recent Advances. *International Journal of Molecular Sciences*, 17(11), 1818. <https://doi.org/10.3390/ijms17111818>
17. Nasibullin, I., Smirnov, I., Ahmadi, P., Vong, K., Kurbangalieva, A., & Tanaka, K. (2022). Synthetic prodrug design enables biocatalytic activation in mice to elicit tumor growth suppression. *Nature Communications*, 13(1), 39. <https://doi.org/10.1038/s41467-021-27804-5>
18. Smith, C. B., Days, L. C., Alajroush, D. R., Faye, K., Khodour, Y., Beebe, S. J., & Holder, A. A. (2021). Photodynamic Therapy of Inorganic Complexes for the Treatment of Cancer. *Photochemistry and Photobiology*. <https://doi.org/10.1111/php.13467>
19. Trachootham, D., Alexandre, J., & Huang, P. (2009). Targeting cancer cells by ROS-mediated mechanisms: a radical therapeutic approach? *Nature Reviews Drug Discovery*, 8(7), 579–591. <https://doi.org/10.1038/nrd2803>
20. Senapati, S., Mahanta, A. K., Kumar, S., & Maiti, P. (2018). Controlled drug delivery vehicles for cancer treatment and their performance. *Signal Transduction and Targeted Therapy*, 3(1). <https://doi.org/10.1038/s41392-017-0004-3>

RENEWABLE ENERGY: A PATHWAY TO A SUSTAINABLE FUTURE

Bindesh Kumar Shukla

Department of Physics,

Govt. Sanjay Gandhi Smriti Post Graduate College, Ganj Basoda

Corresponding author E-mail: bindeshshukla@gmail.com

Abstract:

Global demand for energy is rising, but reliance on fossil fuels has led to serious environmental problems. Renewable energy, which comes from sources like sunlight, wind, water, biomass, and geothermal heat, provides a sustainable and cleaner option. It helps reduce greenhouse gases, improves energy security, and supports economic growth. This paper gives an overview of renewable energy technologies, their benefits, challenges, and future prospects. A comparison of different renewable sources is also presented. The role of renewable energy in achieving global climate targets and the United Nations Sustainable Development Goal 7 is discussed.

Keywords: Renewable Energy, Sustainable Development, Climate Change, Energy Transition, Green Technology.

Introduction:

Energy is essential for human life and economic growth. Most of today's energy still comes from fossil fuels such as coal, oil, and natural gas (IEA, 2023). While these fuels powered industrial revolutions and modern development, they also caused greenhouse gas emissions, air pollution, and resource depletion (IPCC, 2023).

Burning fossil fuels contributes nearly three-quarters of all human-made greenhouse gas emissions, which drive global warming and extreme weather events (IPCC, 2023). To reduce these risks, the world needs to move toward cleaner energy systems. Renewable energy such as solar, wind, hydropower, geothermal, and biomass is naturally replenished and much less harmful to the environment (REN21, 2023). Falling costs of solar and wind technologies, along with better energy storage, have made renewables more practical worldwide. In 2022, renewables provided around 30% of global electricity, with solar and wind leading the growth (REN21, 2023).

In addition to reducing emissions, renewable energy strengthens energy security by lowering dependence on imported fuels and stabilizing energy prices (United Nations, 2024). It also creates jobs and supports local economies (IRENA, 2023). This transformation is central to achieving UN Sustainable Development Goal 7, which calls for affordable and clean energy for all by 2030.

2. Types of Renewable Energy

2.1 Solar Energy

Solar energy is one of the most abundant renewable resources on Earth. It can be harnessed in two major ways:

- **Photovoltaic (PV) Systems:** These directly convert sunlight into electricity using semiconductor materials such as silicon. When sunlight hits the PV cell, photons excite electrons, creating an electric current. PV systems are modular, making them suitable for applications ranging from rooftop panels for households to massive utility-scale solar farms (Ellabban *et al.*, 2014).
- **Concentrated Solar Power (CSP):** CSP systems use mirrors or lenses to concentrate sunlight onto a small receiver. The concentrated heat produces steam that drives a turbine to generate electricity. CSP is typically used in sunny, arid regions with high solar radiation.

Solar energy is clean, scalable, and increasingly affordable. The cost of solar PV has dropped by more than 85% between 2010 and 2022 (IEA, 2022). However, solar generation is intermittent since it depends on sunlight availability, requiring effective storage systems such as lithium-ion batteries or integration with other energy sources for stable supply.

2.2 Wind Energy

Wind energy captures the kinetic energy of moving air and converts it into mechanical or electrical energy using wind turbines.

- **Onshore Wind:** Installed on land, these turbines are cost-effective and widely deployed.
- **Offshore Wind:** Installed in oceans or seas, where wind speeds are stronger and more consistent, offshore wind farms generate higher power but require higher investment.

Advances in turbine blade design, height, and efficiency have made wind one of the fastest-growing renewable technologies. By 2021, the global wind sector had become cost-competitive with fossil fuels in many regions (IRENA, 2021).

Despite its potential, wind energy faces some limitations. Large-scale farms may cause noise, visual impact, and land-use conflicts. Offshore projects can affect marine ecosystems. Nonetheless, wind power remains a key player in reducing carbon emissions and supplying large-scale clean electricity (Gonzalez *et al.*, 2020).

2.3 Hydropower

Hydropower is the oldest and most widely used renewable energy source. It works by channelling water through turbines to generate electricity.

- **Large Hydropower Dams:** These can produce gigawatts of electricity and provide base-load power. Examples include China's Three Gorges Dam and Brazil's Itaipu Dam.
- **Small and Micro Hydropower:** These systems provide electricity to rural or off-grid areas and are less disruptive to the environment.
- **Pumped Storage Hydropower:** Stores energy by pumping water uphill during low demand and releasing it during peak demand.

Hydropower is highly reliable and efficient, with capacity factors often exceeding 50% (World Bank, 2020). However, large dams may cause serious ecological and social issues, including river ecosystem disruption, habitat loss, and community displacement (Zarfl *et al.*, 2015). Modern designs are moving toward run-of-river systems and low-impact hydropower to minimize damage.

2.4 Biomass Energy

Biomass energy is derived from organic materials such as crop residues, forestry waste, animal manure, and algae. It can be used in several ways:

- **Direct Combustion:** Burning biomass (wood, crop waste) to produce heat and electricity.
- **Biogas Production:** Anaerobic digestion of organic waste to produce methane-rich gas, which can fuel generators.
- **Biofuels:** Conversion of crops into liquid fuels such as ethanol and biodiesel for transport.

Biomass energy is considered carbon neutral because the CO₂ released during combustion is roughly balanced by CO₂ absorbed during plant growth (Demirbas, 2011). However, unsustainable sourcing, deforestation, or land-use change can undermine its benefits. When managed properly, biomass can help reduce agricultural waste, provide rural income, and contribute to circular economies.

2.5 Geothermal Energy

Geothermal energy utilizes heat stored beneath the Earth's surface. This heat originates from natural radioactive decay and the Earth's internal energy.

- **Electricity Generation:** High-temperature reservoirs are drilled to access steam, which drives turbines.
- **Direct Heating:** Geothermal systems can directly heat buildings, greenhouses, and industrial processes.

Unlike solar or wind, geothermal energy provides a continuous and stable power supply with high-capacity factors (70–90%). It has a small land footprint and minimal emissions (Lund & Boyd, 2016). However, geothermal plants are limited to geologically active regions (e.g., Iceland, Indonesia, parts of the U.S.), and drilling costs are high.

2.6 Ocean Energy

The oceans hold vast energy potential, which can be harnessed through different technologies:

- **Tidal Energy:** Captures predictable rises and falls of tides caused by gravitational interactions between the Earth, Moon, and Sun.
- **Wave Energy:** Uses the motion of surface waves to drive turbines.
- **Ocean Thermal Energy Conversion (OTEC):** Exploits temperature differences between warm surface water and cold deep water to generate electricity.

3. Benefits of Renewable Energy

Environmental protection: Reduces greenhouse gases and improves air quality (REN21, 2022; Jacobson et al., 2017).

Energy security: Locally available and reduces dependence on imported fuels (IEA, 2021).

Economic growth and jobs: Millions of jobs created worldwide, especially in solar and wind sectors (IRENA, 2022).

Flexibility: Can be deployed from small household systems to large farms (Ellabban et al., 2014).

Falling costs: Solar and wind are now among the cheapest sources of new electricity (Lazard, 2021).

4. Challenges of Renewable Energy

Intermittency: Solar and wind are weather-dependent (Denholm et al., 2010; IRENA, 2020).

Storage needs: Batteries and other storage technologies are costly (Chen et al., 2009)

High upfront costs: Initial investment is often expensive (REN21, 2022).

Land use and environment: Large projects may disrupt ecosystems (Turney & Fthenakis, 2011).

Grid integration: Requires modernized grids and infrastructure (IEA, 2021).

Policy support: Growth depends on stable government policies and incentives (IRENA, 2022).

5. Future Outlook

Renewables are expected to dominate global energy growth by 2030, providing nearly 90% of new capacity (IEA, 2023). Hybrid systems combining solar, wind, and storage will deliver reliable clean power even in variable conditions (Bhattacharyya, 2018). Green hydrogen, advanced bioenergy, and carbon capture integration may help decarbonize industries like steel and aviation. To achieve this vision, continued investment in grid upgrades, storage solutions, and skilled workforce training will be crucial. Strong policies and public support will ensure that renewable energy becomes the backbone of a sustainable and resilient future.

Conclusion:

Renewable energy is no longer an alternative it is becoming the foundation of the global energy system. With falling costs, technological progress, and growing demand for sustainability, renewables are central to fighting climate change, improving health, and driving economic growth. Overcoming challenges like intermittency, financing, and policy uncertainty will require cooperation across governments, industries, and communities. If managed well, renewable energy can secure a cleaner, healthier, and more equitable future for all.

References:

1. Bhattacharyya, S. C. (2018). Mini-grids for the base of the pyramid market: A critical review. *Energies*, 11(4), 813. <https://doi.org/10.3390/en11040813>
2. Chen, H., Cong, T. N., Yang, W., Tan, C., Li, Y., & Ding, Y. (2009). Progress in electrical energy storage system: A critical review. *Progress in Natural Science*, 19(3), 291–312. <https://doi.org/10.1016/j.pnsc.2008.07.014>

3. Cherp, A., & Jewell, J. (2014). The concept of energy security: Beyond the four As. *Energy Policy*, 75, 415–421. <https://doi.org/10.1016/j.enpol.2014.09.005>
4. Demirbas, A. (2011). Competitive liquid biofuels from biomass. *Applied Energy*, 88(1), 17–28. <https://doi.org/10.1016/j.apenergy.2010.07.016>
5. Denholm, P., Ela, E., Kirby, B., & Milligan, M. (2010). The role of energy storage with renewable electricity generation. National Renewable Energy Laboratory (NREL). <https://doi.org/10.2172/2142047>
6. Ellabban, O., Abu-Rub, H., & Blaabjerg, F. (2014). Renewable energy resources: Current status, future prospects and their enabling technology. *Renewable and Sustainable Energy Reviews*, 39, 748–764. <https://doi.org/10.1016/j.rser.2014.07.113>
7. Gonzalez, E., et al. (2020). Offshore wind energy: A review of the current status, challenges and future development in Spain. *Renewable and Sustainable Energy Reviews*, 132, 110042. <https://doi.org/10.1016/j.rser.2020.110042>
8. Green, M. A., Dunlop, E. D., Hohl-Ebinger, J., Yoshita, M., Kopidakis, N., & Hao, X. (2022). Solar cell efficiency tables (Version 60). *Progress in Photovoltaics: Research and Applications*, 30(1), 3–12. <https://doi.org/10.1002/pip.3506>
9. International Energy Agency (IEA). (2021). *World energy outlook 2021*. Paris: IEA.
10. International Energy Agency (IEA). (2022). *Renewables 2022: Analysis and forecast to 2027*. Paris: IEA.
11. International Energy Agency (IEA). (2023). *World energy outlook 2023*. Paris: IEA.
12. International Renewable Energy Agency (IRENA). (2021). *Renewable capacity statistics 2021*. Abu Dhabi: IRENA.
13. International Renewable Energy Agency (IRENA). (2022). *World energy transitions outlook 2022*. Abu Dhabi: IRENA.
14. International Renewable Energy Agency (IRENA). (2023). *World energy transitions outlook 2023*. Abu Dhabi: IRENA.
15. Jacobson, M. Z., Delucchi, M. A., Bauer, Z. A., Goodman, S. C., Chapman, W. E., Cameron, M. A., ... & Chen, C. C. (2017). 100% clean and renewable wind, water, and sunlight (WWS) all-sector energy roadmaps for 139 countries of the world. *Joule*, 1(1), 108–121. <https://doi.org/10.1016/j.joule.2017.07.005>
16. Kumar, A., Samadder, S. R., Kumar, N., & Singh, C. (2020). Estimation of the generation rate of different types of plastic wastes and possible revenue recovery from informal recycling: A case study from India. *Waste Management*, 113, 362–370. <https://doi.org/10.1016/j.wasman.2020.05.009>
17. Lewis, A., Estefen, S., Huckerby, J., Musial, W., Pontes, T., & Torres-Martinez, J. (2011). Ocean energy. In O. Edenhofer et al. (Eds.), *IPCC Special Report on Renewable Energy Sources and Climate Change Mitigation* (pp. 497–534). Cambridge University Press.

18. Liu, H., Wang, X., & Lin, X. (2019). Floating solar photovoltaics: Assessing the technical potential of FPV in China. *Renewable and Sustainable Energy Reviews*, 104, 130–141. <https://doi.org/10.1016/j.rser.2019.01.012>
19. Lund, J. W., & Boyd, T. L. (2016). Direct utilization of geothermal energy 2015 worldwide review. *Geothermics*, 60, 66–93. <https://doi.org/10.1016/j.geothermics.2015.11.004>
20. Luo, X., Wang, J., Dooner, M., & Clarke, J. (2015). Overview of current development in electrical energy storage technologies and the application potential in power system operation. *Applied Energy*, 137, 511–536. <https://doi.org/10.1016/j.apenergy.2014.09.081>
21. Mengelkamp, E., Gärttner, J., Rock, K., Kessler, S., Orsini, L., & Weinhardt, C. (2018). Designing microgrid energy markets: A case study: The Brooklyn Microgrid. *Applied Energy*, 210, 870–880. <https://doi.org/10.1016/j.apenergy.2017.06.054>
22. Musial, W., Beiter, P., Schwabe, P., & Tian, T. (2016). Offshore wind energy resource assessment for the United States. National Renewable Energy Laboratory (NREL). <https://www.nrel.gov/docs/fy16osti/66599.pdf>
23. Panwar, N. L., Kaushik, S. C., & Kothari, S. (2011). Role of renewable energy sources in environmental protection: A review. *Renewable and Sustainable Energy Reviews*, 15(3), 1513–1524. <https://doi.org/10.1016/j.rser.2010.11.037>
24. REN21. (2022). *Renewables 2022 global status report*. Paris: REN21 Secretariat.
25. REN21. (2023). *Renewables 2023 global status report*. Paris: REN21 Secretariat.
26. Smil, V. (2017). *Energy and civilization: A history*. MIT Press.
27. Turney, D., & Fthenakis, V. (2011). Environmental impacts from the installation and operation of large-scale solar power plants. *Renewable and Sustainable Energy Reviews*, 15(6), 3261–3270. <https://doi.org/10.1016/j.rser.2011.04.023>
28. United Nations. (2024). *Sustainable Development Goals Report 2024*. New York: UN.
29. World Bank. (2020). *Hydropower sustainability assessment protocol*. Washington, DC: World Bank.
30. Zakeri, B., & Syri, S. (2015). Electrical energy storage systems: A comparative life cycle cost analysis. *Renewable and Sustainable Energy Reviews*, 42, 569–596. <https://doi.org/10.1016/j.rser.2014.10.011>
31. Zarfl, C., Lumsdon, A. E., Berlekamp, J., Tydecks, L., & Tockner, K. (2015). A global boom in hydropower dam construction. *Aquatic Sciences*, 77(1), 161–170. <https://doi.org/10.1007/s00027-014-0377-0>
32. Zhang, Y., Wang, J., & Wang, X. (2018). Big data and machine learning in smart grid: A review. *Renewable and Sustainable Energy Reviews*, 79, 1–18. <https://doi.org/10.1016/j.rser.2017.05.071>

TRANSITION METAL OXIDES: STRUCTURAL INSIGHTS, UNIQUE PROPERTIES AND EMERGING APPLICATIONS FOR A SUSTAINABLE FUTURE

Amarsinha Babasaheb Gorepatil

Department of Chemistry,

S. G. R. G. Shinde College, Paranda Dist. Dharashiv-413502

Corresponding author E-mail: abgorepatil@gmail.com

Introduction:

It is seen that, transition metal oxides (TMOs) have emerged as one of the most versatile and widely studied classes of inorganic materials due to their structural diversity, variable oxidation states, and fascinating physicochemical properties. Furthermore, TMOs are proven to be significant class of material which is at the forefront of modern technological innovations due to its catalysis and energy storage to electronics and environmental remediation. Their multifunctionality is primarily derived from the interplay of crystal structure, metal–oxygen bonding, and redox flexibility, which imparts catalytic activity, semiconducting properties and magnetic responses. TMOs, with their tunable properties and multifunctional behavior advances in renewable energy technologies, including lithium-ion and sodium-ion batteries, supercapacitors, fuel cells, and photocatalytic hydrogen generation. Historically, TMOs have played critical roles in human civilization, from their early use as pigments and dyes to metallurgical applications and catalysis. For example, oxides of iron, copper, and manganese were utilized in pigments for artistic and functional purposes.

The study of TMOs demonstrates the convergence of science, technology and societal needs. With rising worries about the environment, energy insecurity and the urgent demand for sustainable materials, transition metal oxides offer viable solutions through photocatalysis, heterogeneous catalysis and renewable energy systems. In the context of “*Next Gen Research*,” we should explore here, to understand the structure and bonding principles of TMOs, and with investigating their advanced applications establish a significant connection between fundamental chemistry and sustainable development goals.^[1,2]

We have come within reach that, researchers are now able design next-generation TMOs by systematically studying their crystal chemistry, electronic structure and defect chemistry. Such modified TMOs perform efficiently in energy and environmental applications align with principles of green chemistry. This approach encourages innovation that meets societal needs and also contributes to a cleaner, more sustainable future.

Transition Metal Oxides: Their Structure and Chemistry

The structural chemistry of TMOs is remarkably rich and diverse, reflecting the influence of metal ionic size, oxidation state, and preferred coordination geometry. Simple TMOs such as NiO, CoO, and MnO crystallize in a rock-salt structure, where each metal cation is octahedrally coordinated by oxygen anions. This arrangement provides structural stability and facilitates redox processes, particularly in catalytic and electrochemical applications. Another common motif is the rutile structure, exemplified by TiO₂, where edge-sharing octahedra form a dense lattice, imparting semiconducting behavior and high photocatalytic efficiency.

Perovskite oxides, with the general formula ABO₃, are among the most studied structures due to their structural flexibility and tunable properties. The A-site can accommodate large cations such as lanthanum or strontium, while the B-site hosts transition metals like titanium, manganese, or cobalt. By carefully selecting or substituting these cations, researchers can adjust electronic conductivity, magnetic ordering, and catalytic performance. Perovskites such as LaMnO₃ or SrTiO₃ are extensively explored for applications ranging from catalysis to solar energy conversion.

