Perspectives on Multidisciplinary Research in Science and Technology:

Concepts and Statistical Approaches

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PREFACE

The pursuit of knowledge in the twenty-first century is defined by the convergence of diverse disciplines. Traditional boundaries between fields of science, engineering, mathematics, and technology are steadily dissolving, giving rise to a multidisciplinary approach that offers both depth and breadth in addressing contemporary challenges. This book, ***Perspectives on Multidisciplinary Research in Science and Technology: Concepts and Statistical Approaches***, reflects this dynamic evolution by bringing together research contributions that blend conceptual foundations with analytical and computational methods.

One of the central themes of this volume is the use of quantitative and statistical approaches to decode complex real-world problems. From analyzing economic patterns in the food and beverage sector to exploring algorithmic strategies for traffic and energy optimization, the chapters illustrate how data-driven insights can guide practical decision-making. Such statistical and computational perspectives not only enhance prediction and efficiency but also strengthen the link between theoretical research and societal applications.

At the same time, the book underscores the importance of mathematical frameworks and graph-theoretic explorations, which remain the backbone of computational sciences. Studies on domination numbers, solvability in combinatorial games, and chromatic properties of graphs highlight how abstract mathematical concepts continue to shape modern applications in cryptography, optimization, and network systems. These works

remind us that innovation is deeply rooted in rigorous conceptual foundations.

Another significant dimension of the book lies in its focus on emerging technologies such as Artificial Intelligence (AI) and metaheuristic algorithms. By demonstrating how machine learning can transform workforce performance prediction or how swarm intelligence methods like krill herd and flower pollination algorithms optimize energy dispatch, the book showcases the transformative power of intelligent systems. Such advances are not merely technical triumphs but also harbingers of sustainable solutions to pressing global concerns.

The book also ventures into biomedical research and computational drug discovery, reflecting the growing synergy between life sciences and computational modeling. Chapters dedicated to in silico multi-targeting of cancer pathways and structure-based drug design highlight how multidisciplinary collaboration can accelerate therapeutic innovation. These contributions bridge chemistry, biology, and informatics, exemplifying how science can directly contribute to improved healthcare outcomes.

Altogether, this collection of fourteen chapters serves as a testament to the integrative spirit of modern research. By uniting perspectives from statistics, mathematics, computer science, engineering, and life sciences, the book provides a platform for scholars, researchers, and practitioners to appreciate the interconnectedness of knowledge. It is our hope that the insights offered herein will not only advance academic inquiry but also inspire further multidisciplinary collaborations that address the challenges and opportunities of our rapidly evolving world. We

would like to extend our sincere thanks to our publisher, Scientific Research Reports, Chennai, India, for their dedicated efforts in preparing this book, which provides enriched content.

Wishes and Regards,

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Chapter 1

Time Series Analysis of Sales Prices in the Food and Beverage Sector in India

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Abstract

This study investigates the sales price trends of food and beverages in India using time series analysis techniques. The objective is to identify patterns, seasonal variations, and long-term trends to aid in understanding market behavior and forecasting future prices. The dataset, sourced from reliable governmental publications, covers multiple years and reflects the influence of economic, seasonal, and policy-driven factors on price fluctuations. Statistical tools such as trend analysis, seasonal decomposition, and ARIMA modelling are employed to evaluate the data and produce accurate forecasts. The ARIMA (2,1,2) model was selected based on statistical criteria, including the highest MAPE values, and demonstrated strong predictive performance The results reveal significant seasonal components and an upward trend in prices over the study period, with ARIMA providing robust short-term predictions. These findings can assist policymakers, industry stakeholders, and researchers in making informed decisions regarding price stabilization, supply chain planning, and market interventions in the food and beverage sector.

Keywords: *Time Series Analysis, Sales Price, Food and Beverages, ARIMA, Forecasting.*

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1. Introduction

In India sales price of food and Beverages recently acquires 32% of the country's total food market. Food and Beverages means raw, in whole or in part, used or intended for human consumption, including ice, water, spirits, wine, mixed drinks, beer, soft drinks, sodas, and other beverages. Food and beverage means a cooked or processed edible substance. Food and Beverage means any meal, snack or edible substance or drinkable liquid, including related services. Food and Beverage means all opened and unopened food and Beverages that are in use or in reserve storage for future use in connection with the operation of the golf course as part of the normal course of business. Food and Beverages industry is one of the largest industries in India. India ranks fifth in terms of Production, consumption and exports. The food and potables assiduity includes all companies involved in processing, packaging, and distributing raw food accoutrements. In addition to packaged foods, this also includes fresh, set foods and alcoholic and nonalcoholic potables. Any product meant for mortal consumption, away from medicinal, passes through the food and potables assiduity.

1.1. Food Industry-An Introduction

Food is an integral part of our lives. The food industry is a complex global network of diverse businesses that supply most of the food consumed by the world's population. Today's food industry is highly diversified, from small, traditional, labour-intensive, family-run businesses to large-scale, capital-intensive, highly mechanized industrial processes. Many food industries depend almost entirely on local agriculture, produce, or fisheries.

Finding a comprehensive method that covers all aspects of food

production and sale is difficult. The UK Food Standards Agency describes it as “the entire food industry from agriculture and food production, packaging and distribution to retail and food service”. The USDA Economic Research Service uses the term “food system” to describe the same thing. The U.S. food system is a complex network of farmers and related industries. These links include companies providing services to agribusiness, such as manufacturers of agricultural equipment and chemicals, as well as transportation and financial services providers. It includes

- Agriculture: Growing crops, livestock and seafood.
- Agricultural economy.
- Manufacturing: pesticides, agricultural construction, agricultural machinery and materials, seeds, etc.
- Wholesale and food distribution: logistics, transportation, warehousing Foodservice (which includes catering) Grocery, farmers' markets, public markets and other retailing.
- Regulation: local, regional, national, and international rules and regulations for food production and sale, including food quality, food security, food safety, marketing/advertising, and industry lobbying activities
- Education: academic, consultancy, vocational.
- Research and development: food science, food microbiology, food technology, food chemistry, and food engineering Financial services: credit, insurance.
- Areas of study such as food selection, food preservation and food theology and food storage are directly related to quality

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and quality maintenance and overlap with many of the above processes.

- Outside the realm of the modern food industry, only subsistence farmers, subsistence farmer and hunter-gatherers can be considered.

The food industry is a major and important of all countries. It is one of 17 nationally important sectors of the US economy. It plays an important role in public health, food safety, food security, social development and nutrition. Product quality, health and hygiene issues are the top issues in the food industry. The double pyramid that provides an effective model for promoting sustainable food for health and the environment.

The food industry encompasses a variety of activities including food supply, production, harvesting, processing, packaging, transportation, distribution, consumption and disposal. The development of the food industry began in the early 1900's. The most profitable segments of the food industry are meat processing, vegetable and fruit processing, confectionery, dairy products, sausages, winemaking and bakeries. The food industry is dominated by multinational corporations such as Kraft's Foods, Cadbury, Heinz, Nestlé, Food World, DuPont, McDonalds, Pizza Hut and KFC.

2. Methodology

This chapter explains the methods and procedure followed in this study. Without proper methodology, results are likely to be undependable and defective.