Spinel oxides, represented by AB₂O₄, offer another level of structural adaptability. Cations are distributed between tetrahedral and octahedral sites, which creates intrinsic redox flexibility and contributes to excellent electrical conductivity and catalytic activity. Notable examples include Fe₃O₄ and NiCo₂O₄, which are used in energy storage and electrocatalysis. Layered oxides, such as MoO₃ and LiCoO₂, provide fast ion transport channels, making them ideal candidates for lithium-ion battery cathodes.

The rich variety of structures allows TMOs to be modified for specific applications. Defect engineering, cation substitution and lattice distortion are key strategies to optimize material properties. The interplay between structure and functionality is central to understanding why TMOs remain crucial in both fundamental research and applied technology.^[3]

Unique Properties and Bonding Dynamics

The unique properties of TMOs arise from the combination of their variable oxidation states, mixed ionic–covalent bonding, and strong metal–oxygen orbital interactions. These factors enable TMOs to undergo facile electron transfer, which is essential for redox reactions in catalysis and electrochemical processes. TMOs can accommodate oxygen vacancies or cation deficiencies, which significantly modify their electronic, optical, and catalytic properties.

For instance, cobalt and manganese oxides cycle efficiently between multiple oxidation states, making them effective catalysts for oxygen evolution and reduction reactions in water splitting and fuel cells. Similarly, wide bandgap semiconductors like TiO₂ and ZnO are highly effective photocatalysts for solar-driven pollutant degradation and hydrogen generation. The strong hybridization between metal d orbitals and oxygen 2p orbitals further enables conductivity

modulation, magnetic ordering, and optical activity, depending on the composition and structure of the oxide.^[4]

The coupling of electronic, magnetic, and catalytic properties further distinguishes TMOs from conventional single-function materials. This multifunctionality allowing them to serve as catalysts, energy storage media and electronic or magnetic components. Understanding these bonding dynamics provides insight into how structure, defects, and electronic properties can be engineered to optimize performance for next-generation technologies.^[4]

Technological Applications

The technological impact of TMOs is both diverse and profound, with applications in multiple fields.

- **Heterogeneous Catalysis:** TMOs serve as robust catalysts in organic synthesis, oxidation reactions, and green transformations. Their high surface area and redox flexibility enable efficient catalytic performance with reusability.^[5]
- **Environmental Remediation:** In environmental remediation, TMOs such as TiO₂, ZnO, and Fe₂O₃ are widely used in photocatalytic degradation of dyes, pharmaceuticals, and other pollutants in water. Spinel oxides and iron-based TMOs also adsorb and reduce toxic metals such as Cr⁶⁺ and Pb²⁺, contributing to safer and cleaner water systems.
- **Energy Storage and Conversion:** In energy storage and conversion, perovskite and spinel oxides serve as cathodes, anodes or electrolytes in lithium-ion batteries, supercapacitors, and fuel cells. Their ability to mediate oxygen evolution and reduction reactions is critical for electrochemical performance and energy efficiency.
- **Electronics and Magnetism:** Due to their tunable electronic and magnetic properties TMOs are also used in electronics and magnetism, functioning in resistive switching devices, sensors and spintronic components, further demonstrating their versatility in modern technology.^[6]

Overall, these applications underscore how TMOs bridge fundamental science with practical technology, addressing urgent societal needs such as renewable energy, environmental sustainability, and technological innovation.

Next Generation Research Opportunities

The future of TMO research lies in the design and engineering of nanostructured, hybrid and multifunctional materials. Several emerging directions can be highlighted:

- **Nanostructured TMOs:** Nanoscale design enhances surface reactivity, charge transfer, and selectivity, improving catalytic and photocatalytic performance.
- **Hybrid and Composite Systems:** Integration of TMOs with carbon materials, polymers, or other oxides creates synergistic properties, offering superior performance in energy storage and catalysis.^[7]

- **Computational and AI-Driven Materials Design:** Machine learning and computational modeling are increasingly applied to predict new TMO structures, optimize catalytic pathways, and accelerate discovery.
- **Green Synthesis Approaches:** The development of eco-friendly, low-energy synthetic methods and recyclable TMO catalysts aligns with global goals of green chemistry and sustainable technology.

These opportunities represent show how transition metal oxide chemistry research meets societal needs, making them a true example of “Next Gen Research.”

Conclusion:

Transition metal oxides are very important at the interface of science, technology and society. Their structural diversity, bonding versatility and unique physicochemical properties make them essential in fields ranging from catalysis and energy storage to environmental remediation. As research moves towards nanostructured, composite and computationally designed oxides, TMOs promise to play a central role in addressing future global challenges related to sustainability, clean energy and environmental protection.

References:

1. Rao, C. N. R., & Gopalakrishnan, J. (1997). *New Directions in Solid State Chemistry*. Cambridge University Press.
2. Goodenough, J. B. (2004). Electronic and ionic transport properties and other physical aspects of perovskites. *Reports on Progress in Physics*, 67(11), 1915–1993.
3. Li, M., Chen, Z., & Xu, H. (2020). Structural diversity and catalytic properties of transition metal oxides. *Chemical Reviews*, 120(10), 6783–6819.
4. Fujishima, A., & Honda, K. (1972). Electrochemical photolysis of water at a semiconductor electrode. *Nature*, 238, 37–38.
5. Behrens, M., & Schlögl, R. (2013). Heterogeneous catalysis with transition metal oxides. *Advanced Catalysis*, 55, 1–84.
6. Wang, D., Li, X., & Wu, J. (2021). Transition metal oxides in energy storage and conversion. *Energy & Environmental Science*, 14, 112–140.
7. Singh, R., & Chandra, A. (2022). Emerging opportunities in nanostructured transition metal oxides: Catalysis, energy, and environment. *Materials Today Advances*, 13, 100202.

MATHEMATICAL MODELING IN CHEMICAL SYSTEMS

Anand Kumar Mishra* and Shiv Kumar Verma

Deen Dayal Upadhyay Gorakhpur University, Gorakhpur, India

*Corresponding author E-mail: anandkmishra.ddugu@gmail.com

Introduction:

The intersection of chemistry and mathematics has given rise to powerful tools that enable scientists to understand, predict, and optimize complex chemical phenomena. Mathematical modeling serves as a critical bridge between theoretical chemistry and practical applications, offering a systematic framework to describe the behavior of chemical systems using mathematical language.

In chemical systems, reactions occur dynamically over time, involving numerous variables such as concentration, temperature, pressure, and energy. Capturing these interactions requires the development of models that can reflect both the qualitative mechanisms and the quantitative behavior of such systems. Whether it's modeling reaction kinetics using differential equations, describing equilibrium conditions through algebraic expressions, or simulating molecular dynamics with numerical algorithms, mathematical modeling allows chemists to go beyond empirical observation and into predictive analysis.

This chapter provides an introduction to the foundational principles and methods used in mathematical modeling within chemical contexts. We will explore the role of modeling in areas such as chemical kinetics, thermodynamics, transport phenomena, and reaction engineering. Emphasis is placed on the formulation of models, selection of appropriate assumptions, and the use of analytical and computational techniques to solve them.

The goal is not only to equip the reader with the tools necessary to construct and analyze chemical models, but also to foster an understanding of when and why certain models are appropriate. By the end of this chapter, readers will appreciate the value of mathematical modeling as a unifying approach in modern chemical research and industry.

Keywords: Mathematical Modeling, Reactor Design, Reaction Kinetics, Mathematical Tools, Modeling Technique, Drug Design, ODEs/ PDEs

1. Motivation and scope of mathematical modeling in chemical systems:

1.1. Motivation:

Mathematical modeling in chemical systems is driven by the need to 'understand, predict, and optimize' chemical processes. As chemical systems are often complex, involving multiple reactions, species, and phases, a mathematical model provides a systematic way to represent this complexity in a manageable form. The key motivations include:

a. Predictive Capability: Models allow prediction of system behavior under different conditions without the need for costly or time-consuming experiments. Examples: reaction rates, concentration profiles, temperature changes, and product yields.

b. Process Design and Optimization: Mathematical models help in designing efficient reactors, separation units, and entire chemical plants. They are used to optimize operating conditions to maximize yield, minimize waste, and reduce costs.

c. Safety and Environmental Compliance: Modeling hazardous reactions or pollutant dispersion can help prevent accidents and ensure environmental regulations are met.

d. Scale-Up from Lab to Industry: Models bridge the gap between laboratory-scale experiments and full-scale industrial production by accounting for changes in scale, mixing, heat transfer, etc.

e. Insight and Understanding:

They help in gaining fundamental insights into reaction mechanisms, kinetics, and thermodynamics that may not be directly observable.

1.2. Scope:

The scope of mathematical modeling in chemical systems is broad and interdisciplinary, encompassing various fields within chemical engineering and chemistry:

a. Reaction Kinetics: Modeling the rate laws and mechanisms of chemical reactions, including homogeneous and heterogeneous reactions.

b. Transport Phenomena: Incorporates mass, momentum, and heat transfer equations to describe how species and energy move through the system.

c. Reactor Design: Development of models for batch, CSTR (Continuous Stirred Tank Reactor), PFR (Plug Flow Reactor), etc., to predict performance and optimize design.

d. Multiphase Systems: Modeling gas-liquid, liquid-solid, and gas-solid systems, such as in catalysis, absorption, and distillation.

e. Thermodynamic Modeling: Understanding phase equilibria, activity coefficients, fugacity, and energy balances.

f. Process Control and Simulation: Dynamic modeling for real-time control, fault detection, and optimization in chemical plants.

g. Computational Tools and Techniques: Utilization of numerical methods, simulation software (like Aspen Plus, COMSOL, MATLAB), and machine learning to solve complex models.

Mathematical modeling is an essential tool in modern chemical engineering and chemistry. It allows for efficient design, deeper understanding, safer operations, and innovation in chemical processes. With the increasing availability of computational resources and data, the scope and impact of modeling will continue to grow, making it a cornerstone of chemical system analysis and development. Computation plays a central role in the development, analysis, and application

of mathematical models in chemical systems. As chemical processes often involve complex, nonlinear, and coupled equations, analytical solutions are rarely possible. Computational tools and techniques enable the simulation, optimization, and visualization of these systems efficiently and accurately.

2. Fundamental principles of mathematical modeling in chemical systems:

Mathematical modeling plays a vital role in understanding, predicting, and optimizing chemical processes. By translating chemical phenomena into mathematical language, models enable chemists and engineers to simulate behaviors, test hypotheses, and design processes with precision. This paper outlines the fundamental principles that govern mathematical modeling in chemical systems, offering a framework for both theoretical exploration and practical application.

2.1. Conservation Laws:

At the core of chemical modeling are conservation laws, particularly those for mass, energy, and momentum. These laws serve as the foundation for developing differential equations that describe the dynamic behaviour of chemical systems.

Mass Conservation: Ensures that mass is neither created nor destroyed in a closed system. This principle leads to mass balance equations used extensively in reactor design and process simulation.

Energy Conservation (First Law of Thermodynamics): Energy is conserved in chemical reactions and processes, guiding the formulation of energy balance equation.

Momentum Conservation (Newton's Second Law): Essential in modeling fluid flow, especially in chemical engineering applications involving transport phenomena (Bird *et al.*, 2007).

2.2. Reaction Kinetics:

Chemical kinetics describes the rate at which reactions proceed. Modeling reaction kinetics involves determining rate laws based on empirical or mechanistic approaches.

Rate Laws: Mathematical expressions that relate the rate of reaction to the concentration of reactants.

Arrhenius Equation: A temperature-dependent model used to describe the rate constant of chemical reactions. Kinetic models are essential in reactor design, catalyst development, and control of industrial processes (Levenspiel, 1999).

2.3. Thermodynamics:

Thermodynamics provides constraints for feasible chemical transformations. It defines equilibrium conditions and the directionality of processes.

Equilibrium Models: Use Gibbs free energy minimization or equilibrium constants to determine the composition of a system at equilibrium.

Phase Equilibria: Important in multiphase systems where mass transfer occurs between phases. These principles ensure that models reflect real chemical limitations and predict behavior accurately (Smith, Van Ness, & Abbott, 2005).

2.4. Transport Phenomena:

Transport processes such as diffusion, convection, and conduction are modeled using partial differential equations derived from Fick's, Fourier's, and Newton's laws, respectively.

Mass Transfer: Modelled using Fick's law of diffusion.

Heat Transfer: Modelled using Fourier's law.

Momentum Transfer: Modelled using Navier-Stokes equations.

These are particularly important in heterogeneous reactions, catalysis, and membrane systems (Bird *et al.*, 2007).

2.5. Mathematical Tools and Numerical Methods:

Chemical systems often lead to complex mathematical problems that require computational tools for solutions.

Differential Equations: Used for dynamic systems modeling.

Algebraic Equations: Arise in steady-state or equilibrium problems.

Numerical Methods: Finite difference, finite element, and Runge-Kutta methods are commonly employed for solving systems that lack analytical solutions. Model validation and sensitivity analysis are also critical steps to ensure robustness and reliability (Chapra & Canale, 2015).

2.6. Model Validation and Sensitivity Analysis:

Model predictions must be validated against experimental data to ensure accuracy. Sensitivity analysis identifies the influence of input parameters on model output, guiding parameter estimation and experimental design.

Validation Techniques: Include residual analysis, cross-validation, and comparison with experimental or industrial data.

Sensitivity Analysis: Helps prioritize variables that significantly impact system behaviour (Saltelli *et al.*, 2008).

2.7. Applications in Chemical Engineering and Chemistry:

Mathematical models are widely applied in various fields: Chemical Reactor Design, Environmental Engineering, Pharmaceutical Process Modeling, Materials Science, Systems Biology. Each application leverages the discussed principles to simulate and optimize complex chemical systems.

3. Core modeling techniques in mathematical modeling of chemical systems:

Mathematical modeling in chemical systems involves constructing mathematical representations of physical, chemical, and biological processes to gain insight, make predictions, and optimize operations. Core modeling techniques are built upon physical laws, experimental data, and numerical methods that help simulate and control chemical processes efficiently. Mathematical

modeling of chemical systems involves developing mathematical representations to simulate, analyze, and predict the behaviour of chemical processes. Core modeling techniques used in this field typically draw from various areas of applied mathematics, chemical engineering, and physical chemistry. Here's a breakdown of core modeling techniques.

Mass and Energy Balance Models:

Mass Balance: Mass balance models are based on the law of conservation of mass, ensuring that the total mass entering a system equals the mass leaving plus any accumulation or consumption within the system. Mass balances are used in designing reactors, separation units, and entire process plants.

$$\text{Input} - \text{Output} + \text{Generation} - \text{Consumption} = \text{Accumulation}$$

Energy Balance: These models apply the first law of thermodynamics to calculate the energy exchange due to heat, work, and enthalpy changes in chemical systems. They are essential in thermal design and optimization of chemical reactors and heat exchangers (Smith, Van Ness, & Abbott, 2005).

3.2. Reaction Kinetics Models:

Reaction kinetics models describe how fast chemical reactions occur under various conditions.

Rate Laws: Rate laws relate the rate of reaction to the concentration of reactants. These models can be:

- Empirical, based on experimental data.
- Mechanistic, based on reaction pathways.

Summary Table:

Technique Type	Mathematical Tool	Application Example
Mass Balance	ODEs / Algebraic Equations	Reactor modelling
Energy Balance	ODEs / PDEs	Temperature prediction
Reaction Kinetics	ODEs	Rate of reaction modeling
Transport Phenomena	PDEs	Diffusion in porous media
Thermodynamics	Algebraic Equations	Phase equilibrium
Population Balance	Integro-differential equations	Crystallization
Stochastic Models	SDEs / Monte Carlo	Biochemical systems
Parameter Estimation	Optimization	Kinetic model fitting
Model Reduction	Linear algebra, Approximation	Fast simulation
Numerical Methods	Discretization, Solvers	General solution of ODEs/PDEs
Process Control	Linear systems, Control theory	Reactor control
CFD	PDEs, Mesh generation	Flow in reactors

4. System complexity and network analysis in mathematical modeling of chemical systems:

Chemical systems often involve numerous interacting components, non-linear relationships, and feedback loops. Mathematical modeling enables scientists to analyze, predict, and control the behavior of these complex systems. System complexity refers to the intricate interdependencies and behaviors that emerge from the interactions among parts of a chemical system. Network analysis, in this context, provides a framework for understanding these interactions by representing chemical species and their reactions as nodes and edges in a graph.

1. System Complexity in Chemical Systems:

- Chemical systems are complex due to:
- Large numbers of species and reactions
- Non-linear kinetics Stochastic effects in small-scale reactions
- Emergent behavior, such as oscillations or chaos (e.g., Belousov-Zhabotinsky reactions)
- Mathematical models are essential to manage this complexity, often utilizing:
- Ordinary Differential Equations (ODEs) for deterministic models
- Stochastic models such as the Gillespie algorithm for probabilistic behavior
- Partial Differential Equations (PDEs) for spatial and temporal variations

“Complexity in chemical reaction networks arises from non-linear dynamics and feedback structures, which are essential for understanding biochemical regulation” (Feinberg, 2019).

2. Network Analysis of Chemical Systems:

Network analysis treats chemical systems as graphs where:

- Nodes represent chemical species or reactions
- Edges represent interactions or dependencies (e.g., reaction pathways)

There are different types of networks:

- Reaction networks (species as nodes, reactions as links)
- Metabolic networks (representing entire pathways in organisms)
- Regulatory networks (showing gene-protein-chemical regulation)

Mathematical tools used include:

- Stoichiometric matrices
- Graph theory metrics (e.g., centrality, clustering coefficients)
- Flux Balance Analysis (FBA) in systems biology

“Network-based approaches allow for the identification of key pathways and bottlenecks in metabolic systems, enabling targeted intervention strategies” (Palsson, 2015).

3. Applications and Implications

- **Drug design:** Modeling pathways helps identify target enzymes.

- **Synthetic biology:** Predicting the impact of genetic modifications on metabolic networks.
- **Environmental chemistry:** Modeling pollutant interactions and transformations. For example, in metabolic engineering, network models guide the design of microbial strains for optimal production of biofuels or pharmaceuticals.

5. Numerical solution in mathematical modeling of chemical system:

Chemical systems are often governed by complex differential equations (ordinary or partial) derived from laws like mass conservation, reaction kinetics, and thermodynamics. Analytical solutions are rarely possible, so numerical methods are essential. Numerical Solution of Mathematical Modeling in Chemical Systems is a broad and important topic in chemical engineering, computational chemistry, and applied mathematics. It involves the use of numerical methods to solve mathematical models that describe chemical processes, systems, or reactions. Most real-world chemical systems are non-linear, coupled, and often too complex to solve analytically. Therefore, numerical methods are used.

5.1. Common Mathematical Models in Chemical Systems:

Model Type	Description
ODEs (Ordinary Differential Equations)	Often used for batch reactors, kinetics, etc
PDEs (Partial Differential Equations)	Used in modeling transport processes in space and time
Algebraic Equation	Used in equilibrium, stoichiometry, process constraints
DAEs (Differential-Algebraic Equations)	Common in chemical process modeling with constraints

5.2. Key Numerical Methods Used:

Problem Type	Numerical Method Examples
ODEs	Euler's method, Runge-Kutta methods (RK4), adaptive methods
PDEs	Finite Difference Method (FDM), Finite Volume Method (FVM), Finite Element Method (FEM)
Non-linear equations	Newton-Raphson, Broyden's method
Optimization problems	Gradient descent, Genetic algorithms, Simulated annealing
DAEs	Implicit solvers (e.g., DASSL, IDA)

5.3. Software Tools:

Software	Capabilities
MATLAB	Built-in solvers (ODE45, ODE15s), symbolic math
Python (SciPy/NumPy)	solve_ivp, odeint, PDE solvers
COMSOL Multiphysics	GUI-based FEM modeling for complex systems
Aspen Plus/HYSYS	Process simulation with built-in models
CFD tools (ANSYS Fluent, OpenFOAM)	Transport phenomena simulation

5.4. Applications:

- Reactor Design (CSTRs, PFRs, batch reactors)
- Pollution Modeling
- Pharmaceutical Reaction Modeling
- Combustion and Heat Transfer
- Separation Processes (distillation, absorption)

5.5. Challenges:

- Stiffness in ODEs
- Model validation
- Parameter estimation
- Multiscale modeling (nano to macro)
- Computational cost

6. Application of mathematical modeling in chemical systems (chemical engineering):

6.1. Reactor Design and Analysis: Mathematical models are essential for designing and scaling up chemical reactors. They describe mass and energy balances, reaction kinetics, and transport phenomena. (Levenspiel., 1999).

Example: Modeling plug flow reactors (PFR) and continuous stirred tank reactors (CSTR) to predict conversion rates and temperature profiles.

Use: Optimizing reactor size, residence time, and thermal control.

6.2. Process Simulation and Optimization: Engineers use models to simulate entire chemical plants or individual units, allowing prediction of behavior under different conditions and optimization of performance. (Biegler et al ., 1997)

Example: Using Aspen Plus or gPROMS to simulate distillation columns or heat exchangers.

Use: Reducing energy use, improving yield, and optimizing raw material usage.

6.3. Reaction Kinetics Modeling: Modeling chemical kinetics helps in understanding reaction mechanisms and predicting product distributions. (Froment, G. F., & Bischoff, K. B., 2010)

Example: Modeling catalytic reactions or polymerization processes using differential equations.

Use: Designing catalysts, controlling product selectivity.

6.4. Transport Phenomena: Models describe the transfer of momentum, heat, and mass in chemical systems, which are fundamental to equipment design. (Bird *et al.*, 2007)

Example: Modeling heat transfer in tubular reactors or mass transfer in packed beds.

Use: Designing heat exchangers, separation processes.

6.5. Environmental and Safety Engineering: Mathematical models help assess pollutant dispersion, chemical leak scenarios, or combustion byproducts. (Fogler, H. S. 2016).

Example: Modeling the dispersion of pollutants from a chemical plant into the atmosphere.

Use: Regulatory compliance, risk assessment, emergency response planning.

6.6. Biochemical and Pharmaceutical Engineering: In biochemical systems, modeling is used to simulate fermentation, enzyme kinetics, or drug release mechanisms. (Nielsen & Villadsen, 2011).

Example: Modeling microbial growth and substrate consumption in a bioreactor.

Use: Optimizing yield in bioprocesses, ensuring consistent drug formulation.

6.7. Process Control and Automation: Dynamic models help in developing control strategies (like PID or model predictive control) to maintain system stability. (Seborg *et al.*, 2010)

Example: Controlling temperature or pH in a batch reactor using feedback loops.

Use: Enhancing product quality and process safety.

7. Model validation and sensitivity analysis in mathematical modeling of chemical systems:

Mathematical models are vital for simulating and optimizing chemical systems. However, for models to be trusted and used in decision-making, they must be validated and their sensitivity understood. These two steps ensure reliability and robustness in chemical engineering applications.

7.1. Model Validation: Model validation is the process of ensuring that a mathematical model accurately represents the real-world chemical system it is intended to simulate.

Purpose: Verify model accuracy, ensure predictive capability, Build confidence for use in design and control

Common Validation Techniques:

- **Comparison with Experimental Data:** Check if model outputs agree with laboratory or plant data.
- **Cross-Validation:** Divide data into training and testing sets to assess predictive performance.

- **Goodness-of-Fit Metrics:** Use statistical indicators such as R^2 , RMSE (Root Mean Square Error), and AIC (Akaike Information Criterion).

Example in Chemical Engineering: A reaction kinetics model for a catalytic reactor is validated by comparing predicted conversion rates with data from lab-scale experiments. (Aris, 1999).

7.2. Sensitivity Analysis: Sensitivity analysis (SA) quantifies how variation in model input parameters affects the output. It helps identify which parameters most influence model behavior.

Purpose: Determine critical parameters, Reduce model complexity, Guide experimental design, Support uncertainty analysis. (Saltelli *et al.*, 2008)

Types of Sensitivity Analysis:

- **Local Sensitivity Analysis:** Small perturbations around a nominal value to assess local effects (e.g., partial derivatives).
- **Global Sensitivity Analysis:** Examines parameter influence over the entire input space (e.g., Sobol indices, Morris method).

Example in Chemical Systems: In a batch reactor model, SA can show how variations in activation energy or initial concentration affect product yield.

7.3. Integration of Validation and Sensitivity in Model Development:

Both validation and sensitivity analysis are essential steps in a model's life cycle. Together, they:

- Improve model reliability and interpretability
- Help focus data collection efforts on influential parameters
- Reduce risk in design, scale-up, or control strategies

Case Study Example: In modeling pollutant dispersion from a chemical plant, validation is done using sensor data, and sensitivity analysis reveals that wind speed and temperature gradients are the most influential factors. (Beck & M. B., 1987).

8. Advanced topics and emerging directions in mathematical modeling of chemical systems:

8.1. Multiscale Modeling: Multiscale modeling integrates phenomena across different time and length scales—from molecular (nanoseconds, nanometers) to reactor (hours, meters) scales. (Najm, H. N. 2009).

Applications: Bridging quantum chemistry, molecular dynamics, and continuum models, Modeling catalytic surface reactions from first principles, Linking microscopic transport with macroscopic reactor performance.

8.2. Machine Learning and AI-Enhanced Modeling: Machine learning (ML) augments traditional modeling by identifying patterns in large datasets or creating surrogate models. (Jablonka *et al.*, 2021).

Applications: Surrogate modeling of complex kinetics, Data-driven property prediction (e.g., viscosity, diffusivity), Hybrid physics-based + ML models for real-time control.

8.3. Stochastic Modeling and Uncertainty Quantification (UQ): Stochastic methods account for randomness and uncertainties in model parameters or operating conditions. (Smith & R. C. 2013).

Applications: Monte Carlo simulations in reaction networks, UQ in reactor safety and scale-up, Risk-based process optimization. (Gutenkunst *et al.*, 2007)

8.4. Dynamic and Real-Time Modeling for Process Control: Real-time models are used in closed-loop systems for monitoring, diagnostics, and adaptive control. (Rawlings *et al.*, 2017).

Applications: Model predictive control (MPC), Digital twins of chemical plants, Sensor fusion for online parameter estimation.

8.5. Population Balance Modeling (PBM): PBM tracks the distribution of properties like size, age, or composition within particle systems or molecular populations.(Ramkrishna, 2000).

Applications: Crystallization and precipitation, Polymerization processes, Aerosol dynamics

8.6. Green Process Modeling and Sustainability: Mathematical modeling aids the development of sustainable and energy-efficient chemical processes. (Varjani., et al. 2022).

Applications: Modeling CO₂ capture systems (e.g., amine absorption), Process intensification and life-cycle analysis, Integration of renewable energy sources.

8.7. Cyber-Physical Systems and Digital Twins: Digital twins are virtual replicas of chemical processes updated in real time through sensor data. (Tao *et al.*, 2019).

Applications: Predictive maintenance, Remote monitoring and control, Smart manufacturing (Industry 4.0)

8.8. Integration with Systems Biology and Biochemical Networks: Mathematical modeling is increasingly applied to biochemical pathways, metabolic networks, and synthetic biology.

Applications: Genome-scale metabolic modelling, Enzyme kinetics and cell signaling networks, Biopharmaceutical process development.(Palsson & B. Ø., 2015).

Conclusion:

Mathematical modeling in chemical systems integrates principles of physics, chemistry, and mathematics to analyze and predict system behaviour. Grounded in conservation laws, kinetics, thermodynamics, and transport phenomena, these models are indispensable tools in both academic research and industrial practice.

Chemical system modeling integrates a variety of core techniques—ranging from classical mass and energy balances to cutting-edge machine learning. The proper combination of these models enables process design, optimization, safety, and control in chemical engineering practice. Mastery of these modeling tools is essential for engineers and scientists working on modern chemical systems.

The integration of system complexity and network analysis in the mathematical modeling of chemical systems offers a powerful framework to analyze and control chemical and biochemical

behaviour. These tools enable scientists to go beyond simple linear reaction chains to understand the full scope of dynamic and adaptive chemical networks.

Mathematical modeling plays a crucial role in chemical engineering, helping engineers design, analyze, optimize, and control chemical processes and systems. Below is an overview of applications of mathematical modeling in chemical systems within chemical engineering, along with examples and APA-style references to support the discussion.

Mathematical modeling is foundational in chemical engineering, offering insights that are not easily obtainable through experiments alone. It enables prediction, optimization, and control of complex chemical systems, driving innovation and efficiency in industries such as petrochemicals, pharmaceuticals, energy, and biotechnology.

Validation and sensitivity analysis are core components of developing robust mathematical models in chemical engineering. They enhance model accuracy, support decision-making, and guide future experimentation. Without these steps, model-based predictions risk being inaccurate or misleading. As the chemical industry moves toward automation, sustainability, and integration with data science, mathematical modeling is evolving beyond traditional boundaries. Emerging methods like multiscale modeling, machine learning integration, real-time optimization, and digital twins are setting new directions for the field.

References:

1. Brunton, S. L., & Kutz, J. N. (2019). *Data-driven science and engineering: Machine learning, dynamical systems, and control*. Cambridge University Press.
2. Gutenkunst, R. N., Waterfall, J. J., Casey, F. P., Brown, K. S., Myers, C. R., & Sethna, J. P. (2007). Universally sloppy parameter sensitivities in systems biology models. *PLoS Computational Biology*, 3(10), e189. <https://doi.org/10.1371/journal.pcbi.0030189>
3. Jablonka, K. M., Ongari, D., Moosavi, S. M., & Smit, B. (2021). Big-data science in porous materials: Materials genomics and machine learning. *Chemical Reviews*, 121(16), 11035–11074. <https://doi.org/10.1021/acs.chemrev.0c00084>
4. Najm, H. N. (2009). Toward a predictive science of multiscale modeling. *SIAM News*, 42(9).
5. Palsson, B. Ø. (2015). *Systems biology: Constraint-based reconstruction and analysis*. Cambridge University Press.
6. Ramkrishna, D. (2000). *Population balances: Theory and applications to particulate systems in engineering*. Academic Press.
7. Rawlings, J. B., Mayne, D. Q., & Diehl, M. (2017). *Model predictive control: Theory, computation, and design* (2nd ed.). Nob Hill Publishing.
8. Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., ... & Tarantola, S. (2008). *Global sensitivity analysis: The primer*. Wiley.

9. Smith, R. C. (2013). *Uncertainty quantification: Theory, implementation, and applications*. SIAM.
10. Tao, F., & Qi, Q. (2019). Digital twin and big data towards smart manufacturing and Industry 4.0: 360-degree comparison. *IEEE Access*, 6, 3585–3593. <https://doi.org/10.1109/ACCESS.2018.2793265>
11. Varjani, S. J., Upasani, V. N., & Awasthi, M. K. (2022). Modeling and optimization for green chemical processes. *Bioresource Technology*, 344, 126250. <https://doi.org/10.1016/j.biortech.2021.126250>
12. Weinan, E. (2011). *Principles of multiscale modeling*. Cambridge University Press.
13. Chapra, S. C., & Canale, R. P. (2015). *Numerical methods for engineers (7th ed.)*. McGraw-Hill Education.
14. Kreyszig, E. (2011). *Advanced engineering mathematics (10th ed.)*. Wiley.
15. Elnashaie, S. S. E. H., & Garhyan, P. (2003). *Numerical techniques for chemical and biological engineers using MATLAB®: A simple bifurcation approach*. Springer.
16. Rice, R. G., & Do, D. D. (2012). *Applied mathematics and modeling for chemical engineers (2nd ed.)*. Wiley.
17. Fogler, H. S. (2016). *Essentials of chemical reaction engineering (2nd ed.)*. Pearson Education.
18. Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. (2007). *Numerical recipes: The art of scientific computing (3rd ed.)*. Cambridge University Press.
19. Feinberg, M. (2019). *Foundations of Chemical Reaction Network Theory*. Springer. <https://doi.org/10.1007/978-3-030-03858-8>
20. Palsson, B. Ø. (2015). *Systems Biology: Constraint-based Reconstruction and Analysis*. Cambridge University Press.
21. Gillespie, D. T. (1977). Exact stochastic simulation of coupled chemical reactions. *The Journal of Physical Chemistry*, 81(25), 2340–2361. <https://doi.org/10.1021/j100540a008>
22. Barabási, A.-L., & Oltvai, Z. N. (2004). Network biology: Understanding the cell's functional organization. *Nature Reviews Genetics*, 5(2), 101–113. <https://doi.org/10.1038/nrg1272>
23. Kitano, H. (2002). Systems biology: A brief overview. *Science*, 295(5560), 1662–1664. <https://doi.org/10.1126/science.1069492>
24. Bird, R. B., Stewart, W. E., & Lightfoot, E. N. (2007). *Transport phenomena (2nd ed.)*. John Wiley & Sons.
25. Chapra, S. C., & Canale, R. P. (2015). *Numerical methods for engineers (7th ed.)*. McGraw-Hill Education.
26. Levenspiel, O. (1999). *Chemical reaction engineering (3rd ed.)*. Wiley.

27. Saltelli, A., Chan, K., & Scott, E. M. (2008). *Sensitivity analysis*. Wiley.
28. Smith, J. M., Van Ness, H. C., & Abbott, M. M. (2005). *Introduction to chemical engineering thermodynamics* (7th ed.). McGraw-Hill Education.
29. Bird, R. B., Stewart, W. E., & Lightfoot, E. N. (2007). *Transport phenomena* (2nd ed.). John Wiley & Sons.
30. Chapra, S. C., & Canale, R. P. (2015). *Numerical methods for engineers* (7th ed.). McGraw-Hill Education.
31. Levenspiel, O. (1999). *Chemical reaction engineering* (3rd ed.). Wiley.
32. Saltelli, A., Chan, K., & Scott, E. M. (2008). *Sensitivity analysis*. Wiley.
33. Smith, J. M., Van Ness, H. C., & Abbott, M. M. (2005). *Introduction to chemical engineering thermodynamics* (7th ed.). McGraw-Hill Education.
34. Aris, R. (1999). *Mathematical modeling techniques*. Dover Publications.
35. Beck, M. B. (1987). Water quality modeling: A review of the analysis of uncertainty. *Water Resources Research*, 23(8), 1393–1442. <https://doi.org/10.1029/WR023i008p01393>
36. Kremling, A. (2013). *Systems biology: Mathematical modeling and model analysis*. CRC Press.
37. Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., ... & Tarantola, S. (2008). *Global sensitivity analysis: The primer*. Wiley.
38. Turanyi, T., & Tomlin, A. S. (2014). *Analysis of kinetic reaction mechanisms*. Springer.

ALCOHOL TECHNOLOGY FOR A SUSTAINABLE BIOFUEL FUTURE

Pratapsinha Gorepatil

Sangameshwar College, Solapur (Autonomous)

Corresponding author E-mail: dr.pratapgorepatil@gmail.com

Introduction:

The global energy landscape is undergoing a significant transition, driven by the need to balance economic growth with environmental sustainability. With rising concerns about climate change, limited fossil fuels, and energy insecurity, the focus is now shifting toward cleaner and renewable energy alternatives. Among these, biofuels have emerged as a strategic solution, since they offer an alternative to petroleum-based fuels and simultaneously contributing to rural development, waste utilization, and greenhouse gas (GHG) reduction.^[1]

As the world's third-largest energy consumer, India is facing tremendous pressure to diversify its energy portfolio. The country's energy demand has been growing at an average rate of over 5% annually, mostly because of rapid industrialization, urbanization, and a growing middle-class population.^[2] Currently, India's energy basket dominated by coal and oil, contributing nearly 85% of the total; whereas the share of renewable energy remains below the global average.^[3] This overreliance on fossil fuels not only accelerates environmental degradation but also makes the country exceptionally sensitive to changes in global oil prices, given that nearly 80% of its crude oil requirement is imported.^[4]

To overcome these challenges, India has been proactive in developing policies to promote renewable energy, especially **biofuels**, as part of its commitment to decarbonization and energy independence under the Atmanirbhar Bharat vision. The National Policy on Biofuels (2018) set out a clear plan for increasing the use of biodiesel, blending ethanol, and bio-CNG production. This legislation made the biofuel ecosystem more resilient and sustainable by diversifying feedstock, ranging from conventional molasses and sugarcane juice to non-food sources like damaged grains and lingo-cellulosic biomass.^[2]

Globally, Biofuels are becoming more popular as a sustainable energy source. For example, the United States and Brazil have large-scale ethanol blending programs that not only make energy more secure but also boost rural economies.^[5] Inspired by these global models, India has set ambitious goals, such as achieving 20% ethanol blending with petrol by 2025 and scaling up bio-CNG production to 15 million tons per annum. These kinds of projects are expected to create significant socio-economic impact, by generating new business opportunities in the distillery sector, raising farmers' incomes, and reducing rural suffering by adding value to agricultural waste.^[4]

The strategic function of alcohol technology is at the center of this change. Ethanol, being the most widely used liquid biofuel, and to make it efficiently and sustainably, you require advanced fermentation, distillation, and microbial engineering skills. As the India is the fourth largest producer of alcohol in the world, the demand for skilled manpower and technological expertise in this field has surged. India can not only secure its energy future but also emerge as a global leader in the biofuel sector, by integrating science, innovation, and education.^[6]

Need for Biofuels

The necessity of biofuels arises from three fundamental reasons: environmental sustainability, energy security, and socio-economic development.

First, biofuels significantly reduce environmental pollution by lowering emissions of carbon dioxide, carbon monoxide, particulate matter, and sulfur oxides. Biofuels are made from renewable biomass, so the carbon they release is mostly canceled out by the carbon that plants take in as they grow. This makes them relatively carbon-neutral. This is a crucial step for India, which has pledged to achieve net-zero carbon emissions by 2070.^[3]

Second, biofuels address the issue of energy security. India's heavy reliance on crude oil imports places enormous stress on the economy, particularly when international oil prices fluctuate. By blending domestically produced ethanol and biodiesel with conventional fuels, the nation can reduce its dependency on foreign oil and enhance its energy self-sufficiency.^[4] Third, biofuels contribute to economy and society development i. e. socio-economic development. They create new avenues for farmers to generate additional income through the sale of crop residues, non-edible oil seeds, or damaged food grains. Biofuel production plants and distilleries also create rural employment opportunities, foster entrepreneurship, and support the concept of waste-to-wealth, where agricultural residues and municipal waste are transformed into valuable energy resources.^[2]

Thus, biofuels are not just an energy alternative—they are an integrated solution that connects environmental responsibility, economic resilience, and social inclusivity.