2.1 Aim

Aim of this project is "Time Series Analysis of Sales Price of Food

and Beverages in India".

2.2 Statistical Tool

Time Series Analysis - Autoregressive Integrated Moving Average (ARIMA).

2.3 Objectives

The objectives of this project are

- To analyze Sales Price data for Food and Beverages in India.
- To predict the future Sales Price of Food and Beverages in India.
- To forecast Sales Price value for Food and Beverages in India.

2.4 Data Collection

Statistical data may be classified as primary and secondary. Primary data are those which are collected for the first time and they are original in character. If an individual or an office collects the data to study a particular problem, the data are the raw materials of the enquiry. They are primary data collected by the investigator himself to study any particular problem. Secondary data are those which are already collected by someone for some purpose and are available for the present study. For instance, the collected during census operations are primary data to department of census and the same data, if used by a researcher worker for some study, are secondary data.

Secondary data are those data which have been already collected and analysed by some earlier agency for its own use; and later the same data are used by a different agency. A secondary source is a publication, reporting the data with have been gathered by other

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authorities and for which others are responsible.

2.5 Limitations

Some major disadvantages of ARIMA forecasting are: first, some of the traditional model identification techniques for identifying the correct model from the class of possible models are difficult to understand and usually computationally

In this study, a four-step ARIMA model was used, consisting of identification, estimation, diagnostic checking, and forecasting. Model parameters were considered to fit the ARIMA models.

AR process of order (p) is, $Y_t = \mu + \phi_1 Y_{t-1} + \phi_2 Y_{t-2} + ... + \phi_p Y_{t-p} + \varepsilon_t$;

MA process of order (q) is, $Y_t = \mu - \theta_1 \varepsilon_{t-1} - \theta_2 \varepsilon_{t-2} - .... - \theta_q \varepsilon_{t-q} + \varepsilon_t$; and

ARIMA process of order (p, d, q) is,

$$Y_t = \phi_1 Y_{t-1} + \phi_2 Y_{t-2} + ... + \phi_p Y_{t-p} + \mu - \theta_1 \varepsilon_{t-1} - \theta_2 \varepsilon_{t-2} - .... - \theta_q \varepsilon_{t-q} + \varepsilon_t$$

ε_t's - independently and normally distributed with zero mean and constant variance σ^2 for t = 1,2,..., n; d - the fraction differenced while interpreting AR and MA, and ϕ's and θ's - coefficients to be valued.

Trend Fitting: The Box-Ljung Q statistics was used to convert the non-stationary data into stationarity data and also to validate the adequacy for the residuals. For evaluating the adequacy of AR, MA and ARIMA processes, a range of reliability statistics like R squared, Stationary R squared, RMSE, MAPE and BIC were applied. The reliability statistics viz. RMSE, MAPE, BIC and Q statistics were computed as below:

$$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \widehat{Y}_i\right)^2\right]^{1/2} ;$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{Y_i - \hat{Y}_i}{Y_i}\right| \text{ and}$$

$$BIC(p,q) = \ln v^*(p,q) + (p+q)\left[\frac{\ln(n)}{n}\right]$$

where p and q - order of AR and MA processes; n - number of observations; and v* - approximate of white noise variance σ^2.

$$Q = \frac{n(n+2)\sum_{i=1}^{k} rk^2}{(n-k)}$$

where n - number of residuals and rk - residuals autocorrelation at lag k.

2.6. Source of Data

In this study, sales price of food and beverage data were collected from Department of Food and Public Distribution, Government of India for the period 1992 to 2015 and applied for various ARIMA models. The sales price of food and beverage in India from 1992-2015 is represented in the Table 4.1.

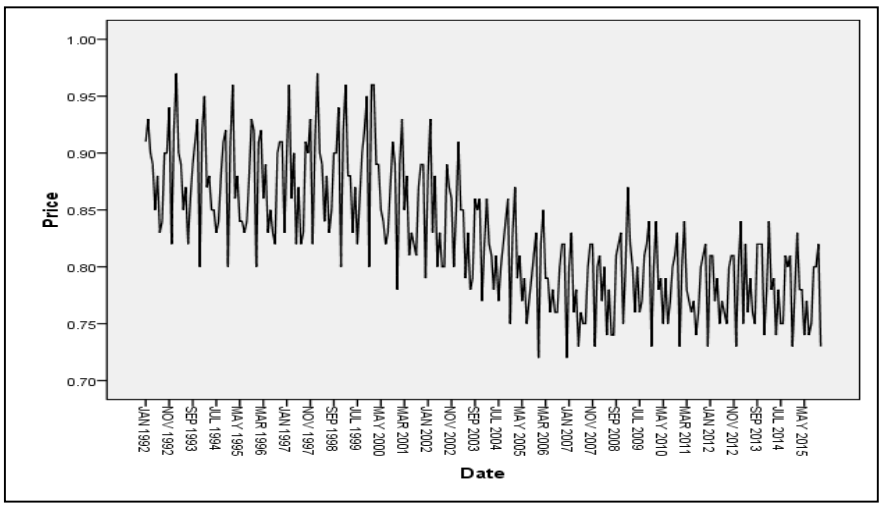

Figure 1 - Actual Time plot of food and beverage sales price

Figure 1 depicts that the data were used for time plot of Food and beverage sales price, the time plot is non-stationary.

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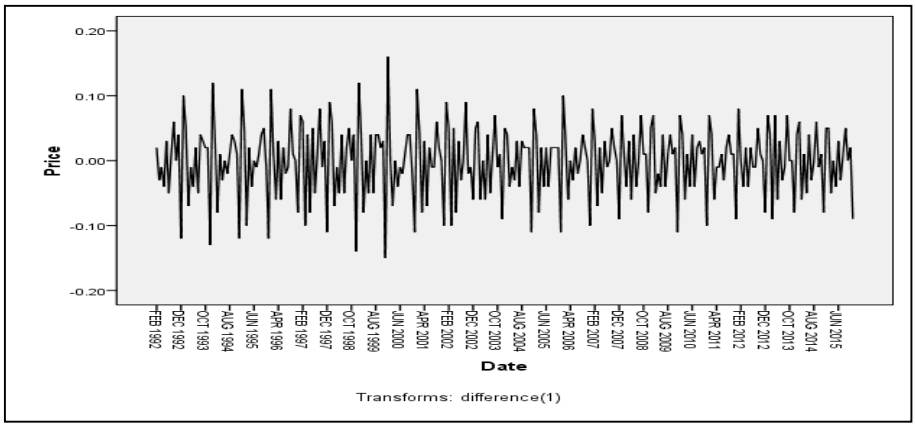

Figure 2 - Time plot for sales price of food and beverage with d=1

Figure 2 reveals the non-stationarity in mean was corrected through first differencing of the data. The newly constructed variable Y_t could now be examined for Stationarity. Since, Y_t was stationary in mean, the next step was to identify the values of p and q. For this, the ACF and PACF of various orders of Y_t were computed.