Types of Biofuels

Biofuels can be broadly classified into three categories: solid, liquid and gaseous.

- **Solid Biofuels:** These include things like firewood, charcoal, crop residues, and agricultural waste that are used to make biofuels.
- **Liquid Biofuels:** Liquid biofuels are quite important for the transportation industry. The best choices are ethanol, biodiesel, and butanol. Ethanol is generally made from feedstock that is high in sugar or starch, while biodiesel is made from animal fats and vegetable oils.

- **Gaseous Biofuels:** This group includes biogas, syngas and bio hydrogen. They are produced through anaerobic digestion, gasification, or microbial fermentation and are used in power generation and household cooking.^[5]

Another way to classify biofuels is by generation of feedstock:

- **First-generation biofuels:** Derived from edible crops like sugarcane, corn, or vegetable oils.
- **Second-generation biofuels:** Second-generation biofuels are made from lingo-cellulosic biomass, which includes sugarcane bagasse, corn stalks, sorghum straw, and forestry leftovers.^[6]
- **Third-generation biofuels:** These are made from algal biomass or genetically modified microorganisms that offer higher productivity.
- **Fourth-generation biofuels:** Using carbon capture and synthetic biology together to make the environment as sustainable as possible.^[3]

This history of biofuel generations shows a change from food-based to waste-based and more modern technologies that promise to be more efficient and have less of an impact on the environment.

Necessity of Ethanol as a Sustainable Biofuel

Among all biofuels, Ethanol is the most useful and impactful biofuel in the near future. Its use as a transport fuel, either directly or blended with petrol, which makes it a key contributor to reducing urban air pollution and fossil fuel dependency. Ethanol has a high-octane rating, which improves engine performance and reduces harmful exhaust emissions.^[5]

The Ethanol Blending Programme (EBP) of the Government of India, has a target of achieving 20% blending by 2025, is a landmark initiative. This scheme is expected to establish an ethanol market worth over ₹840 billion annually. This will help not only the energy sector but also rural economies by getting farmers participation.^[4]

The National Policy on Biofuels (2018) made it possible to make ethanol production by allowing multiple feedstocks. While sugarcane molasses remains a major source, now additionally damaged grains, maize, broken rice, and lingo-cellulosic biomass are being utilized. This makes the system more versatile and sustainable.^[2]

The expansion of ethanol as a biofuel has made Alcohol Technology even more important. This interdisciplinary field includes advanced fermentation techniques, enzyme technology, distillation improvements, and microbial engineering, all of which aim to maximize yield and efficiency. India is the fourth-largest producer of alcohol in the world, thus it is in a unique position to use its knowledge in this sector. Therefore, making skilled manpower through specialized education and training programs in alcohol technology has become a top national priority.^[6]

Conclusion:

Biofuels represent a transformative opportunity for India's energy future and contribute to rural economic growth. They also assist to protect the environment and reduce reliance on foreign oil. Among these, ethanol is particularly significant due to its compatibility with existing fuel infrastructure, its environmental benefits, and its potential to support both farmers and industry. Ethanol and alcohol technology can make India a global leader in the renewable energy sector with the help of strong government policy support, innovative technologies and skilled human resource development.

References:

1. NITI Aayog. *India's Bio-Energy Roadmap: Vision 2047*. New Delhi, 2021.
2. Ministry of New and Renewable Energy (MNRE). *National Policy on Biofuels – 2018*. Government of India.
3. Kumar, A., Singh, J., & Sharma, P. (2020). Biofuels in India: Current Status, Challenges, and Opportunities. *Renewable and Sustainable Energy Reviews*, 119, 109611.
4. Government of India, Ministry of Petroleum and Natural Gas. *Ethanol Blending Programme*. New Delhi, 2022.
5. Balat, M., & Balat, H. (2009). Recent trends in global production and utilization of bio-ethanol fuel. *Applied Energy*, 86(11), 2273–2282.
6. Sarkar, N., Ghosh, S. K., Bannerjee, S., & Aikat, K. (2012). Bioethanol production from agricultural wastes: An overview. *Renewable Energy*, 37(1), 19–27.

RAINBOW CONNECTION NUMBER OF THE ENHANCED POWER GRAPH

Richa Jain

Department of Mathematics,

Govt. P. G. College Guna Madhya Pradesh INDIA

Corresponding author E-mail: rj455001@gmail.com

Abstract:

$P_e(G)$, the enhanced power graph of a finite group G , is a simple undirected graph with G as its vertex set and two different vertices x, y that are adjacent if and only if $x, y \in \langle z \rangle$ for some z that resides in G . The enhanced power graph with finite degree, independence number, and matching number is examined in this work, and the results about the rainbow connection number and strong metric dimension of the enhanced power graph are presented.

Introduction:

A graph is a pair (V, E) , where V is a set with elements called vertices and E is a set of edges, i.e., unordered pairs of vertices. As usual, for a graph Γ , we use $V(\Gamma)$ and $E(\Gamma)$ to denote its vertex and edge sets, respectively. The underlying graph of a digraph is the simple undirected graph obtained by replacing each arc by an edge with the same end-vertices. Kelarev and Quinn established the idea of a group's power graph as a directed graph in [1], and later expanded it to semigroups in [2, 3]. The vertices of the undirected, simple power graph $P(G)$ of a group G are its elements, and two vertices are adjacent if one of them is a power of the other. Cameron and Ghosh [10] showed that two finite abelian groups with isomorphic power graphs are isomorphic. More generally, they shown that directed power graphs of two finite groups are also isomorphic if their power graphs are isomorphic. For any group G , G is periodic if and only if $P(G)$ is connected. Furthermore, for a finite group G , $P(G)$ is complete if and only if G is cyclic group of order one or prime power. There have been numerous more noteworthy findings about power graphs in the literature; see [4,15] and the references therein. Aalipour et al. [6] introduced the enhanced power graph of a group. For every group G , it can be seen that the graph $P(G)$ is a spanning subgraph of $P_e(G)$. An edge colouring or edge labeling of Γ is an assignment of some colours or labels to the edges of Γ . In 2006 Chartrand et al. [7] introduced the concept of rainbow connection of graphs. After the terrorist attacks of September 11, 2001, information sharing between American government agencies served as the inspiration for this notion. Let $V(\Gamma)$ and $E(\Gamma)$ be the vertex and edge sets of a nontrivial connected graph Γ . We define an edge-coloring for $k \in \mathbb{N}$ as: $f: E(\Gamma) \rightarrow \{1, \dots, k\}$, with adjacent edges being allowed to share the same color. If there are no edges with the same color on a path P , the path is a rainbow. An edge-colored graph Γ is rainbow connected if every two distinct vertices are connected by a rainbow. An edge-coloring under which Γ is rainbow connected is called rainbow coloring. The rainbow

connection number of Γ , denoted by $rc(\Gamma)$, is the smallest number of colors that are needed in order to make Γ rainbow connected. A vertex of a graph Γ is called a dominating vertex if this vertex is adjacent to every other vertex of Γ .

The cyclic graph of a semigroup S is a graph whose vertex set is S and two vertices u and v are adjacent if $\langle u, v \rangle \in \langle w \rangle$ for some $w \in S$. When S is a group, it can be seen that the concepts of enhanced power graph and cyclic graph coincide.

If there is a shortest path from vertex z to vertex u containing vertex v or a shortest path from vertex z to vertex v containing vertex u for vertices u and v in a graph Γ , then we say that z strongly resolves u and v . A subset Q of $V(\Gamma)$ is a strong resolving set of Γ if every pair of vertices of Γ is strongly resolved by some vertex of Q . The least cardinality of a strong resolving set of Γ is called the strong metric dimension of Γ .

Results and Discussion:

Lemma[8] 2.1. For any finite group G , $P_e(G) = P(G)$ if and only if every cyclic subgroup of G has prime power order.

The clique number of enhanced power graphs was determined in [8] in terms of the ordering of the associated groups' constituents.

We write (a, b) as the greatest common divisor of the integers a and b . It is commonly known that the Euler's totient function φ has the following result (for instance, see [5]):

Theorem 2.2. For any finite group G , the independence number of enhanced power graph equals to the number of maximal cyclic subgraphs of G . Furthermore, if G is isomorphic to a direct product of its Sylow subgroups and the prime factors of $|G|$ are p_1, p_2, \dots, p_n then the independence number $\alpha(P_e(G)) = m_1, m_2, \dots, m_n$, where m_i is the number of maximal subgroups of a Sylow- p_i subgroups.

Proof. Suppose $M(G)$ be the number of maximal cyclic subgroups of G . If a and b be any two elements generating two different maximal cyclic subgroups of G , then they are non-adjacent in $P_e(G)$. This will implies, $\alpha(P_e(G)) \geq M(G)$. Now let's look at an independent set S in $P_e(G)$. Remember that each group can be expressed as the union of all of its cyclic maximum subgroups. Since no two elements of an independent set in $P_e(G)$ belong to the same maximum cyclic subgroup since a maximal cyclic subgroup creates a clique. As a result, $\alpha(P_e(G)) \leq M(G)$. Thus, we conclude that $\alpha(P_e(G)) = M(G)$.

Since G is isomorphic to a direct product of its Sylow subgroups and M_i be the Sylow- p_i subgroup of G for $1 \leq i \leq n$. Then, we gave $G = p_1.p_2, \dots, p_n$. Then H is a maximal cyclic subgroup of G if and only if $H = H_1 H_2 \dots H_n$, where H_i is a maximal cyclic subgroup of M_i for $1 \leq i \leq n$ (see [11]).

Let P_i, P'_i be the maximal cyclic subgroups of M_i for $1 \leq i \leq n$. If $P_i \neq P'_i$ for any $1 \leq i \leq n$, then $P_1 P_2, \dots, P_n = P'_1 P'_2, \dots, P'_n$. This is possible since the generators of P_i belong to

P_1P_2, \dots, P_n , but not to $P'_1P'_2, \dots, P'_n$. Thus, if the number of maximal subgroups of M_i is m_i , then $\alpha(P_e(G)) = m_1, m_2, \dots, m_n$.

Theorem 2.3. Let G be any finite abelian p -group with exponent p^x with order n . Then the strong metric dimension of $P_e(G)$ is (i) $|G| - 1$, if G has an element of order n , (ii) $|G| - (x + 1)$, otherwise.

Proof. When G has an element of order n , the proof is simple. Now we will discuss the second case. For some cyclic p -groups C_1, C_2, \dots, C_m , $m \geq 2$, we have $G \sim C_1 \times C_2 \times \dots \times C_m$. Now let us assume two distinct elements $a = (a_1, a_2, \dots, a_m)$ and $b = (b_1, b_2, \dots, b_m)$ in G with $O(a) \geq O(b)$.

Case 1: If $N[a] = N[b]$ then, $a \sim b$.

Case 2: If $N[a] \neq N[b]$

If $a = e$, then we have $N[a] = N[b] = G$. However, this rises a contradiction. Similarly, this situation occurs when $b = e$. Thus, a and b cannot be identity elements.

If $O(a) = 2$. Then $O(b) = 2$, since $O(a) \geq O(b)$. As $a \sim b$, we thus have $\langle a \rangle = \langle b \rangle$. Then $a = b$, which is a contradiction

Now Suppose $O(a) \geq 3$ and $O(a) > O(b)$. Then as $a \sim b$, there exists an integer k with $p \mid k$ such that $b = ak$. We have the following cases

Case I: If $a_i = e$ for some i such that $1 \leq i \leq m$. We define an element $q = (q_1, q_2, \dots, q_m)$ such that q_i is an element of order p in C_i and $q_j = a_j$ for $1 \leq i \leq m, j \neq i$. Then notice that $O(q) = O(a)$ and $\langle a \rangle = \langle q \rangle$. As a result, $q \not\sim a$. However, as $b = ak$, we have $q \sim b$. This contradicts our assumption that $N[a] = N[b]$.

Case II. If $a_i \neq e$ for some i such that $1 \leq i \leq m$. Let $1 \leq j \leq m$ be such that $O(a_j) \leq O(a_k)$ for all $1 \leq k \leq m$. We define an element $q = (q_1, q_2, \dots, q_m)$ such that $q_j = a_j^{p^{\beta-1}+1}$, where $O(a_j) = p^\beta$, and $q_k = a_k$ for $1 \leq k \leq m, j \neq k$. Then $b = qk$, so that $q \sim b$. Moreover, as $O(a) = O(q)$, we have $q = ar$ for some $(r, p) = 1$. Accordingly, $O(a_i) \mid (r - 1)$ for all $1 \leq k \leq s, j \neq k$. Since $O(a_i) \leq O(a_k)$ for all $1 \leq k \leq m$, we thus get $p\beta \mid (r - 1)$. This implies $a_j^{p^{\beta-1}+1} = a_j$, which is not possible. As a result, $q \not\sim a$. This again results in a contradiction. Consequently, $O(a) = O(b)$. Hence as $a \sim b$, we have $\langle a_i \rangle = \langle b_i \rangle$. Since converse is trivial, we therefore conclude that $N[a] = N[b]$ if and only if $O(a) \geq 3$ and $\langle a_i \rangle = \langle b_i \rangle$. Thus, we get $e^\wedge = \{e\}$. Moreover, if $p = 2$, then $a^\wedge = \{a\}$. For every element a of order 2 in G . Now consider a clique C in $\hat{P}(G)$ with at least two vertices. Then for any pair of distinct vertices \hat{a}, \hat{b} in C , we have $O(a) \neq O(b)$. Additionally, for any $a \in G$, we have $O(a) = p^i$ for some $0 \leq i \leq x$. Since G is p -group of exponent p^x , there exists $z \in G$ of order p^x . We observe that $\{\hat{e}\} \cup \{\hat{z}^{a^i} : 0 \leq i \leq x - 1\}$ is a clique in $\hat{P}(G)$. Therefore, we get $\omega(\hat{P}(G)) = x + 1$ and subsequently, strong metric dimension is $|G| - (x + 1)$.

We will use the concept of calculating the rainbow connected number of enhanced power graph through graphs, as was done by the authors from [15] about the power graph, using the set of maximum involutions; denoted by M_G the set of maximal involutions of G , whose significant role will be discussed later. We can enumerate the following theorem:

Theorem 2.4. Let G be a finite group of order at least 3 and let $M_G \neq \emptyset$. Then

$$rc(\text{power graph}) = \begin{cases} 3, & \text{if } 1 \leq |M_G| \leq 2, \\ |M_G|, & \text{if } |M_G| \geq 3 \end{cases}$$

If $|M_G| = \emptyset$, let G be a finite group

1. If G is cyclic, then

$$rc(\text{power graph}) = \begin{cases} 1, & \text{if } |G| \text{ is a prime power,} \\ 2, & \text{otherwise.} \end{cases}$$

2. If G is noncyclic, then $rc(\text{power graph}) = 2$ or 3 .

The vertex connectivity $\kappa(\Gamma)$ of a graph Γ , also called "point connectivity" or simply "connectivity," is the minimum size of a vertex cut i.e., a vertex subset $S \subseteq V(\Gamma)$ such that $\Gamma - S$ is disconnected or has only one vertex. A graph Γ with $\kappa(\Gamma) \geq 1$ or on a single vertex is said to be connected, a graph with $\kappa(\Gamma) \geq 2$ is said to be biconnected, and in general, a graph with vertex connectivity $\kappa(\Gamma) \geq k$ is said to be k -connected. From the definition of an enhanced power graph, the following statement follows.

Proposition 2.5. $rc(P_e(G)) = 1$ if and only if $P_e(G)$ with n vertices has vertex connectivity $n - 1$.

Proof. We have $rc(P_e(G)) = 1$ and suppose $E = E_1 \cup E_2$ be the set of edges of $P_e(G)$ and a 1-coloring given and let $M_G = \{a_1, a_2, \dots, a_m\}$ be an independence cyclic set of $P_e(G)$, thus there is $h \in \langle a_i \rangle \cap \langle a_j \rangle$ such that $\{a_i, h\} \in E_1$ and $\{h, a_j\} \in E_2$ (or $\{a_i, h\} \in E_2$ and $\{h, a_j\} \in E_1$). Let us consider $h_{i,j} = h$, moreover $H_i := \{h_{i,1}, h_{i,2}, \dots, h_{i,m}\} =: U_i \cup V_i$ such that $U_i = \{h_{i,j} | \{a_i, h_{i,j}\} \in E_1\}$ and $V_i = \{h_{i,j} | \{h_{i,j}, a_j\} \in E_2\}$. Thus $P_e(G)$ has vertex connectivity $n-1$.

Now Suppose $M_G = \{a_1, a_2\} \neq b$, and $b \in \langle a_1 \rangle \cap \langle a_2 \rangle$, then $\langle g \rangle = \langle a_1 \rangle$ or $\langle g \rangle = \langle a_2 \rangle$. Without loss of generality suppose that $\langle g \rangle = \langle a_1 \rangle$, then $\langle a_1 \rangle = \langle g \rangle \subset \langle a_2 \rangle$, but that is a contradiction because M_G is an essential cyclic set. Therefore $|\langle a_1 \rangle \cap \langle a_2 \rangle| = 1$. Since $P_e(G)$ is not complete, we have $rc(P_e(G)) \geq 2$, then, $E_1 = \{\{a, b\} | a, b \in \langle a_1 \rangle\}$, $E_2 = \{\{a, b\} | a, b \in \langle a_2 \rangle\}$. We notice that the only path between a_{1_i} and a_{2_i} for all $a_{1_i} \in \langle a_1 \rangle$, and $a_{2_i} \in \langle a_2 \rangle$ is (a_{1_i}, e, a_{2_i}) , then, the 1-coloring is given by $\zeta : E(G) \rightarrow \{1, 2\}$ with $f \mapsto i$, if $f \in E_i$ is a rainbow 1-coloring of $P_e(G)$.

subgraph Γ' of Γ is called hole if Γ' is a cycle as an induced subgraph, and Γ' is called an antihole of Γ if Γ' is a hole in Γ . For any finite group G , e does not belong to the vertex set of any hole of length greater than 3, or any antihole of $P_e(G)$. For $n \geq 1$, the group U_{6n} is defined as the presentation $U_{6n} = \{x, y : x^{2n} = y^3 = e, xy = yx^{-1}\}$. The order of group U_{6n} is $6n$. It should be remembered that the order of U_{6n} is $6n$ if and only if y does not belongs to $\langle x \rangle$.

Theorem 2.6. The enhanced power graph $P_e(U_{6n})$ does not contain hole or antihole of odd length at least 5.

Proof. First suppose that $P_e(U_{6n})$ contains a hole H given by $a_1 \sim a_2 \sim \dots \sim a_l \sim a_1$, where $l \geq 5$. Then we have the following two cases:

Case 1. $a_i \notin \langle z \rangle$ for all i . We have either $a_1 \in P_j \setminus \langle z \rangle$ or $a_1 \in Q_j \setminus \langle z \rangle$ for some j . Without loss of generality, we suppose that $a_1 \in P_j \setminus \langle z \rangle$ for some j . Since $a_1 \sim a_2 \sim \dots \sim a_l$, then, we have $a_1, a_2 \in P_j$. Consequently, $a_1 \sim a_2$.