3. Conclusion

ARIMA: In this analysis, sequence plot shows the production data of food and beverage in India from the year 1992-2015. Hence, we differentiate data to make it non-stationary to stationary. Here in this step, we start with the initial processing of the data to make it stationary and then we choose possible values of p and q which we can of course adjust as model fitting progresses. The test is carried out on the SPSS software. For food and beverages, with the value of difference (d=1), the model which has the minimum MAPE was selected. The value of MAPE of the chosen ARIMA was **3.795**. Hence the most suitable model for the production of food and beverages was ARIMA (2, 1, 2) as this model has the lowest MAPE value. The forecast is obtained from ARIMA (2,1,2) because it has a low MAPE value compared to other models. We can clearly see that the model chosen can be used for modeling and forecasting the future demand, but

each time we need to feed the historical data with the new data to enrich it in order to improve the new model and forecasting.

ARIMA-Intervention: For sales price of food and beverages data with the value of difference (d=1), we have estimated the fit statistics values of the fitted model ARIMA-Intervention (2,1,2) contains Stationary R-squared, RMSE, MAPE, MaxPE, MaxAE and Normalised BIC. We have estimated the parameters value of the ARIMA-Intervention model. The forecast is obtained from ARIMA-Intervention (2,1,2) are given in the table: We compared the MAPE value of ARIMA and ARIMA-Intervention model to conclude the appropriate model for forecasting.

Table 1: MAPE value of ARIMA and ARIMA-Intervention

MODEL	MAPE VALUE
ARIMA	3.795
ARIMA-Intervention	**0.954**

From table 1 it can be inferred that the accuracy of forecasting of ARIMA- intervention model is better than ARIMA model. ARIMA-Intervention model has the low MAPE value compared to the ARIMA model, hence it is a better model to forecast with low percentage error. The results from the ARIMA intervention model showed that prices would not remain stable throughout the year. From the temporal data, it can be found that forecasted prices would decrease to Rs. 0.727 (in million dollar) in December 2024 from Rs. 0.764 (in million dollar) in January 2016 in India. The results will be useful to the farming community and other relevant stakeholders. Using time series data from January 1992 to December 2015 on Sales Prices of food and Beverage, this study provides an evidence on future Sales

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prices of Food and Beverage in the country, which can be considered for future policy making and formulating strategies for augmenting and sustaining prices in India.

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Chapter 2

Arithmetic Concepts in Kanakkatikaram through Translation

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Abstract

The Kanakkatikaram reveals an extensive legacy of Indigenous Mathematical knowledge, demonstrating the profound integration of Arithmetic into the social and economic fabric of medieval Tamil culture. The tasks, which are all encoded in beautiful Tamil culture. The tasks, which are all encoded in beautiful Tamil verse, involve learners in real-life scenarios such as surveying land, calculating crop the shares, allocating pay and answering time-based riddles. They are by no means theoretical or abstract. These puzzles enhance logical reasoning, proportionate thinking and cultural literacy in addition to teach computation. Kanakkatikaram shows that information does not have to imported or elite in order to be rigorous and profound. This is achieved by integrating Mathematics into everyday situations and utilizing, local units and metaphors.

Keywords: Number System; Tamil Literature Poem; Kaṇakkatikaram

1. Introduction

The Kanakkatikaram (கணக்கதிகாரம்) which translates to “Treatise on Arithmetics”, is a classic Tamil work that exemplifies

South India's significant Mathematical legacy. This work is credited to Kari Nayanar of Korukkaiyur in Chola Nadu and is believed to have been written sometime in the 15th century CE. Kannakkatikaram is more than just a mathematical manual. It combines pedagogy, poetry, and real-world problem solving, mirroring the way mathematics was taught and applied in the Tamil-speaking areas of medieval South India. The puzzles place more emphasis on applied thinking than on abstract theories; they teach mathematical concepts such as addition, fractions, proportions and geometry through scenarios involving the division of paddy grain, the weighing of gold, the measurement of textiles and time-related difficulties. Poetic riddles have a lot of issues that need to be interpreted both linguistically and numerically. In order to provide insight into the regional computational culture, the text also introduces local systems of units and measures. Kanakkatikaram served as an interface between Mathematical thinking and everyday life by converting everyday transactions into structured puzzles. Its eternal impact derives from its capacity to communicate Mathematical concepts in understandable, regional and forever poetic ways. The related concepts can be found in [1-5].

2. Arithmetic Concepts in Kaṇakkatikaram

2.1 Structure and Style

Unlike modern textbooks, *Kaṇakkatikaram* is written entirely in Tamil poetic meters, including Venpa, Kattalai kalithurai, and Nurpa. This metrical form made the content easier to memorize and recite, aligning with the oral traditions of the time. The text contains 64 main verses, supplemented by problem sets and puzzles that often reflect real-life scenarios involving trade, measurement, and calculation.

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2.2 Content Overview

The treatise is systematically organized into six key sections, each addressing a different aspect of arithmetic:

1. Number Naming and Counting Systems

- Tamil names for numbers up to large magnitudes
- Use of fractions and decimal-like representations

2. Units and Measures

- Local systems for land, volume, grain, gold, and time
- Conversion between units used in trade and agriculture

3. Basic Operations

- Addition, subtraction, multiplication, and division
- Rule of three, interest calculation, and unit cost problems

4. Geometrical Knowledge

- Area of squares, circles, and triangles
- Concepts similar to the Pythagorean theorem

5. Riddles and Practical Problems

- Problems framed as poetic puzzles involving climbing trees, dividing grain, or measuring cloth
- Use of logic, estimation, and proportional reasoning

6. Applications in Daily Life

- Merchant arithmetic: calculating wages, profit, and loss
- Problems relevant to farming, construction, and temple rituals

2.3 Pedagogical Purpose

Kaṇakkatikaram was not a theoretical mathematical text like those in Greek or Sanskrit traditions, but a practical teaching manual. It was used by teachers and accountants (kanakku pulligal) to train students in temple schools and local institutions. The poetic format allowed students to recite, memorize, and apply the material easily.

This treatise demonstrates how mathematics was embedded in daily life, tied to agriculture, trade, and social duties.

2.4 Comparison with Other Traditions

Although it shares ideas with Sanskrit texts like Bhaskara II's *Lilavati*, *Kaṇakkatikaram* stands out for its localization:

- It uses Tamil terms, rather than Sanskrit.
- It reflects Dravidian measurement systems, such as *muzham* (arm length), *padi* (grain volume), and *kalanju* (gold weight).
- It emphasizes utility over abstraction, making it a rare example of *applied mathematics* in early Indian literature.

2.5 Legacy and Influence

Kaṇakkatikaram was widely copied, adapted, and taught in South Indian schools well into the 19th century. Its influence reached Kerala, where versions of it were integrated into Malayalam manuscripts. Modern scholars consider it a genre of arithmetic teaching texts rather than a single fixed document.

2.6 Examples

Let's look at a Poem:

முப்பத்தி ரெண்டு முழம்உள முட்பனையைத்
தப்பாமல் ஓந்தி தவழ்ந்தேறிச்---செப்பமுடன்
சாணேறி நான்கு விரல்கழியும் என்பரே
நாணா(து) ஒருநாள் நகர்ந்து.
ஓந்தி---ஓணான்.

<u>*Question:*</u> An Oriental Garden Lizard climbs a palm tree 32 muzham high. Its climbing speed is such that if it climbs one saan per day, it descends four fingers. (1 muzham = 2 saan; 1 saan = 12 fingers; 1 muzham = 24 fingers). In how many days will the Oriental Garden Lizard climb the palm tree at this speed to reach the top?

Double the palm tree and divide by twelve to get the answer. That is,

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multiply the height of the palm tree by 2, then multiply by 12 again, and divide the resulting number by 2 (divide by 8).

The height of the palm tree is 32 muzham (Feet).

That is 64(32x2) feet;

that is 768 (64x12) finger heights.

The height climbed per day: 12 finger heights

Subtract (Descending) 4 finger heights

The final height climbed: 8 finger heights

The day it takes to climb 8 finger heights.=1

Days it takes to climb 768 finger heights:

768 divided by 8 = 96 days.

Next, let's look at a riddle-like calculation.

பூசணிக்காய் ஒன்றின் விலை 10 பணம்; கத்தரிக்காய் 2இன் விலை 1 பணம்;பாகற்காய் 3இன் விலை 1 பணம். கையில் 100 பணம் இருப்பு உள்ளது. இந்த 100 பணத்துக்குப் பூசணிக்காய், கத்தரிக்காய் மற்றும் பாகற்காய் எத்தனை எத்தனை எண்ணிக்கையில் வாங்கினால் மொத்தம் 100 காய்கள் கிடைக்கும்?(அதாவது 100 பணத்தைச் செலவழித்து 100 காய்கள் வாங்குதல் வேண்டும்).

Question: The cost of one Pumpkin is 10 paise; the cost of 2 Brinjals is 1 paise; the cost of 3 Bitter gourds is 1 paise. You have 100 paise in your hand. How many Pumpkins, Brinjals and Bitter gourds can you buy for this 100 paise to get a total of 100 fruits? (i.e., you need to spend 100 paise to buy 100 fruits).

Vegetable's Name	Vegetable's Count	Vegetable's Cost
Pumpkin	6	60
Brinjals	52	26
Bitter gourds	42	14
Total	100	100

Kaṇakkatikaram covers topics such as fraction and whole numbers names, Mathematical computations that yield the same result regardless of how they are added and entertaining quizzes. Such a calculation is one of many amusing and strange ones. There are methods for calculating the area of circle and their circumference.

3. Conclusion

Kaṇakkatikaram is a shining example of how traditional knowledge systems merged practicality, poetry, and pedagogy. It reminds us that mathematics is not a modern import but a discipline deeply rooted in India's cultural and linguistic past. Its poetic clarity, real-world focus, and regional identity make it a unique landmark in the global history of mathematics.

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Chapter 3

Hash Functions in Cryptography

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Abstract

Hash functions are introduced in Cryptography as tool to protect the integrand authenticity of information in late seventies. Later it plays a vital role in many fields like Computer science, Communication networks, Password security, Digital signature. This paper discusses the basics of Hash functions and their applications, properties and also discusses the Algorithms of Hash functions and their limitations. Now a day the security and authenticity of information are very essential and Hash functions play a crucial role to solve the emerging challenges.

Keywords: Hash Function; Concept of Cryptography; Integrity; Secure Hashing Algorithm;

1. Introduction

Cryptographic techniques mainly used to protect authenticity of information. Over the past few decades network such as social networks, telecommunication networks etc. has seen a radical change. These evolution demand developed security requirements, that is a new challenge before the cryptologic. Introduction of electronic mediums often offer no protection and privacy in all aspects of our life. Need to implement sufficient design to overcome this

scenario, not for a group but for worldwide systems which go through a wide range of the world. In this paper we will discuss about Hash functions which play a vital role in cryptography in order to protect authenticity of information and protection of privacy. Hash functions are functions that reduce an arbitrary length input into a fixed length output. Hash functions are immensely a useful tool in the development of methods in order to protect the validity of information, provided that they meet additional requirements. The term Hash functions was first introduced in computer science, referred that a function compress arbitrary input string into a fixed length string. They distribute storage for files records. The related concepts can be found in [1-8].

2. Hash Functions

Hash functions is an essential tool in cryptography, Digital signature, message authentication codes are some of its applications. In this technology era Hash functions can apply many different contexts that need advanced characteristics. Collision resistance and pre image are two important characteristics because in this context it is computationally challenging to identify two inputs with similar output or to flip a Hash function. Moreover, Hash functions are often applied for entirely random functions, where Collision protection is adequate.

2.1 Definition

A Hash function is a function$C: H \rightarrow D$, Where the Domain

$H = \{0,1\}*$ and $D = \{0,1\}^n$ for some$n \geq 1$.

The two main categories of cryptographic Hash Functions are Keyed Hash functions and un-keyed Hash functions. Keyed Hash functions, which operate under a secret key, and un- Keyed Hash functions or simply Hash functions are not.

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2.2 One Way Hash Functions

A one-way Hash function is a function c satisfying the given conditions:

- Take any length of input and produce an image c(u) has a fixed size of n bits.
- Given a t in the image of c it is a challenge to find an input p such that c (u) = v This property is one way property or pre-image resistance. and given u and c(u) it is challenge to find a message u′ ≠ u such that c(u′) = c(u). This property is known as second pre-image resistance property.

2.3 Collision Resistant Hash Functions

Collision Resistant Hash Functions is a type of Hash function that is a one-way Hash function that satisfies an additional property called Collision resistance property given below: "There is no computational way to find a pair (u, v) such that c(u) =c(v) for the given c."

2.4 Universal One Way Hash Functions

The idea of Universal one-way Hash functions was introduced by Mani Naor and Moti Yung [5], which is a type of Hash function that's designed to be a target collision- resistant keyed Hash function which is mainly used for Digital signature, message authentication codes.

2.5 Security of Hash functions

The three main features collision resistant, second pre-image resistance, and pre- image resistance combine to make the strongest type of security for Hash functions. Any Hash functions which is second pre- image resistance is also a pre- image resistant. But the converse need not be true. Also, the Hash functions which is collision resistance also hold for second pre-image resistance and it follow pre-

image resistance. As the same above reverse is not true. Thus, in order to find a collision resistant Hash functions is the challenge, which provide a secure Hash function. That is a collision Resistant Hash function give a secure message authentication or a secure message transmission.

3. Application of Hash functions

Hash functions have many applications in various fields such as computer information security and communication networks etc. Some of the applications are:

Cryptography: In Cryptography, Hash Functions play an important role in Digital signature, Block chain technology and password storage. A strong password helps us to store data or information securely. Hash value used to create such a password instead of plane password. Like this Hash functions used in Digital signature which ensure the authenticity and integrity of the message. Bitcoins heavily rely on cryptographic Hash Functions.

Deduplication of Data: Identifying duplicate files help us to optimize storage size in a system. Hash functions can identify such files and delete them.

4. Cryptographic Hash Algorithms

There are many algorithms in cryptographic Hash Functions which are widely used in many fields. Some of them are discussed here:

Message Digest Algorithm 5: This algorithm is a commonly used algorithm in data integrand digital signature. But now it is not much familiar since it is very simple to make hash collision by the attackers and its speed. Thus, now it is considered as an insecure algorithm.

Secure Hash Algorithms 1: A longer Hash length and better collision resistance Secure Hash Algorithms 1 is a better than Message Digest

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Algorithm 5. But in computing power and cryptoanalysis lead to collision attacks. Since SHA 1 is no longer advised for security applications.