Case 2. $a_i \in \langle z \rangle$ for some i . Without loss of generality, we assume that $a_1 \in \langle z \rangle$. Since a_4 is not adjacent with a_1 so either $a_4 \in P_j \setminus \langle z \rangle$ or $a_4 \in Q_j \setminus \langle z \rangle$ for some j . Also, $a_3 \sim a_4 \sim a_5$, and, we have either $a_3, a_5 \in P_j$ or $a_3, a_5 \in Q_j$. We have $a_3 \sim a_5$. Now suppose C' is an antihole of order at least 5 in $P_e(U_{6n})$ that is, we have a hole $b_1 \sim b_2 \sim \dots \sim b_l \sim b_1$, where $l \geq 5$, in $P_e(U_{6n})$. Then, again we arrive at contradiction in each of the following cases.

Case I. $b_i \notin \langle z \rangle$ for all i . then, either $b_1 \in P_j \setminus \langle z \rangle$ or $b_1 \in Q_j \setminus \langle z \rangle$ for some j . Since $b_1 \sim b_3$ and $b_1 \sim b_4$ in $P_e(U_{6n})$. we obtain either $b_3, b_4 \in P_j$ or $b_3, b_5 \in Q_j$. Thus, we have $b_3 \sim b_4$ in $P_e(U_{6n})$.

Case II. $b_i \in \langle z \rangle$ for some i . Without loss of generality, we assume that $b_1 \in \langle z \rangle$. Notice that we have $b_1 \not\sim b_2$ in $P_e(U_{6n})$. Consequently, either $b_2 \in P_j \setminus \langle z \rangle$ or $b_2 \in Q_j \setminus \langle z \rangle$. Moreover, $b_2 \sim b_4$ and $b_2 \sim b_5$ in $P_e(U_{6n})$, as C' is an antihole in $P_e(U_{6n})$. Thus either $b_4, b_5 \in P_j$ or $b_4, b_5 \in Q_j$. As a result, $b_4 \sim b_5$ in $P_e(U_{6n})$.

Conclusion:

We conclude by mentioning a few relevant sources that support the findings mentioned above and may possibly be used in future research. If D is the set of dominating vertices of the enhanced power graph of G then The proper enhanced power graph of a group G is the induced subgraph of the enhanced power graph on the set $G \setminus D$. All nilpotent groups were categorized by Bera and Dey [9] such that their correct enhanced power graphs are connected, and their diameters were established. Additionally, they explicitly discovered the domination number of a finite nilpotent group's correct improved power graph. Several graph theoretical aspects of the enhanced power graph of semigroups, such as the dominant number, independence number, genus, connectedness, minimum degree, chromatic number, and others, were investigated in [11,12,13].

Acknowledgement:

The author would like to convey heartfelt gratitude to Mr. Sanjeev Singh Parihar for his tremendous support and assistance in the completion of this work. The author also wishes to thank Dr. B.K. Tiwari, Principal of Government P.G. College, Guna, Madhya Pradesh, for his guidance. We sincerely appreciate the valuable comments on our manuscript and the excellent editing provided.

References:

1. Kelarev, A. V., & Quinn, S. (2000). A combinatorial property and power graphs of groups. *Contributions to General Algebra*, 12(58), 3–6.
2. Kelarev, A. V., Quinn, S., & Smolikova, R. (2001). Power graphs and semigroups of matrices. *Bulletin of the Australian Mathematical Society*, 63(2), 341–344.
3. Kelarev, A. V., & Quinn, S. J. (2002). Directed graphs and combinatorial properties of semigroups. *Journal of Algebra*, 251(1), 16–26.
4. Curtin, B., & Pourgholi, G. R. (2014). Edge-maximality of power graphs of finite cyclic groups. *Journal of Algebraic Combinatorics*, 40(2), 313–330.
5. Burton, D. M. (2006). *Elementary number theory*. Tata McGraw-Hill Education.
6. Aalipour, G., Akbari, S., Cameron, P. J., Nikandish, R., & Shaveisi, F. (2016). On the structure of the power graph and the enhanced power graph of a group. *Electronic Journal of Combinatorics*, 24(3), 3.16,18.
7. Chartrand, G., Johns, G. L., McKeon, K. A., & Zhang, P. (2008). Rainbow connection in graphs. *Mathematica Bohemica*, 133, 85–98.
8. Aalipour, G., Akbari, S., Cameron, P. J., Nikandish, R., & Shaveisi, F. (2017). On the structure of the power graph and the enhanced power graph of a group. *Electronic Journal of Combinatorics*, 24(3), 3.16,18.
9. Bera, S., & Dey, H. K. (2021). On connectivity, domination number and spectral radius of the proper enhanced power graphs of finite nilpotent groups. *arXiv*. <https://arxiv.org/abs/2108.05175v1>
10. Cameron, P. J., & Ghosh, S. (2011). The power graph of a finite group. *Discrete Mathematics*, 311(13), 1220–1222.
11. Chattopadhyay, S., Patra, K. L., & Sahoo, B. K. (2018). Minimal cut-sets in the power graph of certain finite non-cyclic groups. *arXiv*. <https://arxiv.org/abs/1802.07646v1>
12. Dalal, S., & Kumar, J. (2020). Chromatic number of the cyclic graph of infinite semigroup. *Graphs and Combinatorics*, 36, 109–113.
13. Dalal, S., Kumar, J., & Singh, S. (2021). On the enhanced power graph of a semigroup. *arXiv*. <https://arxiv.org/abs/2107.11793v1>
14. Dalal, S., Kumar, J., & Singh, S. (2021). The cyclic graph of a semigroup. *arXiv*. <https://arxiv.org/abs/2107.11021v1>
15. Ma, X., Feng, M., & Wang, K. (2016). The rainbow connection number of the power graph of a finite group. *Graphs and Combinatorics*, 32, 1495–1504.
16. Ma, X., Feng, M., & Wang, K. (2018). The strong metric dimension of the power graph of a finite group. *Discrete Applied Mathematics*, 239, 159–164.

IMPACT OF GENETICALLY MODIFIED FOODS ON HUMAN HEALTH

Krithika K, Gunavadhana S and Anu Swedha Ananthan*

Department of Microbiology,

Justice Basheer Ahmed Sayeed College for Women, Chennai-600 018, Tamilnadu, India

*Corresponding author E-mail: anuswedha.a@jbascollege.edu.in

Introduction:

Genetically modified foods are derived from Genetically Modified Organisms (GMOs) which have these genes modified or altered through recombinant DNA technology. These foods are safe in most of the cases but there are controversial issues going on which keeps these foods from being sold out worldwide. Like all new technologies, GMOs also possess threats which are both known and unknown. Public concerns on GMO are mainly focused on human and environmental safety, food security and environmental conservation.

This article provides a better view on the general impacts (both positive and negative) of Genetically modified foods for a general study on GMOs.

Gmo Fruits, Vegetable Oils, Sugars:

In order to increase the papaya productivity and to protect from deadly papaya ring spot virus papaya has been genetically modified and it is resulted in being resistant to ringspot virus GM Potatoes was genetically engineered by adding resistance genes like blb1 and blb2. This prevents the late blight disease of potatoes. GM maize has been used for ethanol, sweeteners, food, drinks, alcohol. Corn oil is used as cooking oil and it is sold directly for cooking purposes. In the USA the majority of sugar beet acres were grown with glyphosate - resistant seed. Herbicide tolerant sugar beets were approved in Canada, Japan, Australia, Korea, USA.

Impacts of GMO Foods on Human Health:

GMO foods may cause diseases which are immune to antibiotics. Many businesses minded people do not label these foods as GMO foods so that it would backfire their business profits. Many cultural and religious people are against these foods.

Positive Effects of GMO Foods:

Genetically modified foods offer a number of potential benefits, addressing challenges in both agriculture and nutrition. Let us see in depth about the positive effects of GMO foods,

- **Biofortification to Combat Malnutrition:**

GM crops like Golden Rice are engineered to accumulate essential nutrients (beta-carotene/Vitamin A) to prevent deficiencies (e.g., childhood blindness) in vulnerable populations

- **Reduction of Food Shortage and Chemicals:**

To reduce food shortage and to produce enough food as the population increases. Pesticide and herbicide usage is reduced by GMO foods. Also, it is used to reduce consumer costs.

They are less expensive and have more nutritional values than the traditional crops.

- **Reduced Mycotoxin Exposure:**

Insect-resistant crops like Bt corn suffer less damage. This leads to significantly lower levels of potent fungal toxins such as mycotoxins. This includes aflatoxins/fumonisin. This indirectly reduces human exposure to carcinogens. There is also a good antioxidant combination of the blueberries and the tomatoes which helps to prevent cancer and is also used in medications.

- **Production of Healthier Oils:**

Genetic modification can produce healthy cooking oils, such as soybeans. These are engineered to produce oil with little saturated fat and no trans-fats.

- **Tolerance to Abiotic Stress:**

Engineering crops for drought or salt tolerance are important for adapting to climate change. This ensures more global food security and benefits marginal countries effectively.

Genetically-modified foods have the potential to address global challenges like hunger and malnutrition. But they also present environmental, health, and economic risks. The ongoing debate on negative effects of GMO foods highlights the need for strict regulation and long-term studies to ensure public health and environmental safety.

Negative Effects of GMO Foods:

Genetically modified organisms (GMOs) in food have raised significant health, environmental, and economic concerns worldwide. While they are developed to enhance crop productivity and nutritional value, their potential risks cannot be ignored.

- **Allergenicity:**

IgE mediated immediate allergic responses and skin sensitization to *Bacillus thuringiensis* spore extract have been noticed. It should be done with attention whenever the common allergen's genes are genetically engineered with the foods. Common allergenic foods include milk, eggs, legumes, fish, crustacean, wheat, nuts etc.; In order to add proteins Brazil nut genes were genetically spliced with soybeans, this resulted in anaphylactic shock which can also cause death in people who consume those foods.

- **Antibiotic Resistance:**

When a genetically modified food or plant is ingested the bacteria which lives in the gastrointestinal tract is affected due to the transferred gene from the GMO food to the bacteria so this develops resistance to a specific antibiotic. Not only does it reduce the effectiveness of medication but also speed up the resistance factors. It causes health related issues when consumed for a longer period. High levels of antibiotics lead to allergic reactions.

- **Anti- Nutrient Effect:**

Insertion of new genes may increase the amount of nutrients along with existing nutrients Eg:- Glyphosate resistant roundup ready soybean. Phytoestrogens protect us from cancer and heart diseases. This is low in GMO foods so this leads to infertility, allergic reactions.

Gene insertion can have pleiotropic effects, unintentionally disrupting plant metabolism. This may result in Nutrient Displacement (e.g., reduced vitamins). Or, conversely, an increase in anti-nutrients (e.g., phytic acid) that block nutrient absorption. Studies on GM soybeans, for example, have explored potential reductions in beneficial isoflavones (phytoestrogens).

- **Environmental Effects:**

GMO foods also affect the environments and non- target organisms like worms, fish, birds. The effects include the loss of biodiversity, increased usage of chemicals in agriculture. Widespread use of Herbicide-Tolerant (HT) GM crops has driven the evolution of resistant weeds. This forces farmers to use higher volumes or toxic herbicides.

- **Economic Effects and Legal Issues:**

There will be an increase in price of the seeds for GM crops by patenting new plant varieties, it increases global production levels of the main crops, it leads to endangering of farmers, environment and trade. GMO foods are one of the most controversial topics. Many NGOs have been actively protesting against these GM foods for years.

- **GMO Foods and Cancer:**

FDA In 1993 approved the use of genetically engineered recombinant Bovine Growth Hormone (rBGH). Genetically altered growth hormones are injected into the cows this increases the milk production and can cause colorectal, breast and prostate cancer (IGF-1 causes breast cancer). When GMO foods are consumed, our body is exposed to foreign DNA , this DNA is not fully digested in our stomach or intestine and these DNA fragments are mixed with normal DNA which leads to arthritis, lymphoma (blood cancer). The greater concern is the increased residue of chemicals like Glyphosate on HT crops. IARC classifies glyphosate as "probably carcinogenic to humans" (Group 2A), making this a contentious link between GM technology and potential cancer risk from chemical exposure.

Thus, while GMO foods may offer certain benefits, the associated risks highlight the need for strict regulation and long-term studies. A cautious approach is essential to ensure public health, environmental safety, and ethical agricultural practices.

Conclusion:

Genetically-modified foods have the ability to resolve the world's hunger and malnutrition problems, and to help protect and preserve the environment by increasing yield. GM foods have both positive and negative effects. The potential threats can be expressed as environmental hazards, health problems, economic concerns as well as legal issues. Lately, many countries have

developed many safety measures to regulate the growth of GM foods in order to eradicate their possible risks on biodiversity, human health and environment.

References:

1. Chekol, C. (2021). The health effects of genetically modified foods: A brief review. *International Journal of Nutrition Sciences*, 6(1), 1047.
2. Chagas, C. E. A., Rogero, M. M., & Martini, L. A. (2012). Evaluating the links between intake of milk/dairy products and cancer. *Nutrition Reviews*, 70(5), 294–300.
3. Nordlee, J. A., et al. (1996). Recombinant proteins in newly developed foods: Identification of allergenic activity. *Allergy*, 51(5), 324–331.
4. Nordlee, J. A., Taylor, S. L., Townsend, J. A., Thomas, L. A., & Bush, R. K. (1996). Identification of a Brazil-nut allergen in transgenic soybeans. *The New England Journal of Medicine*, 334(11), 688–692
5. Peyrat, J. P., et al. (1993). Plasma Insulin-like Growth Factor-1 (IGF-1) concentrations in human breast cancer. *European Journal of Cancer*, 29A(4), 492–497.
6. Reddy, K. N., & Nandula, V. K. (2012). Herbicide resistant crops: History, development and current technologies. *Indian Journal of Agronomy*, 57(1), 1–7.
7. USDA Agricultural Research Service. (2005). Line 63-1, a new virus-resistant transgenic papaya for Hawaii. *HortScience*, 40(5), 1196–1199.

NEXT-GENERATION CROP MONITORING WITH SMART TECHNOLOGIES IN PRECISION AGRICULTURE

Yashaswini R*, Sridhara M R, Prem Sagar S P, V C Raghavendra and Sharanabasava

University of Agricultural Sciences, Raichur – 584104 (Karnataka), India

*Corresponding author E-mail: yashaswinirayanki1998@gmail.com

Abstract:

Feeding an estimated nine billion people by 2050 requires innovative, data-driven agricultural practices that transcend traditional methods. Next-generation technologies including unmanned aerial vehicles (UAVs), information and communication technologies (ICTs), remote sensing (RS), big data analytics and machine learning (ML) are transforming crop monitoring and management into precise, sustainable and climate-resilient systems. ICTs enhance farmer connectivity, delivering timely advisories on weather, pests, inputs and markets through mobile platforms, while UAVs equipped with multispectral, hyper spectral, thermal, LiDAR and RGB sensors enable high-resolution, real-time monitoring of crop health, water stress, nutrient status and pest/disease outbreaks. UAV-based RS complements satellite imagery by offering flexible, site-specific and time-series data, facilitating yield forecasting and precision input application. Integration with ML and deep learning improves disease detection, high-throughput phenotyping and yield prediction through multimodal data fusion and attention-based architectures. Big data analytics further empowers decision-making by transforming heterogeneous datasets from sensors, IoTs and satellites into actionable insights. These advancements optimize irrigation, fertilization and pest control, reducing input waste and environmental impact while enhancing productivity. Scaling these technologies through interoperable data infrastructures, farmer-friendly platforms and robust public-private partnerships is crucial to ensure accessibility for smallholders, thereby strengthening global food security and supporting Sustainable Development Goals.

Introduction:

Global agriculture faces the critical challenge of feeding a projected population of nearly nine billion by 2050, necessitating a paradigm shift in how we manage agricultural systems. Traditional farming practices must be supplemented with next-generation technologies that support precision, sustainability and resilience. Integrating remote sensing (RS), unmanned aerial vehicles (UAVs) and machine learning (ML) into agricultural management allows for spatially and temporally precise interventions, ultimately leading to higher productivity, reduced input waste and better environmental stewardship.

Conventional crop monitoring techniques rely on field sampling for parameters like biomass, nitrogen concentration or crop health. While these methods are time-consuming, limited in spatial coverage and often fail to represent field variability accurately. Satellite-based RS has improved agricultural monitoring but suffers from limitations such as high costs, cloud interference, lower revisit frequencies and coarse spatial resolution. In contrast, UAVs offer low-altitude, high-resolution, real-time data collection with greater flexibility, especially under variable weather conditions.

ICTs?

“Is any device, tool or application that permits the exchange or collection of data through interaction or transmission”. Umbrella term that includes anything ranging from radio to satellite imagery to mobile phones or electronic money transfers.

Current Status of ICT in India (MeitY, 2020)

Mobile App/ Web service	Information /Data disseminate
1. Sidilu	Early warning on lightning and thunderstorms.
2. Megadoot	Weather based agro advisories (wind speed and its direction, humidity, rainfall).
3. e-SAP	Insect pest identification, microbial diseases, nutritional deficiencies and weed problems.
4. IFFCO-Kissan	Kissan call centre, Green sim, Samadhan Services, Sampark Services (latest mandi prices, weather forecast, agricultural advisory, animal husbandry, horticulture and agricultural news and schemes).
5. Kissan Suvidha	Weather of current day and next 5 days, dealers, market prices, agro advisories, plant protection, IPM practices etc.
6. M-Kissan (SMS)	Marketing the agriculture produce (buy and purchase).
7. e-Sagu	The agricultural experts' advice the latest information about the crop.
8. Sowing advisories	Land preparation to storage.
9. NADAMS	Provides real-time information on prevalence, severity level and persistence of agricultural drought.
10. AGRI-daksh	Selection of suitable variety.
11. Krishi ganaka	Web based online fertilizer recommendation for different crops through STCR approach.
12. Plantix app	Identifies potential defects and nutrient deficiencies in soil.
13. Krishi Chintana	Agriculture and allied aspects.
14. e-NAM	Farmer can access the prevailing commodity prices information on this app prior to even going to the mandi.

India has the second-largest telecom network in the world after China, with over 1.17 billion connections. Wireless communication dominates, accounting for 98.2% of total phone connections. The overall tele-density is 86.55%, with urban tele-density at 139.01% and rural tele-density at 59.08%, showing steady rural growth.

India implements nearly 45% of global ICT projects and has established a large number of information kiosks in rural areas. The country has 752.09 million internet users and 734.82 million broadband subscribers, reflecting rapid digital penetration.

ICT services provide critical access to the knowledge, information and technology that farmers require to improve the productivity and thus improve the quality of their lives and livelihoods and also helps by collecting and sharing timely and accurate information on weather, inputs, markets, and prices. By feeding information into research and development initiatives and by disseminating knowledge to farmers by connecting producers and consumers. ICT has immense potential to standardize and regulate agricultural processes and address the needs of farmers. It will therefore, definitely serve as an important tool for agricultural development in the near future.

UAVs

Recent advances in information and communication technologies (ICTs) and AI-driven analytics have revolutionized data handling in agriculture. UAVs, equipped with multispectral, hyper spectral or thermal sensors are capable of capturing detailed imagery related to crop health, disease outbreaks, water stress and nutrient status. When integrated with machine learning algorithms, this data can be transformed into actionable insights for early intervention, yield forecasting and variable-rate input application. UAVs thus form a crucial component of digital agriculture ecosystems, enabling site-specific management with unprecedented efficiency.