Secure Hash Algorithms 2 Family (SHA 256 SHA 512): Secure Hash Algorithms 2 family still a standard tool for cryptographic hashing. Which gives a strong security with long Hash outputs in 256 bits and 512 bits. This algorithm is high collision resistant and pre- image resistant thus it is widely used in blockchain technology digital signature etc.

Secure Hash Algorithms 3: Use of unique sponge construction Secure Hash Algorithms 3 is more flexible and secure algorithm. It offers long term security and also defends specific kind of attacks. These are some advance features of Secure Hash Algorithms 3 apart Secure Hash Algorithms 2.

BLAKE 2 and BLAKE 3: Apart from Secure Hash Algorithms 2 and Secure Hash Algorithms 3, BLAKE 2 and BLAKE 3 designed as speed and secure hashing. That is, BLAKE 2 and 3 provide fast hashing that doesn't affect the security. In particular, BLAKE 3 is perfect for current scenarios that need speed and quality in hashing because it enables parallel processing and incremental updates.

5. Conclusion

Hashing plays a fundamental in cryptography providing data authentication security and integrity. This paper provides a basic idea of Hash functions their properties and application of Hash functions and some algorithms for hashing. Collision resistant pre- image resistant hash function provides a secure hashing. Secure Hash Algorithms 2 and Secure Hash Algorithms 3, BLAKE 2 and BLAKE 3 are efficient hash functions that are collision resistance and provide

secure data authentication. This paper underscores the current significance in hashing and development and improvement of hashing is essential for the emerging challenges. As technology advances, Hash functions will continue to be a vital component of digital security, offering the simplicity and robustness required to protect data.

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Chapter 4

AI-Driven Approaches to Transform Workforce Performance Prediction

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Abstract

The emergence of Artificial Intelligence (AI) and Machine Learning (ML) has transformed the way organizations evaluate and forecast workforce performance. Traditional performance appraisal systems, often criticized for subjectivity, limited scope, and lack of real-time feedback, are increasingly inadequate in addressing the complexities of modern work environments. This chapter explores how AI-driven predictive analytics can provide objective, continuous, and data-informed insights into employee performance, bridging the gap between human resource management and advanced technologies. Drawing upon the Job Demands–Resources (JD-R) Model, Human Capital Theory, and the Technology Acceptance Model (TAM), the chapter develops a conceptual framework that integrates job demands, resources, skills, and collaboration as critical predictors of workforce performance, mediated by AI analytics. The framework highlights how AI enables organizations to anticipate performance outcomes, identify risks of burnout or attrition, and design personalized development interventions. The chapter further situates the relevance of AI-driven performance prediction in the post-

pandemic era, where hybrid work, digital collaboration, and employee well-being have redefined performance metrics. Practical implications for managers, policymakers, and researchers are discussed, alongside ethical considerations such as privacy, fairness, and transparency. By synthesizing theory with application, this chapter underscores AI's potential to enhance workforce performance prediction while ensuring human-centred, ethical, and future-ready HR practices.

Keywords: *Artificial Intelligence; Workforce Analytics; Performance Prediction; Job Demands–Resources Model; Human Capital Development;*

1. Introduction

1.1 Background and Motivation

Employee performance is a key driver of organizational success. Traditional appraisal systems such as supervisor evaluations and annual reviews are often criticized for subjectivity, inconsistency, and reactive focus. In the digital era, organizations require predictive, data-driven methods to forecast performance and align workforce development with strategic goals. Artificial Intelligence (AI) and Machine Learning (ML) offer predictive insights by analyzing large-scale workforce data, identifying skill gaps, and recommending interventions.

1.2 Limitations of Traditional Performance Appraisal

Conventional appraisal systems suffer from bias, infrequent feedback, narrow data use, and employee dissatisfaction. They remain reactive rather than predictive, making them less suited for today's dynamic and technology-driven workplaces.

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1.3 The Rise of AI and Machine Learning in HR

AI and ML in HR provide strategic augmentation rather than simple automation. Applications include recruitment screening, performance forecasting, learning personalization, and attrition prediction. Importantly, explainable AI (XAI) enhances transparency and builds trust in AI-driven workforce decisions.

1.4 Relevance in the Post-Pandemic Era

The COVID-19 pandemic accelerated remote work, hybrid models, and digital collaboration. Traditional performance reviews became ineffective, making AI essential for real-time monitoring, well-being tracking, skill-gap forecasting, and ensuring fairness in distributed environments.

2. Research Objectives and Scope

2.1 Defining the Problem Statement

Despite abundant digital workforce data, organizations struggle to convert it into actionable insights. Traditional appraisals remain subjective and limited, while AI adoption faces challenges of bias, explain ability, and privacy. The core problem is how AI-driven predictive models can enhance fairness, accuracy, and transparency in workforce performance prediction.

2.2 Objectives of the Study

The study aims to explore and demonstrate AI-driven performance prediction. Objectives include:

- Examine limitations of traditional systems.
- Analyze AI and ML applications in workforce analytics.
- Develop a conceptual framework integrating JD-R, HCT, and TAM.
- Identify predictors of employee performance.

- Assess managerial and policy implications.
- Provide recommendations for adoption in post-pandemic contexts.

2.3 Scope and Boundaries of AI in Workforce Analytics

The scope covers knowledge-intensive sectors, E-HRM data, and supervised ML with explainable AI. Boundaries include limited applicability in low-digital industries, ethical considerations, and emphasis on AI as augmenting, not replacing, human judgment.

3. Theoretical Foundations

3.1 Job Demands–Resources (JD-R) Model

The JD-R model is a widely applied framework for explaining employee performance, motivation, and well-being. It classifies workplace factors into job demands (workload, deadlines, emotional strain) and job resources (support, autonomy, development opportunities). High demands deplete energy and lead to burnout (health impairment process), while adequate resources stimulate engagement and motivation (motivational process).

In AI-driven performance prediction, this model provides a structured basis for selecting variables. For instance, digital workload, overtime, and call volume represent demands, while training access, supervisory support, and collaboration tools represent resources. Feeding these variables into machine learning models enables organizations to forecast outcomes such as performance, burnout, and attrition in a theoretically grounded way.

3.2 Human Capital Theory (HCT)

Human Capital Theory, introduced by Becker (1964), views employees as assets whose value increases with investment in education and training. Skills, knowledge, and experience drive

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productivity and competitive advantage. Organizations that invest in workforce development enhance long-term performance and adaptability.

In an AI context, HCT justifies predictive modelling by linking employee learning and development data with future performance outcomes. AI tools can identify skill gaps, recommend targeted training, and estimate the return on investment from such programs. This positions human capital as a measurable, strategic resource that organizations can optimize through predictive analytics.

3.3 Technology Acceptance Model (TAM)

The Technology Acceptance Model (TAM) explains why individuals adopt or reject new technologies. It emphasizes perceived usefulness and perceived ease of use). In AI-driven HR, adoption depends on whether employees and managers trust and find value in predictive systems.

Acceptance increases when AI tools are transparent, easy to interpret, and demonstrate fairness. Explainable AI (XAI) frameworks such as SHAP or LIME strengthen trust by clarifying why predictions are made. TAM thus highlights the human dimension of AI adoption, ensuring that technological sophistication aligns with workforce acceptance.