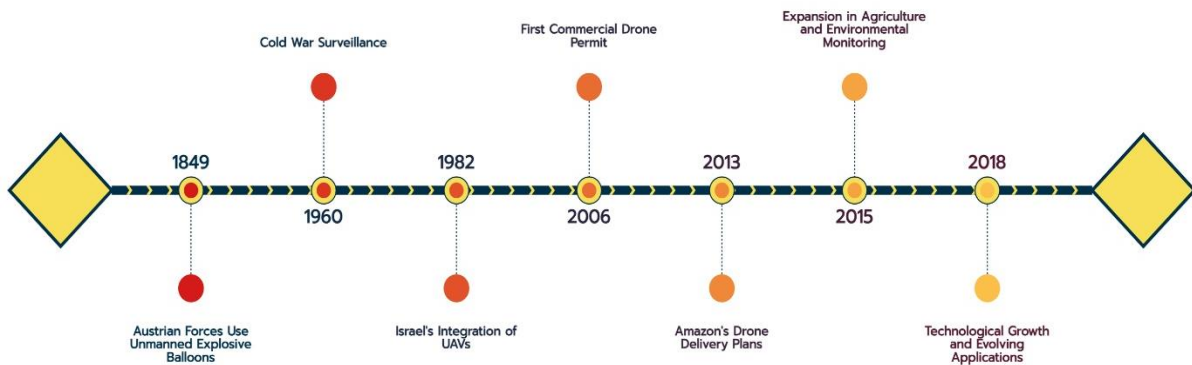
While UAVs are not poised to completely replace satellite or manned aerial surveys, they complement these platforms with high-frequency, high-precision monitoring as a critical capability for dynamic crop environments. Moreover, as UAV software becomes more autonomous and data processing tools become more accessible, these technologies are increasingly scalable and affordable, even for smallholder farmers. Together, UAVs, RS and ML represent the cornerstone of smart, climate-resilient agriculture, supporting the achievement of Sustainable Development Goals (SDGs) and long-term food security.

History of Drone Development

Unmanned Aerial Vehicles (UAVs), commonly known as drones, originated primarily from military applications. The first known use of UAVs for aerial reconnaissance dates back to 1955, when the Radioplane was deployed in the United States for photographic intelligence. Throughout the following decades, similar UAV capabilities were developed by France (late 1950s), Italy (1960s) and the Soviet Union (early 1970s). Although radar and television systems

were integrated into UAVs as early as 1941, their use was initially limited to guidance, not surveillance.

UAV-based aerial imagery gained prominence during the Vietnam War (1960s–1970s), when high-altitude reconnaissance became a critical military tool. Many of the technologies developed during this period laid the groundwork for future civilian UAV applications. By the mid-1980s, UAVs began to be tested for non-military tasks, such as forest fire monitoring in Montana (1986). Notable advancements include the Condor UAV, capable of autonomous take-off and landing, and the Predator UAV, which delivered imagery with 30 cm spatial resolution which is a breakthrough in real-time aerial intelligence.



In India, significant progress was marked by the development of NETRA, a lightweight autonomous UAV co-developed by DRDO and IdeaForge. Designed for surveillance and reconnaissance, NETRA is equipped with thermal imaging and real-time communication systems. It has been utilized in border security, law enforcement, search and rescue, disaster management and aerial monitoring. Over the years, the scope of UAV applications has expanded rapidly into the civilian domain. Modern uses include precision agriculture, traffic monitoring, environmental research, archaeological surveys, disaster response and public safety operations. The timeline of major UAV milestones includes:

Types of drones based on wings/ rotor

Type	Advantages	Disadvantages	Typical Uses
Fixed-Wing Drones	<ul style="list-style-type: none"> • Long flight time • Fly at high altitude • Carry more weight • Stable in air 	<ul style="list-style-type: none"> • Expensive • Require training • Need launcher in most cases • Harder to land • Can only move forward • Can't hover 	Aerial mapping, Inspection, Agriculture, Construction, Security, Surveillance

Single-Rotor Drones	<ul style="list-style-type: none"> • More efficient than multi-rotors • Can use gas motor for longer endurance • Simple design (main rotor + tail rotor) 	<ul style="list-style-type: none"> • More complex than multi-rotors • Higher safety risks due to large rotor blades 	Surveying, Heavy-lift operations, Agriculture, Research
Multi-Rotor Drones	<ul style="list-style-type: none"> • Easy to control & maneuver • Can hover • Vertical takeoff/ landing • Very stable • Cheapest and easiest to manufacture 	<ul style="list-style-type: none"> • Short flight time • Small payload capacity • Energy mostly used to fight gravity 	Aerial photography & video, Inspections, Leisure, Agriculture, Filmmaking, Construction, Security

(A)



(B)



(C)



The unmanned aerial vehicle (UAV) types used in precision phenotyping: (A) rotary wings (Inspired flight IF1200A); (B) fixed-wing (senseFly eBee SQ) & (C) hybrid, VTOL fixed-wing (DeltaQuad Evo) (Dragonfly Aerospace, 2022).

Types of drones based on cost

Category	Price range	Typical features / Uses
Low-Cost Drones	\$ 20 – \$ 100	Mainly toy drones for fun and casual flying; no advanced equipment
Mid-Range Drones	\$ 150 – \$ 500	Used for both hobby and semi-professional tasks; can support basic mapping and light data collection
High-Cost Drones	\$ 600 – \$ 2000	Purchased for professional purposes; suitable for surveillance, photography, and specialized projects
Premium Drones	\$ 3000+	Advanced models for military, industrial, or geo-mapping applications

Types of drones based on size

Category	Approx. Size	Description / Typical Uses
Nano	Up to 50 cm (insect-sized)	Extremely small; used for research, reconnaissance, or hobby purposes
Small	Less than 2 m in length	Compact drones; common for hobbyists, photography and light professional use
Medium	Portable by two people	Professional-grade; used for mapping, agriculture and inspections
Large	Comparable to small aircraft	Military, long-range surveillance and heavy-duty operations

Types of drones based on range

Category	Range	Endurance	Typical Uses
Very Close Range	Up to ~5 km	20 minutes – 1 hour	Hobby flying, short inspections, basic observation
Close Range	Up to ~50 km	Up to 6 hours	Extended inspections, mapping, reconnaissance
Short Range	Up to ~150 km	Up to 12 hours	Spying, surveillance, security operations
Mid-Range	Up to ~650 km	Long endurance (varies)	Scientific research, weather studies, geological data collection

How drone technology works in agriculture

Modern agricultural drones combine navigation systems, GPS, sensors, cameras and on-board controllers to collect and process field data. They provide more precise and real-time insights than traditional satellite imagery, supporting precision farming.

Key steps in agricultural drone operation (Yallappa, 2018):

1. Field Analysis & Boundary Setup

Define the area of interest. Upload GPS coordinates and boundaries into the drone’s navigation system.

2. Autonomous Flight & Data Collection

Drones follow pre-programmed flight paths. Sensors (e.g., multispectral, RGB, thermal) capture images and field information.

3. Data Processing

Collected images and sensor readings are uploaded to specialized agri-tech software. Software analyzes plant health, soil conditions and crop variability.

4. Output & Visualization

Processed data is converted into farmer-friendly outputs. Results are often displayed through 3D mapping or photogrammetry for easy interpretation.

UAVs in Agriculture

Unmanned Aerial Vehicles (UAVs), commonly known as drones, have become integral to modern agricultural practices, especially in the context of smart or precision agriculture. These systems offer a flexible, low-cost and high-resolution alternative to traditional data collection methods such as manual field surveys or satellite remote sensing. UAVs can be equipped with a variety of sensors - multispectral, hyper spectral, thermal, LiDAR and RGB that enables rapid and accurate monitoring of crop health, soil conditions, moisture levels and pest or disease outbreaks. These sensors capture spectral data based on how plants reflect light particularly in relation to chlorophyll content and biomass which allowing vegetation indices like NDVI to assess plant health and stress levels. Their ability to fly at low altitudes allows for data collection at very high spatial and temporal resolutions, essential for detecting subtle variations within fields and making site-specific management decisions (Huang *et al.*, 2013).

Compared to satellite imagery, UAV-based remote sensing has several technical advantages, including reduced atmospheric interference, full user control over data acquisition timing, and higher flexibility in cloudy or variable weather conditions. UAVs also allow for repeated flights over the same area, making them ideal for time-series monitoring and growth stage assessment. When integrated with advanced analytical tools such as machine learning and deep learning, UAV data can be used to generate vegetation indices, 3D crop models and predictive maps that inform precision input application and yield forecasting. These capabilities make UAVs a powerful tool for enhancing efficiency, reducing environmental impact and ensuring sustainable agricultural productivity in the face of increasing global food demand.

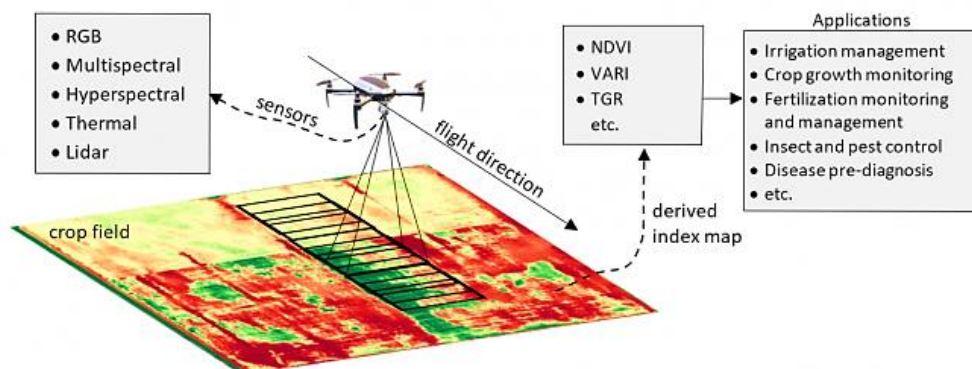


Figure 1: A visualization of the use of UAVs in agriculture

Best Drone Practices in Agriculture

1. **Irrigation Monitoring:** Drones use thermal and multispectral sensors to detect water stress, leaks, and over-irrigation, helping optimize water usage.

2. **Crop Health Monitoring:** Multispectral and NIR imaging identify early signs of crop stress, pests, or disease for timely intervention.
3. **Crop Damage Assessment:** RGB and multispectral data quantify affected areas, enabling precise chemical use and accurate loss estimation.
4. **Field Soil Analysis:** Drone-based 3D mapping and imaging evaluate soil moisture, nutrients, and planting suitability for precision farming.
5. **Planting:** Drone seed-pod systems deploy seeds and nutrients directly into soil, reducing costs and improving planting efficiency.
6. **Agricultural Spraying:** Drones perform targeted fertilizer and pesticide spraying, increasing speed and reducing chemical exposure.
7. **Livestock Tracking:** Thermal cameras track livestock movement, detect illness, and locate missing animals for efficient herd management.

Remote Sensing in Agriculture

Agriculture provides raw materials, fuel, fibers and food to humanity. However, this crucial role must be carried out in the face of climate change and environmental sustainability challenges, all while accommodating a growing population and ensuring the continued viability of agricultural activities to sustain livelihoods.

The application of remote sensing in agriculture plays a crucial role in the evolution of farming practices, helping to address various challenges by providing real-time information about crop status at different scales throughout the growing season.

The art and science of obtaining information about an object without any physically contact between the object and sensor. Remote sensing and agriculture go hand in hand. The basic operation of this technology, using UAVs (Unmanned Aerial Vehicles), satellites and other platforms, is similar across the board. Energy, in the form of light, travels from the sun to Earth. Just like ocean waves, light waves travel in a pattern – the distance between the peaks of one wave to the peak of the next is known as wavelength. The energy emitted by the sun is electromagnetic energy, which forms part of the electromagnetic spectrum. The wavelengths used for agricultural applications occupy a small portion of this spectrum. When electromagnetic energy interacts with plants during hyper spectral remote sensing in agriculture, one of three things can happen: the energy will be reflected, absorbed, or transmitted. The outcome depends on both the wavelength of the energy and the specific characteristics of the plant. Remote sensing technology can detect the reflected, absorbed and transmitted energy (Peace *et al.*, 2019). The interplay between these three interactions creates the plant's spectral signature, which is unique to different species. By analysing these spectral signatures, remote sensing in agriculture helps identify stressed areas by comparing the signatures of healthy plants.

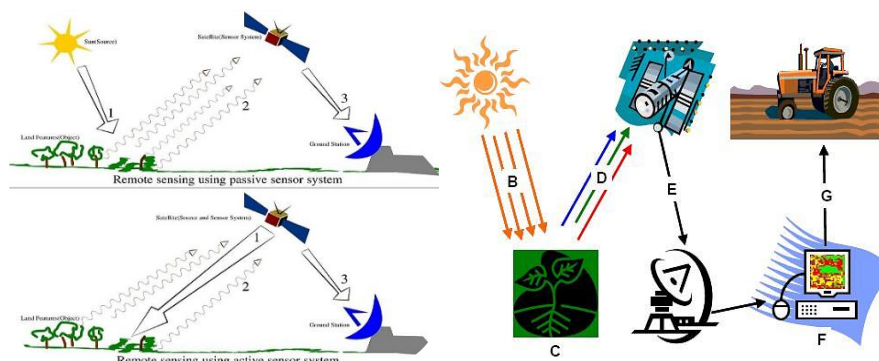


Figure 2: Working of remote sensing in agriculture

Process of remote sensing

Energy source or illumination (A), Radiation and the atmosphere (B), Interaction with the target (C), Recording of energy by the sensor (D), Transmission, Reception and Processing (E), Interpretation and Analysis (F) and Application (G).

The UAV platform (DJI Matrice 600 Pro) is equipped with a multi-sensor payload designed for high-resolution remote sensing. It integrates a Headwall Nano-Hyperspec VNIR hyperspectral camera (400-1000 nm, 270 bands) for capturing detailed spectral information, a Velodyne VLP-16 LiDAR for 3D canopy and terrain structure mapping, and a Sony Alpha 7R RGB camera for high-resolution imaging and photogrammetry. An APX UAV GNSS/IMU module ensures accurate geo-referencing of all datasets. Together, these sensors enable simultaneous acquisition of spectral, structural and visual data for precise monitoring of crop growth and yield prediction (Aierken *et al.*, 2024).



Types of Remote Sensing

Type	Energy source	Key feature	Example
Passive Remote Sensing	Natural energy (mainly sunlight)	Works only when the Sun illuminates the Earth	Sun, Optical sensors
Active Remote Sensing	Artificial energy (emitted by sensor)	Can operate anytime, day or night, in any season	LASER, RADAR

Applications of Remote Sensing in Agriculture

Remote sensing technology has found numerous applications in fields such as forestry, geology, surveying and photography. However, its most significant impact has been in agriculture. The use of remote sensing in agriculture has proven to be highly beneficial, with various applications that include, but are not limited to, the following.

1. Crop Monitoring and Health Assessment

Remote sensing plays a crucial role in monitoring crop health by using technologies like optical and infrared (VIR) sensors. These sensors can detect crop vigor, stress and damage, even before it's visible to the naked eye. This allows farmers to assess crop conditions in real-time and respond promptly to issues such as weather changes, pests or disease, improving overall crop management.

2. Soil Condition Monitoring

Monitoring soil conditions is crucial for precision agriculture. Key parameters like soil organic matter, texture, pH and moisture content, along with data on canopy health, growth stages and biomass, help optimize crop management. Remote sensing allows farmers to analyse the connection between soil health and crop performance, enabling better decisions for improved yields and resource efficiency.

3. Monitoring Water Resources

As irrigated land expands to meet growing food demand, monitoring water resources becomes essential for sustainable agriculture. Remote sensing provides accurate data on water bodies, irrigated areas and crop water status, helping farmers manage water use efficiently and adapt to changing environmental conditions.

4. Weather Prediction

Accurate weather data is vital for crop management and irrigation planning. Remote sensing enables precise weather forecasts, allowing farmers to anticipate conditions and adjust their practices, reducing unnecessary costs and preparing for potential natural disasters.

5. Air Quality Monitoring

Remote sensing helps monitor air conditions that impact crop growth. By assessing factors like wind and temperature, farmers can predict environmental changes and take preventive actions to protect crops from adverse weather conditions.

6. Precision Farming

Advancements in precision farming, supported by remote sensing, enable better crop mapping and yield optimization while minimizing environmental impact. Technologies like AI and IoT further enhance farm efficiency, making agriculture more sustainable and resource-efficient.

7. Climate Change Monitoring

Remote sensing plays a crucial role in tracking climate change, offering precise data on shifts in land, oceans and atmosphere. In agriculture, this technology helps predict climate impacts on crop yields, guiding more informed farming decisions and climate adaptation strategies.

UAV-Based Remote Sensing in Agriculture

UAV-based remote sensing has emerged as a transformative tool in agriculture, offering high-resolution, real-time data for crop and environmental monitoring. Unlike traditional methods, such as satellite imaging or field surveys, UAVs provide targeted, on-demand data collection, enabling precise monitoring of crop health, soil conditions and environmental factors. With various sensors like multispectral and thermal cameras, UAVs can assess growth stages, detect stress and identify issues like pest infestations, all of which are crucial for timely and effective crop management.

The integration of machine learning (ML) and deep learning (DL) further enhances the capabilities of UAV-based systems, automating data analysis and improving accuracy in yield prediction and disease detection. These advancements enable farmers to make data-driven decisions for irrigation, fertilization and pest control, ultimately leading to more efficient and sustainable agricultural practices. UAV remote sensing is revolutionizing precision farming by providing cost-effective, adaptable and highly detailed insights that drive improved crop management and productivity.

Sensors used in agriculture drones

Sensor Types	Main Applications
Visual Sensors	Aerial mapping, 3D reconstruction, plant counting, surveillance, emergency response, land use surveys
Thermal Sensors	Heat signature detection, livestock monitoring, security, water source detection, emergency response
Multispectral Sensors	Plant health assessment, water quality analysis, vegetation index calculation, plant counting
Hyperspectral Sensors	Advanced plant health monitoring, water quality assessment, vegetation index, full-spectrum sensing, R&D, mineral and surface composition surveys
LiDAR Sensors	Short-range laser scanning, 3D surface modeling, flood mapping, surface variation detection, plant height and canopy analysis

Geographic Information System (GIS)

GIS is a toolset used to collect, store, analyse and display spatial data linked with attribute information. It integrates multiple data layers (e.g., roads, parcels, zoning, demographics, flood

zones) into maps, revealing spatial patterns and relationships that support decision-making and location analysis.

Global Positioning System (GPS)

GPS is a satellite-based navigation system that provides accurate position and timing information anywhere on Earth. It supplies essential data (points, lines, polygons) for GIS and is often combined with remote sensing imagery.

Spectral Signature

A spectral signature describes how a material reflects or emits electromagnetic radiation across different wavelengths, serving as a unique identifier for remote sensing applications.