3.4 Integration of Theories

Together, these theories create a multidimensional framework. The JD-R model guides variable selection by balancing demands and resources. HCT provides economic justification for predicting and enhancing human potential. TAM ensures acceptance and trust in AI adoption. Their integration ensures that predictive models are psychologically grounded, strategically relevant, and behaviourally

acceptable.

4. Conceptual Framework

4.1. Independent Variables

- Job Demands – workload intensity, time pressure, and emotional strain.
- Job Resources – managerial support, autonomy, training, and recognition.
- Skills – depth, breadth, and learning agility derived from HR records and certifications.
- Collaboration – team interaction quality, use of digital platforms, and knowledge sharing.

4.2 Mediating Role of AI-driven Predictive Analytics

AI acts as a mediator between inputs (demands, resources, skills, collaboration) and outputs (performance). By integrating data across HR and digital systems, machine learning detects hidden patterns and forecasts productivity, innovation, and retention. Instead of relying on subjective evaluations, organizations gain evidence-based, actionable insights.

4.3 Dependent Variables

The study focuses on four performance dimensions:

- Task Performance – accuracy and efficiency in assigned duties.
- Innovative Performance – creativity and contribution to problem-solving.
- Engagement and Motivation – enthusiasm and psychological investment.

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- Retention and Career Progression – likelihood of staying and advancing within the organization.

4.4 Conceptual Model Explanation

The framework shows how workforce inputs (demands, resources, skills, collaboration) flow through AI-driven analytics as a mediator to produce outputs (performance outcomes). AI transforms raw workforce data into predictive intelligence, making performance evaluation more transparent, fair, and future oriented.

5. Contextual Applications

5.1 Sectoral Relevance

- Technology – predicting developer productivity, preventing burnout, and recommending reskilling.
- Healthcare – forecasting nurse performance, managing fatigue risks, and aligning training with emerging needs.
- Education – evaluating teaching quality and faculty research potential using digital learning data.
- Manufacturing – predicting worker productivity, enhancing safety, and optimizing workforce allocation.
- Logistics – forecasting warehouse and driver efficiency and addressing last-mile delivery attrition.

5.2 Post-Pandemic Workforce Trends

- Remote/Hybrid Work – AI ensures fair evaluation via digital footprints.
- Employee Well-being – predictive models detect burnout risks early.

- Digital Skill Acceleration – AI forecasts skill gaps and aligns training.
- Outcome-based Evaluation – emphasis on project results over presence.
- Resilience and Agility – adaptability becomes a core performance metric.

5.3 Ethical and Privacy Considerations

- Data Privacy – strict compliance with GDPR and local data laws, with anonymization protocols.
- Bias and Fairness – adoption of bias-mitigation and XAI frameworks.
- Transparency and Consent – employees must know what data is collected and how it is used.
- Human Oversight – AI should support, not replace, human judgment.

6. Contributions and Implications

6.1 Managerial Implications

- Enables data-driven talent management.
- Optimizes workforce allocation and project matching.
- Provides real-time monitoring instead of annual reviews.
- Supports engagement and retention through early risk detection.

6.2 Policy Implications

- Necessity of fairness audits and bias monitoring.
- Strong data privacy and security frameworks.

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- Possible standardization of AI use in HR.
- Use of predictive analytics for workforce development policies.

6.3 Research Implications

- Theoretical: Integrates JD-R, HCT, and TAM in AI-based HR research.
- Methodological: Encourages machine learning with explainability.
- Practical: Opens scope for cross-sectoral and longitudinal studies.

7. Conclusion and Future Directions

7.1 Key Findings

- Traditional appraisals lack objectivity and timeliness.
- AI-driven methods offer predictive, transparent, and continuous insights.
- JD-R, HCT, and TAM together provide strong theoretical grounding.
- The framework emphasizes AI as a mediator linking inputs to multidimensional performance.
- Applications span across sectors with universal relevance.

7.2 Challenges and Opportunities

- Challenges – data quality, algorithmic bias, employee resistance, regulatory uncertainty, and integration with legacy systems.
- Opportunities – personalized development, proactive HR, hybrid work optimization, and global talent forecasting.

7.3 Future Directions

- Integration of well-being and mental health metrics.
- Wider adoption of Explainable AI in HR.
- Block chain for secure and transparent workforce data.
- Cross-industry benchmarking using AI models.
- Development of global ethical and governance standards.

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Chapter 5

Investigation of Sisal/Palm Reinforced Composites through Natural Fiber Wastes

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Abstract

Natural fibers have long been utilized in traditional crafts and low-strength structures owing to their wide availability, low cost, and biodegradability. In the modern context, environmental regulations and sustainability concerns are steering industries toward eco-friendly materials to replace synthetic fibers. However, the majority of research has concentrated on virgin natural fibers, leaving agricultural fiber wastes underexplored. This research addresses that gap by investigating the potential of sisal and palm fiber wastes as reinforcements in polymer composites. The outcomes highlight the importance of waste-derived fibers as promising reinforcements, demonstrating both environmental and engineering benefits. The findings establish a pathway for sustainable composites that can find applications in lightweight structures, automotive panels, construction materials, and biodegradable packaging solutions.

Keywords Sisal fiber waste; Palm fiber composites; Natural fiber hybrid composites; Sustainable polymer materials

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1. Introduction

1.1 Background and Relevance

The transition toward sustainable and environmentally responsible materials has become a global priority in recent decades. Synthetic reinforcements such as glass, carbon, and aramid fibers offer excellent performance but suffer from drawbacks including high cost, non-biodegradability, and energy-intensive production processes. Natural fibers, derived from plants, present a compelling alternative due to their renewability, biodegradability, low density, and reasonable mechanical properties. These attributes have positioned natural fibers as candidates for reinforcing polymer composites, particularly in automotive, packaging, and construction sectors.

Among natural fibers, sisal and palm fibers stand out because of their abundance in tropical regions, low production costs, and good mechanical performance. Sisal fibers, obtained from Agave sisalana, possess high cellulose content, making them relatively strong and stiff. Palm fibers, extracted from oil palm tree residues, are lightweight, thermally stable, and widely available as waste from agricultural industries.

1.2 Research Gap and Problem Definition

Despite significant advances in natural fiber composites, a majority of investigations focus on virgin fibers that require deliberate harvesting, processing, and supply chain management. Agricultural and industrial waste fibers—produced in substantial quantities—remain largely underutilized. This not only represents a missed opportunity for value addition but also creates environmental disposal challenges.

Moreover, limited studies have examined hybrid composites reinforced with more than one type of fiber, particularly waste-based hybrids. Hybridization provides a balance between the mechanical and thermal properties of individual fibers, offering synergistic effects that single-fiber composites cannot achieve. The gap lies in systematically investigating waste-based sisal/palm hybrids for engineering applications.

1.3 Objectives of the Study

This chapter investigates the feasibility of utilizing sisal and palm fiber wastes as reinforcements in polymer composites. Specific objectives include

- To extract and chemically treat waste sisal and palm fibers to improve compatibility with polymer matrices.
- To fabricate and characterize composites reinforced with individual and hybrid fibers.
- To evaluate the mechanical, thermal, and water absorption behavior of the developed composites.
- To analyze the influence of fiber hybridization and surface modification on overall performance.
- To propose potential applications and highlight sustainability benefits of natural fiber waste composites.