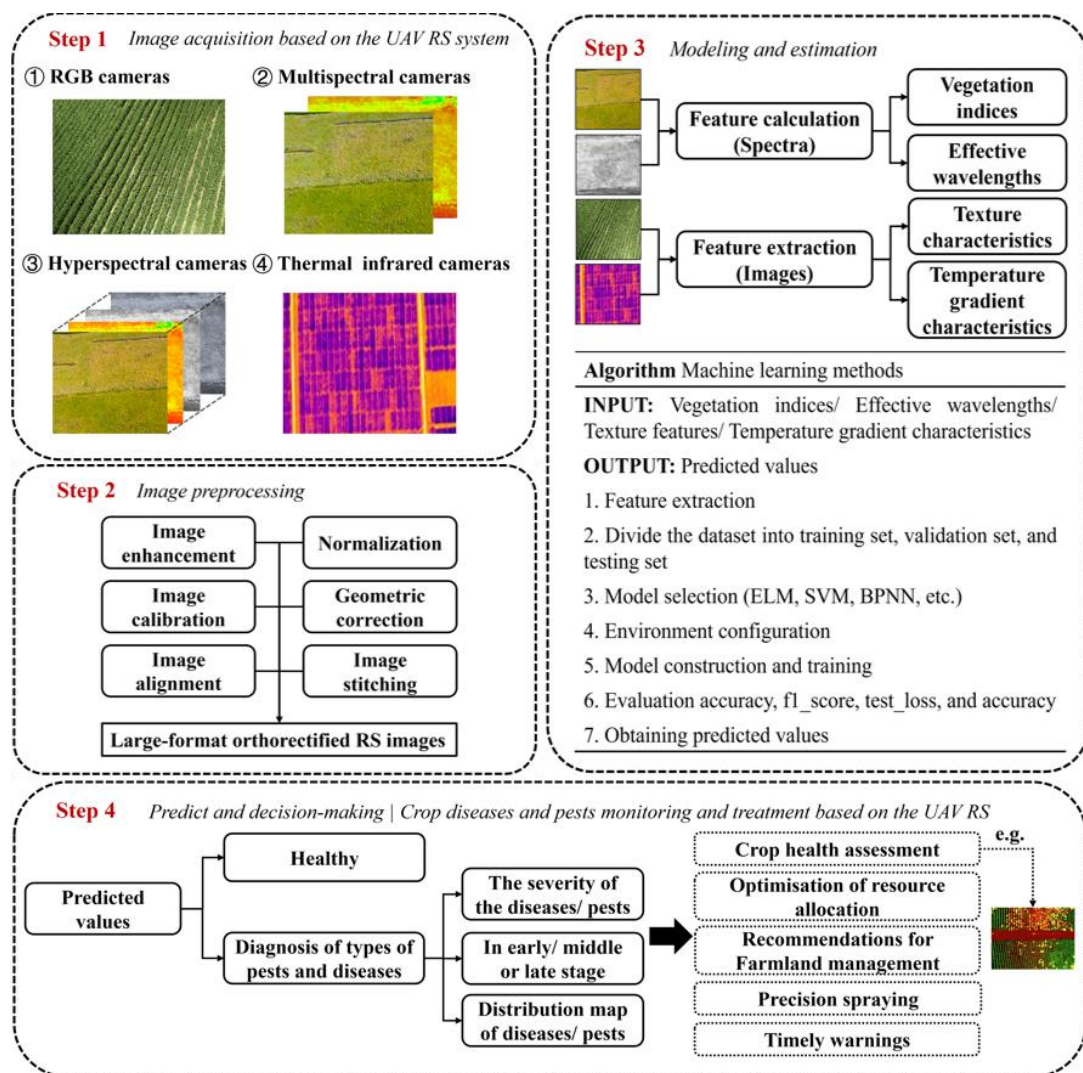


Figure 3: Technology roadmap of crop diseases and pests monitoring (Zhu *et al.*, 2024)

UAV RS in Crop Diseases and Pests

Crop diseases and pests severely affect yield and quality, with varied types and outbreak patterns that are difficult to monitor manually. UAV-based remote sensing integrates RGB, multispectral, hyper spectral and thermal cameras (Step 1) to capture crop health signals. These images

undergo pre-processing (Step 2) such as calibration, alignment and correction to generate accurate datasets. Using machine learning and deep learning models (Step 3), vegetation indices, texture and temperature features are extracted to identify disease severity and spread. The predicted outcomes (Step 4) enable precise diagnosis, distribution mapping and timely management decisions such as health assessment, optimized spraying and resource allocation, making UAV RS a powerful tool for pest and disease control.

Yield Prediction in Field Crops Through Satellite and Remote Sensing

Agriculture remains vital for global food security, especially in countries with large populations and limited arable land. With rising demand for food driven by population growth, accurate crop yield prediction has become essential for planning and resource management. Traditional survey-based methods are time-consuming and often imprecise, whereas satellite and remote sensing technologies provide real-time, large-scale monitoring of crop conditions. By analysing parameters such as vegetation indices, soil moisture, temperature and canopy reflectance, remote sensing enables early detection of stress factors and reliable yield forecasting. This not only supports farmers in optimizing irrigation, fertilizer use and cultivation practices but also assists policymakers in making informed decisions on food imports, exports and overall agricultural planning.

Crop yield prediction has traditionally been carried out using statistical regression models that integrate inputs such as remote sensing (RS) data, weather conditions, soil properties, genetic traits and management practices. Over time, classical machine learning methods including Support Vector Regression (SVR), Partial Least Squares Regression (PLSR), Random Forests (RF) and Boosted Regression Trees (BRT) have been widely applied for estimating grain yield and biomass. Although these approaches improved accuracy compared to simple regression, they face challenges in generalizing beyond the training domain, handling multi-modal time-series inputs and distinguishing between categorical factors like genetics and dynamic variables such as environmental conditions or farm management practices (Figure 4).

Recent advances in deep learning have significantly enhanced yield prediction, particularly at larger spatial scales. Frameworks such as Long Short-Term Memory (LSTM) networks and other neural architectures now enable effective integration of RS time-series data, improving prediction across regions and seasons. UAV-based RS has been successfully applied for plot-level yield forecasting in crops like sorghum and maize, while satellite products such as MODIS have supported county-level predictions. Furthermore, transfer learning approaches are being explored to expand model applicability across diverse geographies and growing periods. Despite this progress, future research must focus on combining multiple RS modalities and improving model interpretability to support more reliable and actionable agricultural decision-making.

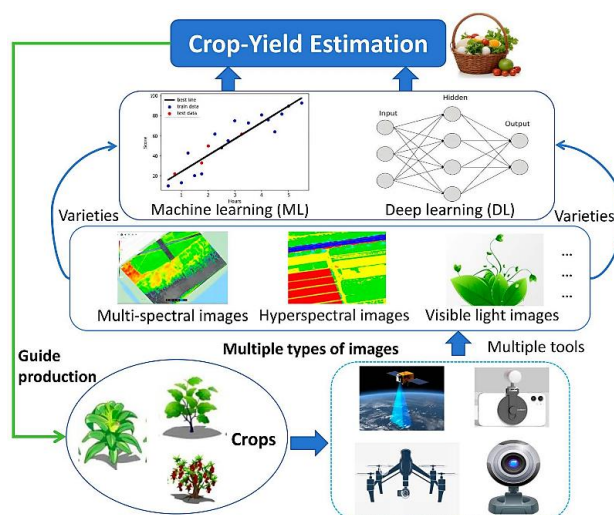


Figure 4: Integration of ML, DL and imaging tools for crop yield estimation

Satellites

A satellite is an artificial object placed into orbit around Earth or another celestial body for purposes such as communication, navigation, weather forecasting, Earth observation and scientific research. Satellites play a crucial role in remote sensing, as they capture data on land, water, atmosphere and vegetation, enabling large-scale monitoring and analysis.

Types of Satellites

1. Geostationary Satellites

Orbit at an altitude of ~35,786 km above the equator. Match the Earth's rotation, appearing fixed over one location. Provide continuous, real-time coverage of the same region. Widely used in weather monitoring, telecommunications and broadcasting.

2. Polar-Orbiting Satellites

Orbit at lower altitudes (~700–1,000 km) passing close to Earth's poles. Cover the entire Earth in multiple passes as the planet rotates beneath them. Provide high-resolution data suitable for **Earth observation, environmental monitoring, and climate studies. Often sun-synchronous, meaning they cross the equator at the same local solar time, ensuring consistent lighting conditions for imagery.

Two main types of strategies used in yield prediction

1. The first strategy incorporates satellite RS data into (existing or advanced) agro meteorological or plant-physiological models.
2. The second type of general strategy is based on direct mathematical relationships between satellite RS data and crop yields.

Challenges for RS based yield prediction

- Often localized & non-transferable.
- Mixed signals (crop/ non crop) and availability of within season crop type masks.
- Scaling up/down models (field level- admin level-national).

- Clouds (for optical systems).
- Temporal and spatial resolution (for complex cropping systems).
- Availability of in situ training/validation data.
- Timing of running model for national scale forecasting.
- Capturing impacts of events that affect yields but not biomass (i.e. late frosts).
- Dependency on availability of planted/ harvest area information.

Remote sensing indices and satellite imagery are efficient tools in predicting yield of rice, wheat, corn etc. Actual yields of crops were well correlated with predicted yields using remote sensing and satellites. Integration of RS data along with crop simulation models are found to be accurate in predicting the yield of field crops.

High-Throughput Phenotyping and Yield Prediction Using Remote Sensing

High-throughput phenotyping refers to the rapid, large-scale measurement of plant traits over time, using technologies like UAVs with advanced sensors, to monitor growth, health and performance. In a recent maize breeding experiment, researchers integrated multi-modal remote sensing (RS) data including hyper spectral imagery, LiDAR point clouds and environmental/ weather info with deep learning to predict end-of-season grain yield with high accuracy (Aviles Toledo *et al.*, 2024).

Key Components and Methods

1. Sensors & Data Collection:

UAV flights gathered hyper spectral data (400-1000 nm, ~270 spectral bands), LiDAR for structural traits (height, canopy cover, volume) and RGB imagery, along with ground truth yield data. Data were captured weekly across critical growth stages throughout the season.

2. Feature Extraction & Selection:

From hyper spectral data: vegetation indices, derivative/ integral features and spectral bands were selected. From LiDAR: canopy height percentiles, volume, cover, etc. Feature selection used methods like DeepSHAP to reduce dimensionality and focus on meaningful predictors.

3. Modeling Architecture:

They tested several deep learning architectures:

1. Vanilla stacked LSTM (long-short term memory) using early fusion (concatenated data inputs),
2. Stacked LSTM with temporal attention mechanism to highlight which time steps are most informative,
3. Multi-modal network with separate processing of each RS modality and then fusion.

Attention mechanisms play a crucial role: they allow the model to assign weights to different time steps and sensor sources, helping identify which growth stages contribute most to yield

prediction, increasing interpretability. For example, LiDAR features were more important in early growth, while hyper spectral features peaked in relevance during grain filling.

Results and Insights

Prediction Accuracy:

Using combined (multi-modal + attention) models achieved R^2 (coefficient of determination) of $\sim 0.82-0.96$ and lower RMSEs compared to simpler models. The best performance came when using full season RS data with late fusion multimodal architecture.

Temporal importance:

The model's attention weights consistently aligned with known physiological stages of maize e.g., emergence, vegetative growth, flowering/reproductive period and grain filling. This confirms that RS data can both predict yield and reflect biological processes.

Data efficiency:

Some scenarios using only subsets of the full season (e.g. mid-season data) gave fairly close accuracies, though full season inputs were best. This suggests potential for reducing data collection burden by targeting key growth stages.

Implications for Phenotyping & Crop Yield Prediction

- High-throughput phenotyping with RS & AI allows early selection of promising hybrids/varieties in plant breeding, accelerating breeding cycles.
- Multi-modal RS (spectral + structural + environmental) gives more reliable predictions than single modality.
- Attention-based deep learning models add interpretability, enabling understanding of when and which traits or sensor data matter most.
- For operational use, focusing RS data collection on key growth periods could reduce costs while retaining strong prediction accuracy.

Big Data Analytics and Artificial Intelligence Methods for Decision Making in Agriculture Data

The quantities, characters or symbols on which operations are performed by a computer, which may be stored and transmitted in the form of electrical signals and recorded on magnetic, optical or mechanical recording media.

Big Data: What it is and why it matters?

Large, hard to manage volumes, both structured and unstructured and growing exponentially with time.

Types of Big Data

1. **Structured Data:** Any data that can be stored, accessed and processed in the form of fixed format is termed as a 'structured' data.

2. **Unstructured Data:** Any data with unknown form or the structure is classified as unstructured data. A typical example of unstructured data is a heterogeneous data source containing a combination of simple text files, images, videos etc.
3. **Semi-Structured Data:** Semi-structured data can contain both the forms of data.

Types of Big Data in Agriculture: Geo-Spatial data, Meta data and Telematics data.

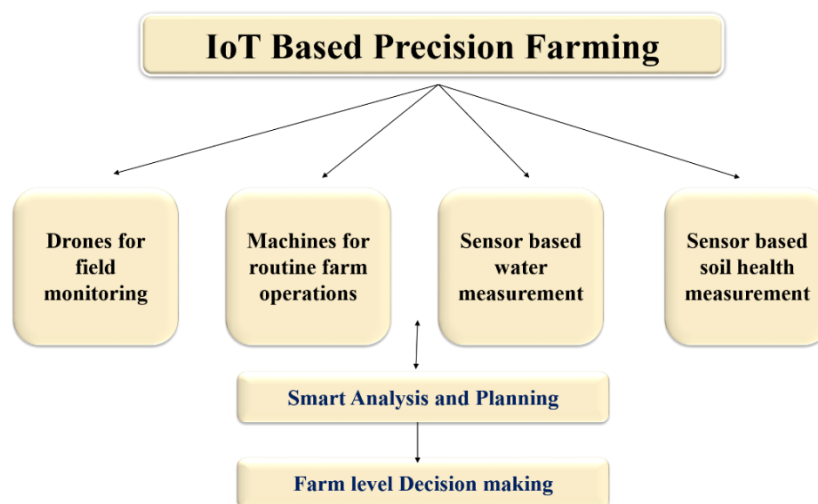
Big Data Analytics

Big data analytics involve computations with predetermined algorithms to solve certain problems. Recently, artificial intelligence-based methods are widely used in various applications in agriculture.

Data Acquisition

Acquisition of quality, real-time and diverse data (weather, soils and crops) is paramount in the use of AI in agriculture. The various means to acquire the data are:

1. **Field data collection:** Traditionally, data are collected from research experiments and farmers' fields by researchers, field personnel.
2. **Sensors:** Various types of sensors which could be fitted to farm equipment such as tractors, hand held, field installed etc. are available that aid in data collection.
3. **Multispectral data from satellites and unmanned aerial vehicles:** Remote sensing has been widely used to capture land features which are used in various sectors.
4. **Internet of Things (IoT) based data collection.**



IoT and Agriculture

- One of the more powerful developments in this regard is NASA's Gravity Recovery and Climate Experiment (GRACE) mission.
- GRACE, launched in 2002, uses two spacecraft to map variations in the Earth's gravity field. The gravitational research is, in part, collecting relevant agricultural data on factors such as groundwater availability and stress as they relate to global agricultural production areas.

- Maps developed using the GRACE data are able to identify the difference between climate-related drought conditions and the depletion of aquifers through groundwater extraction that exceeds recharge.

Artificial Intelligence

Raw data requires analysis for it to have value. Analytics involving artificial intelligence (AI) is required for data mining. AI is a relatively new technical discipline adopted by agricultural research and corporations that assesses the expansion of human intelligence by developing theories, methods, algorithms and applications.

Given the size and complexity of big data which cannot be handled by traditional data-processing systems, AI through machine learning algorithms is designed to extract meaningful value from big data.



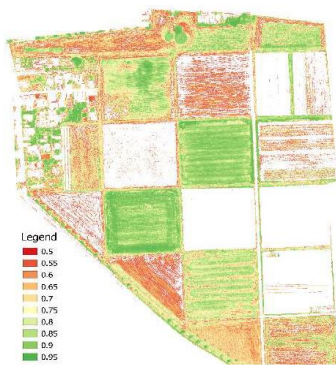
Study site at Muramatsu experimental station



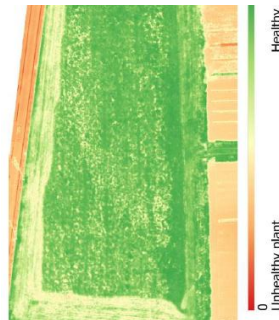
Example of mission planning software display



Example of five-band map



NDVI layer



NDVI layer of cedar seedlings plot



NDRE layer, chlorophyll index value

Representation of Drones for Field Monitoring (Boiarskii & Hasegawa, 2019)

Artificial Intelligence (AI) is emerging as a transformative force in agriculture by enabling data-driven and precise farming practices. Through tools such as drones, sensors and computer vision, AI supports real-time crop monitoring, soil health assessment and predictive analytics for weather, yield and input management. These technologies allow farmers to apply water, fertilizers and pesticides only when and where needed, reducing resource wastage and

environmental stress. AI-driven automation in weed and pest control, coupled with decision-support systems, further enhances efficiency and sustainability.

Evidence from field applications underscores its impact. AI-based pilot projects in India, such as predictive sowing advisories and smart irrigation systems, have improved yields by 10-30% while reducing water consumption by nearly one-third. By combining productivity gains with resource conservation, AI addresses critical challenges of labor shortages, climate variability and input misuse. Thus, AI in agriculture not only increases profitability for farmers but also contributes to long-term food security and sustainable farming systems.

Machine Learning

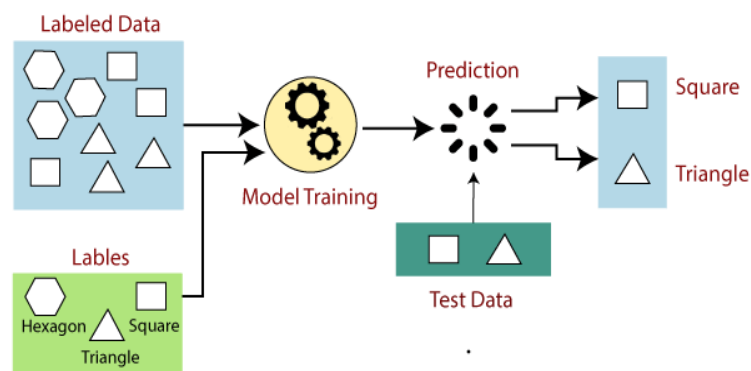
Machine learning is a type of artificial intelligence that provides computers with the ability to learn without being explicitly programmed. They are data driven or phenomenon-based approaches.

Types of Machine Learning

- Supervised
- Unsupervised

These basically are a description of ways in which you can let machines or algorithms loose on a data set. The machines would also be expected to learn something useful out of the process.

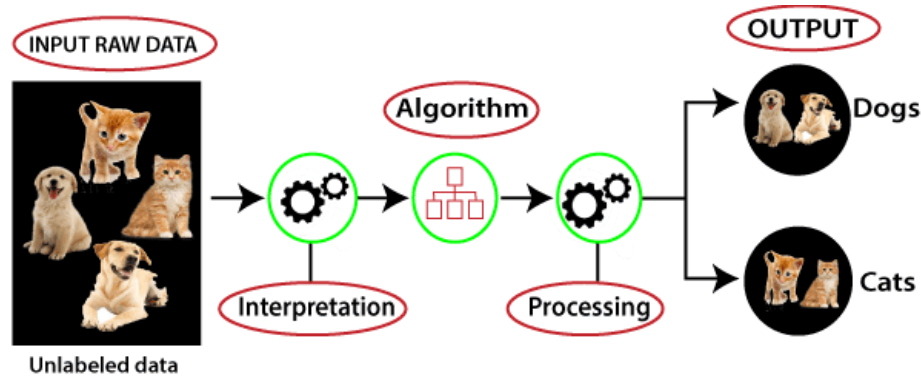
Supervised Learning



- Supervised learning is the types of machine learning in which machines are trained using well “labelled” training data, and on basis of that data, machines predict the output. The labelled data means some input data is already tagged with the correct output.
- In supervised learning, the training data provided to the machines work as the supervisor that teaches the machines to predict the output correctly.
- Supervised learning is a process of providing input data as well as correct output data to the machine learning model.
- The aim of a supervised learning algorithm is to find a mapping function to map the input variable (x) with the output variable (y).

Unsupervised Learning

- Unsupervised learning is a machine learning technique in which models are not supervised using training dataset.
- Instead, models itself find the hidden patterns and insights from the given data.
- It can be compared to learning which takes place in the human brain while learning new things.
- The goal of unsupervised learning is to find the underlying structure of dataset, group that data according to similarities and represent that dataset in a compressed format.



Deep Learning

- Deep learning is a machine learning technique that teaches computers to do what comes naturally to humans.
- It uses machine learning the way a human brain filters information by using artificial neural networks which mimic human neural networks.
- It learns from examples and helps the computer model to filter large data sets to classify and predict information
- Deep Learning is a prime technology behind the technology such as virtual assistants, facial recognition, driverless cars, etc.
- The working of deep learning involves training the data and learning from the experiences.
- The learning procedure is called 'Deep', as with every passing minute the neural networks rapidly discover the new levels of data. Each time data is trained, it focuses on enhancing the performance.

Convolutional Neural Networks

Deep Learning has been constructed and perfected with time, primarily over one particular algorithm - a Convolutional Neural Network (CNN). Convolutional Neural Network (CNN) is the heart of Deep learning. Convolutional neural networks are composed of multiple layers of artificial neurons.

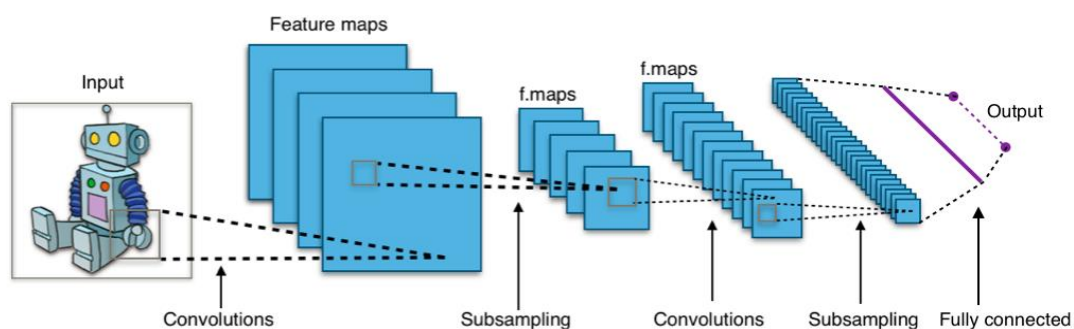


Figure 5: Big-data analytics platform for generating farm advisories

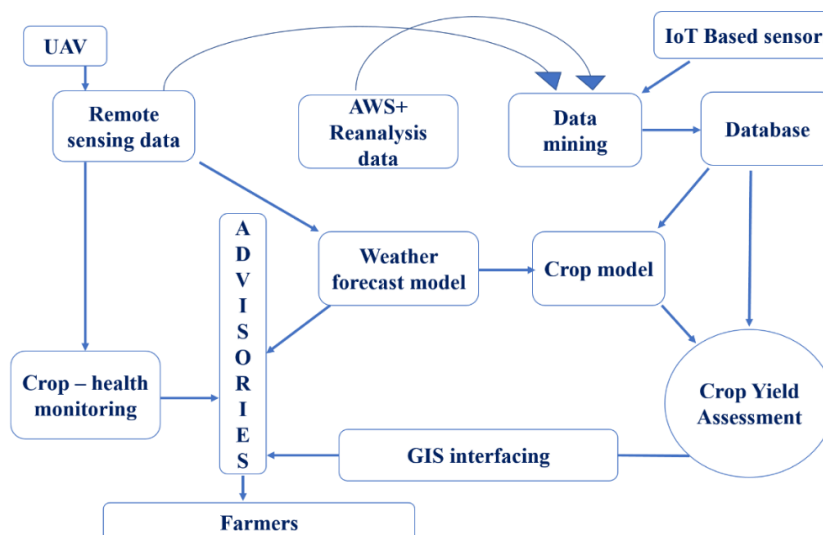


Figure 6: Framework for smart crop monitoring and yield assessment

Autonomous agriculture is a way forward in Indian agriculture. Big data and AI will play a major role in the new paradigm agronomic research and farm advisories. The AI models require continuous and reliable data flow, which is a serious lacuna. An interactive platform consisting of 3 segments of people i.e., developers and engineers, researchers and subject matter specialists need to be developed to address the needs of the ultimate beneficiary.

Building strong public-NGO-private partnerships could help not only to strap up the strengths but also address the weaknesses for ultimate benefit of the farming community. Digital farming or AI-driven Agri-tech projects are to be supported in the country through sustained investment in this sector to bring the technology at marginal land-holding level.

Conclusion:

The integration of UAVs, remote sensing, ICTs, big data analytics and machine learning represents a paradigm shift in modern crop management, enabling precise, timely and site-specific decision-making for sustainable agriculture. UAV-based high-resolution sensing, coupled with satellite imagery and advanced AI models, allows accurate monitoring of crop health, soil conditions, water stress, pest and disease outbreaks and yield prediction. By transforming large, complex datasets into actionable insights, these technologies optimize resource use, enhance productivity and reduce environmental impacts, thereby supporting

climate-resilient and sustainable food systems. Moving forward, scaling these innovations through robust data infrastructures, farmer-friendly platforms and strong public-private partnerships will be crucial to ensure accessibility and adoption, particularly for smallholder farmers, to achieve global food security goals.

References

1. Aierken, N., Yang, B., Li, Y., Jiang, P., Pan, G., & Li, S. (2024). A review of unmanned aerial vehicle based remote sensing and machine learning for cotton crop growth monitoring. *Computers and Electronics in Agriculture*, 227, 109601. <https://doi.org/10.1016/j.compag.2024.109601>
2. Aviles Toledo, C., Crawford, M. M., & Tuinstra, M. R. (2024). Integrating multi-modal remote sensing, deep learning, and attention mechanisms for yield prediction in plant breeding experiments. *Frontiers in Plant Science*, 15, 1408047. <https://doi.org/10.3389/fpls.2024.1408047>
3. Boiarskii, B., & Hasegawa, H. (2019). Comparison of NDVI and NDRE indices to detect differences in vegetation and chlorophyll content. *Journal of Mechanics of Continua and Mathematical Sciences, Special Issue* (4), 20–29. <https://doi.org/10.26782/jmcms.spl.4/2019.11.00003>
4. Dragonfly Aerospace. (2022, May 13). *7 applications of remote sensing in agriculture*. Dragonfly Aerospace. <https://dragonflyaerospace.com/remote-sensing-in-agriculture-what-are-some-applications>
5. Huang, J., Wang, X., Li, X., Tian, H., & Pan, Z. (2013). Remotely sensed rice yield prediction using multi-temporal NDVI data derived from NOAA's-AVHRR. *PLoS ONE*, 8(8), e70816. <https://doi.org/10.1371/journal.pone.0070816>
6. Ministry of Electronics and Information Technology. (2020). *Current status of ICT in India*. Government of India.
7. Peace, K., Khwantri, S., Jetsada, P., Cumnueng, W., & Wongphati, M. (2019). Study of field capacity and variables of UAV operation time during spraying hormone fertilizer in sugarcane field. *IOP Conference Series: Earth and Environmental Science*, 301, 012015. <https://doi.org/10.1088/1755-1315/301/1/012015>
8. Yallappa, D. (2018). *Development and evaluation of drone mounted sprayer for selected field crops* (Master's thesis, University of Agricultural Sciences, Raichur, Karnataka, India).
9. Zhu, H., Lin, C., Liu, G., Wang, D., Qin, S., Li, A., Xu, J.-L., & He, Y. (2024). Intelligent agriculture: Deep learning in UAV-based remote sensing imagery for crop diseases and pests detection. *Frontiers in Plant Science*, 15, 1435016. <https://doi.org/10.3389/fpls.2024.1435016>

THE SCIENCE SHIFT

Manasa C*¹ and Madhusudhan H S²

¹Department of Chemistry,

²Department of Computer Science and Engineering,

Vidyavardhaka College of Engineering, Mysuru

*Corresponding author E-mail: manasac@vvce.ac.in

Abstract:

This chapter examines the evolving relationship between science and society through the lens of next-generation research paradigms. It explores the shift from siloed disciplinary approaches to interdisciplinary, open, and participatory models of scientific inquiry. Key trends such as digital transformation, open science, citizen engagement, and convergence science are analyzed in the context of addressing complex societal challenges like climate change, pandemics, and artificial intelligence. Ethical concerns, public trust, and inclusive governance are emphasized as central to responsible research in the 21st century. By integrating diverse perspectives, promoting transparency, and aligning scientific progress with societal needs, next-generation research offers a more democratic and impactful model for science policy and practice.

Keywords: Next-Generation Research, Science and Society, Interdisciplinary Research, Open Science, Citizen Science, Public Trust, Responsible Research and Innovation, Societal Challenges, Science Policy.

Introduction:

Science has long been a cornerstone of societal development, driving innovation, improving public health, and transforming economies. However, in the 21st century, the relationship between science and society is undergoing a profound evolution. Next-generation research, characterized by interdisciplinarity, open science practices, digital technologies, and increased public engagement, is reshaping how scientific inquiry is conducted and applied. This chapter explores the dynamic interplay between science and society, focusing on how emerging research paradigms are responding to global challenges while demanding greater accountability, inclusivity, and ethical responsibility.

The Shifting Landscape of Scientific Research

Traditional models of scientific research were often siloed within disciplines, guided by internal priorities rather than external societal needs. In contrast, next-generation research is inherently problem-oriented and mission-driven. It tackles complex, "wicked" problems such as climate change, pandemics, and technological disruption—issues that do not fall neatly within disciplinary boundaries (Rittel & Webber, 1973). As such, interdisciplinary and transdisciplinary approaches are now becoming essential.

For instance, addressing global health crises like COVID-19 required not just virologists and epidemiologists, but also data scientists, economists, behavioral psychologists, and policy experts working in tandem (Van Bavel *et al.*, 2020). This convergence of disciplines has led to the emergence of what some scholars call "convergence science," which integrates knowledge from life sciences, physical sciences, engineering, and the social sciences to produce holistic solutions (Sharp *et al.*, 2011).

Furthermore, science today is no longer confined to laboratories or academic institutions. The advent of citizen science, crowdsourced research, and participatory action research has enabled the public to take part in the scientific process. This democratization of science enhances transparency, increases trust, and often leads to more relevant outcomes (Bonney *et al.*, 2016).

Digital Transformation and Open Science

Digital technologies are revolutionizing scientific workflows, from data collection and simulation to dissemination and replication. Big data, artificial intelligence, and machine learning allow researchers to process complex datasets at unprecedented speeds, enabling discoveries that were previously inconceivable. For example, machine learning algorithms are now being used to predict protein folding structures (Senior *et al.*, 2020), a problem that puzzled scientists for decades.

One of the most transformative developments is the rise of open science. Open access publishing, open data repositories, and collaborative platforms like GitHub and preprint servers have broken down the barriers to knowledge sharing. This accelerates scientific progress, reduces duplication, and fosters global collaboration, especially in low- and middle-income countries where access to academic journals is often limited (Tennant *et al.*, 2016).

However, open science also brings new challenges, including concerns about data privacy, intellectual property rights, and the spread of misinformation through non-peer-reviewed channels. Balancing openness with scientific integrity requires robust policies and ethical frameworks.

Ethical and Social Implications

As scientific capabilities expand, so too do the ethical questions they raise. Gene editing technologies like CRISPR-Cas9 have immense potential for treating genetic diseases, but they also raise profound moral concerns about human enhancement and ecological impact (Jinek *et al.*, 2012). Similarly, the use of AI in surveillance, employment, and criminal justice systems poses risks of bias, discrimination, and loss of human agency.

Next-generation research must therefore be embedded within strong ethical guardrails and engage diverse stakeholders, including marginalized communities, in its development and oversight. Concepts such as Responsible Research and Innovation (RRI) emphasize the need for

anticipatory governance, public dialogue, and inclusion in shaping science policy and practice (Owen *et al.*, 2012).

Science Communication and Public Trust

The COVID-19 pandemic laid bare the critical role of science communication in shaping public behavior and policy. Conflicting messages, misinformation, and politicization of science led to widespread confusion and skepticism. Building public trust in science requires more than just disseminating facts it demands transparency, empathy, and cultural sensitivity.

Next-generation science communication must be two-way, enabling dialogue rather than monologue. Researchers are increasingly engaging with communities through social media, podcasts, and storytelling formats, making science more accessible and relatable (Scheufele, 2013). Moreover, training scientists in communication skills is becoming a vital component of research education.

Conclusion:

Next-generation research is not merely a scientific revolution, it is a societal transformation. As science becomes more integrated with societal values, inclusive practices, and global challenges, the boundaries between researcher and citizen, lab and community, and data and decision-making are increasingly blurred. Ensuring that this transformation benefits all requires a renewed commitment to ethical responsibility, public engagement, and interdisciplinary collaboration.

Society must not only support science through funding and education but also shape its direction through democratic participation. In doing so, we can build a scientific enterprise that is not only innovative but also equitable, inclusive, and responsive to the needs of a rapidly changing world.

References:

1. Bonney, R., Phillips, T. B., Ballard, H. L., & Enck, J. W. (2016). *Can citizen science enhance public understanding of science?*. *Public Understanding of Science*, 25(1), 2–16. <https://doi.org/10.1177/0963662515607406>
2. Jinek, M., Chylinski, K., Fonfara, I., Hauer, M., Doudna, J. A., & Charpentier, E. (2012). *A programmable dual-RNA-guided DNA endonuclease in adaptive bacterial immunity*. *Science*, 337(6096), 816–821. <https://doi.org/10.1126/science.1225829>
3. Owen, R., Macnaghten, P., & Stilgoe, J. (2012). *Responsible research and innovation: From science in society to science for society, with society*. *Science and Public Policy*, 39(6), 751–760. <https://doi.org/10.1093/scipol/scs093>
4. Rittel, H. W. J., & Webber, M. M. (1973). *Dilemmas in a general theory of planning*. *Policy Sciences*, 4(2), 155–169. <https://doi.org/10.1007/BF01405730>
5. Scheufele, D. A. (2013). *Communicating science in social settings*. *Proceedings of the National Academy of Sciences*, 110(Supplement_3), 14040–14047. <https://doi.org/10.1073/pnas.1213275110>

6. Senior, A. W., Evans, R., Jumper, J., Kirkpatrick, J., Sifre, L., Green, T., ... & Hassabis, D. (2020). *Improved protein structure prediction using potentials from deep learning*. *Nature*, 577(7792), 706–710. <https://doi.org/10.1038/s41586-019-1923-7>
7. Sharp, P. A., Langer, R., & Lippard, S. J. (2011). *Convergence: The future of health*. *Science*, 333(6042), 527. <https://doi.org/10.1126/science.1207464>
8. Tennant, J. P., Waldner, F., Jacques, D. C., Masuzzo, P., Collister, L. B., & Hartgerink, C. H. J. (2016). *The academic, economic and societal impacts of Open Access: An evidence-based review*. *F1000Research*, 5, 632. <https://doi.org/10.12688/f1000research.8460.3>
9. Van Bavel, J. J., Baicker, K., Boggio, P. S., Capraro, V., Cichocka, A., Cikara, M., ... & Willer, R. (2020). *Using social and behavioural science to support COVID-19 pandemic response*. *Nature Human Behaviour*, 4(5), 460–471. <https://doi.org/10.1038/s41562-020-0884-z>

Science, Technology and Society: Next Gen Research Volume I Volume I

(ISBN: 978-81-993182-2-9)

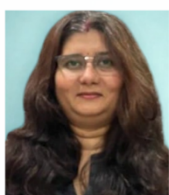
About Editors



Dr. Manoj P. Mahajan is an Assistant Professor in the Department of Physics at V. G. Vaze College of Arts, Science & Commerce (Autonomous), Mulund, Mumbai, with 15 years of teaching experience. He earned his Ph.D. in Nanotechnology from the University of Mumbai in 2019, specializing in Nanotechnology and Material Science. His research contributions include the publication of five research papers in reputed international journals and the granting of one patent in his name. He has actively shared his work by presenting papers at 30 international and national conferences. In addition to his research, Dr. Mahajan has contributed to academic resources by authoring two books designed for science and engineering undergraduates. His academic journey reflects a strong commitment to both innovative research and quality teaching in physics.



Mr. Anand Kumar Mishra is a research scholar currently pursuing his Ph.D. at Deen Dayal Upadhyay Gorakhpur University, Gorakhpur, India, focusing on catalytic treatment for the removal of environmentally harmful metals from industrial wastewater. He completed his M.Sc. in Chemistry in 2021 from M.L.K. P.G. College, Balrampur (affiliated with Siddhartha University, Uttar Pradesh) and earned a B.Ed. degree in 2023, reflecting his dual commitment to chemistry and education. Demonstrating his growing research potential, he has contributed four book chapters published by Bhumi Publishing, India, and also served as an editor for one of its books. His academic interests center on catalysis and its diverse applications in chemical sciences. With a strong focus on advancing his research skills, Mr. Mishra aims to make meaningful contributions through quality publications and academic initiatives.



Dr. Preyoshi Bose, M.Sc., Ph.D. (BARC), is currently serving at Smt. Chandibai Himathmal Mansukhani College, Ulhasnagar – 421003, focusing on Physics Education. With a rich academic and professional background, she has held multiple roles including mentor teacher, DLLE work teacher, and presently serves as NSS Program Officer, fostering close engagement with students and learners. Her work emphasizes holistic student development, combining academic guidance with extracurricular mentorship. Through her varied roles, Dr. Bose has developed strong connections with students, guiding them in both academic pursuits and social responsibilities. Her commitment to education and mentorship reflects her dedication to nurturing well-rounded individuals, supporting their learning journey, and promoting active participation in community and educational initiatives.



Dr. Shikumar Verma is a dedicated scientist, researcher, and educator with extensive experience in the fields of science and research. He has contributed significantly to both academic teaching and innovative research, fostering a strong learning environment for students. His research interests span multiple areas of scientific inquiry, with several publications in reputed journals highlighting his commitment to advancing knowledge. Dr. Verma has actively participated in national and international conferences, presenting his work and collaborating with fellow researchers. In addition to his research, he is deeply involved in mentoring and guiding students, promoting critical thinking and practical understanding of scientific concepts. His professional journey reflects a balanced dedication to research excellence, quality teaching, and the overall development of the scientific community.



ISBN 978-81-993182-2-9



9 788199 318229