2. Natural Fibers in Composites

Natural fibers are primarily composed of cellulose, hemicellulose, and lignin. Cellulose provides strength, while hemicellulose and lignin contribute to flexibility and thermal resistance. Their advantages include low density, low cost, renewability, and biodegradability. However, challenges such as hydrophilicity, poor matrix adhesion,

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and variability in properties limit their performance in structural applications.

2.1 Sisal Fiber Characteristics

Sisal fibers are extracted from the leaves of Agave sisalana. They contain about 65–72% cellulose, 12% hemicellulose, and 10% lignin. Mechanical properties include tensile strength ranging from 400–700 MPa and modulus of 9–22 GPa. Previous research has demonstrated sisal composites with good tensile and flexural properties, but high water absorption and poor interfacial bonding remain critical issues.

2.2 Palm Fiber Characteristics

Palm fibers are by-products of the oil palm industry, primarily extracted from empty fruit bunches. They typically contain 40–50% cellulose, 25% hemicellulose, and 15–20% lignin. Palm fibers exhibit lower tensile strength compared to sisal but possess excellent thermal stability and good toughness. They are widely available as waste, making them attractive for composite applications.

2.3 Fiber Treatments and Modifications

Surface modification is essential to improve fiber–matrix adhesion. Alkaline treatment (NaOH) is the most common method, which removes surface impurities, increases surface roughness, and reduces hemicellulose content, thereby enhancing bonding. Coupling agents such as silanes and compatibilizers have also been explored. Literature consistently reports significant improvements in tensile strength and reduced water absorption after treatment.

2.4 Hybrid Composites

Hybridization combines two or more fibers to harness their complementary strengths. For instance, sisal provides stiffness while

palm offers toughness and thermal resistance. Studies have shown hybrid composites outperforming single-fiber systems in tensile, flexural, and impact tests. However, very few studies have considered waste-derived fibers for hybridization, leaving a gap in sustainable composite development.

2.5 Research Gap Identified

From the reviewed literature, two major gaps are evident

- Insufficient attention to waste-based fibers as reinforcements.
- Lack of systematic studies on hybrid composites made from sisal and palm wastes.

This study aims to address these gaps by fabricating and characterizing sisal/palm hybrid composites, focusing on waste valorization and property enhancement.

3. Methodology

The methodology adopted in this study consisted of four major stages materials selection, fiber extraction and treatment, composite fabrication, and characterization of the fabricated samples. A systematic approach was followed to ensure that the results were reliable, reproducible, and aligned with international testing standards.

3.1 Materials

3.1.1 Matrix

The matrix material chosen was an unsaturated polyester resin (UPR) due to its widespread availability, relatively low cost, and favorable mechanical properties. UPR is known for its ease of processing, good adhesion characteristics, and compatibility with natural fibers. The

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curing agent methyl ethyl ketone peroxide (MEKP) was employed as a hardener, in a typical resin-to-hardener mixing ratio of 1001 by weight, ensuring controlled polymerization.

3.1.2 Fibers

Two different types of waste fibers were utilized in this investigation

- Sisal fibers these were collected from rope-making industries where considerable amounts of short-length sisal fibers are discarded as waste.
- Palm fibers Extracted from oil palm agricultural residues, specifically empty fruit bunches (EFB), which are generally left unutilized after palm oil processing.

Both fiber types were selected based on their availability, mechanical potential, and current underutilization in industrial waste streams.

3.2 Fiber Extraction and Treatment

3.2.1 Sisal Fiber Preparation

The waste sisal fibers were initially cut into lengths of 20–30 mm to ensure uniformity. The fibers were washed with distilled water to remove dirt, oil residues, and surface contaminants, followed by sun-drying for 48 hours. This pre-treatment minimized impurities that could interfere with subsequent chemical modification.

3.2.2 Palm Fiber Preparation

Palm empty fruit bunches were manually processed by mechanical combing and retting to separate individual fibers. These raw palm fibers contained surface wax, lignin, and hemicellulose, which limited effective bonding with polymer matrices.

3.2.3 Chemical Treatment

Both sisal and palm fibers were subjected to alkaline treatment using a 5% NaOH solution at room temperature for four hours. The alkali treatment served multiple purposes

- It removed hemicellulose, wax, and pectin from fiber surfaces.
- It increased surface roughness, enhancing mechanical interlocking with the matrix.
- It exposed cellulose fibrils, thereby improving chemical affinity with the polyester resin.

After treatment, the fibers were thoroughly rinsed with distilled water until a neutral pH was achieved. Finally, they were oven-dried at 60°C for 24 hours to eliminate moisture, as retained water content can cause void formation and poor adhesion during fabrication.

3.3 Composite Fabrication

The composites were fabricated using the hand lay-up method, which is widely recognized for its simplicity, cost-effectiveness, and suitability for natural fiber composites.

3.3.1 Procedure

- A flat glass mold was prepared and coated with a thin layer of polyvinyl alcohol (PVA) as a release agent.
- The resin and hardener mixture was prepared in a 1001 ratio and stirred for uniform consistency.
- The treated fibers were distributed evenly in the mold, either as pure sisal, pure palm, or a hybrid mixture of both.

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- Resin was carefully poured over the fibers, and a roller was used to remove trapped air bubbles and ensure uniform resin impregnation.
- The mold was left to cure at room temperature for 24 hours, followed by post-curing at 80°C for 3 hours to enhance cross-linking.

3.3.2 Configurations Fabricated

- Pure sisal waste composites (30% fiber, 70% resin by weight).
- Pure palm waste composites (30% fiber, 70% resin).
- Hybrid composites (15% sisal + 15% palm, 70% resin).

3.3.3 Specimen Preparation

The cured laminates were cut into standard dimensions using a diamond saw, following ASTM standards for mechanical and physical testing.

3.4 Characterization

To assess the performance of the fabricated composites, comprehensive characterization was conducted under standardized conditions.

3.4.1 Mechanical Testing

- Tensile Testing (ASTM D638) Dog-bone-shaped specimens were tested using a universal testing machine (UTM) at a crosshead speed of 5 mm/min. Parameters measured included tensile strength, tensile modulus, and elongation at break.
- Flexural Testing (ASTM D790) Three-point bending tests were carried out with a span-to-depth ratio of 161. Flexural strength and modulus were evaluated.

- Impact Testing (ASTM D256) Charpy impact tests were performed on notched specimens to evaluate energy absorption capacity.

3.4.2 Thermal Analysis

- Thermogravimetric Analysis (TGA) Conducted under nitrogen atmosphere from room temperature to 600°C at a heating rate of 10°C/min to assess thermal stability.

- Differential Scanning Calorimetry (DSC) Conducted to determine glass transition temperature (Tg) and other thermal transitions.

3.4.3 Water Absorption (ASTM D570)

Specimens were immersed in distilled water at room temperature, and weight gain was recorded periodically until equilibrium was reached. The test provided insights into the hydrophilicity and durability of composites in humid environments.

4. Results

4.1 Mechanical Properties

4.1.1 Tensile Strength

The results demonstrated that sisal/palm hybrid composites exhibited superior tensile strength, showing a 20–25% improvement over pure palm composites and about 10% higher than pure sisal composites. This enhancement can be attributed to the synergistic effect of combining stiff sisal fibers with tough palm fibers. The alkali-treated fibers provided better interfacial bonding, reducing fiber pull-out during loading.

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4.1.2 Flexural Strength

Flexural tests revealed that hybrid composites displayed higher stiffness and load-bearing capability. Sisal fibers contributed to rigidity, while palm fibers enhanced toughness, leading to a balanced flexural response. Pure palm composites showed lower modulus, confirming that sisal fibers were critical in enhancing flexural performance.

4.1.2 Impact Strength

Palm fibers, being more ductile, contributed significantly to impact energy absorption. The hybrid composites achieved the highest impact resistance due to the complementary interaction of sisal (strength) and palm (toughness). This suggests potential applications in components requiring shock resistance.

4.2 Thermal Analysis

4.2.1 Thermogravimetric Analysis (TGA)

The onset of decomposition for hybrid composites was observed at higher temperatures (around 320°C) compared to pure palm (290°C) and pure sisal (305°C) composites. This improvement indicates enhanced thermal stability due to the hybrid effect and stronger fiber–matrix bonding.

4.2.2 Differential Scanning Calorimetry (DSC)

Hybrid composites exhibited a higher glass transition temperature (Tg) compared to individual fiber composites, suggesting restricted polymer chain mobility due to stronger adhesion. This confirmed the effectiveness of fiber treatment and hybridization in improving thermal properties.

4.3 Water Absorption

Water absorption results indicated that untreated composites absorbed significantly more water due to the hydrophilic nature of natural fibers. After NaOH treatment, water uptake decreased by nearly 30%, as surface impurities and hemicellulose responsible for hydrophilicity were removed.

Hybrid composites showed the lowest water absorption, owing to improved interfacial adhesion and reduced void content. This suggests that hybrid composites are more dimensionally stable in moist environments, extending their potential applications in outdoor and packaging materials.

5. Discussion

The study demonstrated that waste-derived sisal and palm fibers can be effectively utilized as reinforcements in polymer composites. Hybridization provided synergistic effects, improving tensile and flexural properties while maintaining good toughness. The results are consistent with earlier studies on natural fiber hybrids but add novelty by emphasizing waste valorization. Fiber treatment played a crucial role in improving adhesion, reducing hydrophilicity, and enhancing mechanical performance. Without surface modification, interfacial bonding would remain poor, leading to inferior properties. A limitation of this study is the variability of waste fibers, which may affect consistency in large-scale production. Furthermore, only polyester resin was considered as a matrix; future studies may explore biodegradable matrices such as polylactic acid (PLA). The outcomes strongly suggest that sisal/palm hybrid composites have potential for automotive interiors, construction panels, and packaging

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materials where moderate strength, lightweight, and eco-friendliness are required.

6. Conclusion

This investigation confirms that sisal and palm fiber wastes, when properly treated and hybridized, can serve as efficient reinforcements for polymer composites. Hybrid composites outperformed single-fiber systems in tensile, flexural, impact, and thermal properties. Chemical treatment significantly reduced water absorption and enhanced fiber–matrix adhesion, contributing to overall performance improvements. The research addresses critical gaps in natural fiber composite development by utilizing waste resources, thereby supporting sustainability and circular economy principles. Applications in lightweight structural panels, automotive parts, and eco-friendly packaging demonstrate the potential for industrial adoption.

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Chapter 6

A Study on the Impact of Smart Traffic Management Systems on Urban Congestion

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Abstract:

Rapid urbanization has led to a significant rise in traffic congestion across metropolitan areas resulting in increased travel times, fuel consumption & environmental pollution. This study explores role of Smart Traffic Management Systems in alleviating urban traffic congestion. These systems utilize real-time traffic data, adaptive signal control, GPS tracking, surveillance cameras & data analytics to monitor & regulate traffic flow efficiently. Research involves a comparative analysis of traffic patterns in urban areas before & after implementation of STMS supported by simulations & case studies from selected cities. Key performance indicators as average travel time, vehicle delay & emission levels were assessed. Findings reveal a considerable reduction in congestion levels with improved travel efficiency & smoother traffic flow. Study highlights importance of integrating smart infrastructure with public transportation networks & urban planning strategies. Results suggest that STMS offer a promising sustainable solution to challenges posed by rapid urban growth & increasing vehicular density. Study concludes that wider adoption of such intelligent systems can enhance mobility reduce environmental impacts & support development of smart livable cities. Research is recommended to address implementation challenges &

cost-efficiency concerns.

Keywords: *Smart Traffic Management Systems, Urban Congestion, Adaptive Signal Control, Intelligent Transportation Systems & Sustainable Urban Mobility*

1. Introduction

Urban traffic congestion has emerged as one of most persistent challenges confronting modern cities. With rapid urbanization, rising car ownership & inadequate urban planning cities are witnessing traffic gridlocks that negatively affect economic productivity, environmental sustainability & quality of urban life. According to World Bank & international urban mobility reports traffic congestion costs cities billions annually in lost productivity & wasted fuel. Traditional traffic management strategies which largely rely on static traffic lights, road widening & manual supervision have proven inadequate to cope with ever-growing demand for urban mobility.

To overcome these limitations Smart Traffic Management Systems (STMS) have emerged as a comprehensive solution by integrating real-time sensing technologies, Artificial Intelligence (AI), Internet of Things (IoT) & cloud-based platforms. These systems enable dynamic monitoring, analysis & control of traffic networks thereby improving flow efficiency, reducing congestion & minimizing environmental footprint of transportation. As cities transition toward becoming "smart cities" STMS are increasingly regarded as essential infrastructure for sustainable urban development.

1.1 Background of Study

Rapid expansion of metropolitan regions has led to unprecedented growth in number of private vehicles on urban roads. According to studies by the International Transport Forum (ITF) urban dwellers

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spend approximately 30–40% of their commuting time trapped in traffic congestion particularly during peak hours. This inefficiency translates into increased stress, reduced work productivity & elevated greenhouse gas emissions.

Traditional road-expansion projects & installation of conventional traffic signals have provided only temporary relief. Reason lies in dynamic nature of traffic which changes hourly, daily & seasonally. A static system cannot adapt to such variations. Cities are increasingly adopting smart mobility solutions where traffic flow management is guided by real-time data acquisition, machine learning algorithms & adaptive control strategies. Background of this highlights transition from a conventional infrastructure-centric approach to a technology-driven data-centric model of traffic management. This paradigm shift is not merely technological but also societal aiming to ensure sustainable urban living by reducing burden of congestion & making transportation more efficient & eco-friendly.

1.2 Need for Study

Despite heavy financial investment in flyovers, expressways & road widening projects, congestion remains a critical urban issue. Core challenge is that infrastructure alone cannot match exponential growth of vehicles. Traffic congestion is not only a transportation issue but also an economic, environmental & social problem. Prolonged traffic jams increase air pollution, elevate fuel consumption & result in lost economic opportunities due to delays in goods & passenger movement.

Need for present study arises from following factors:

- **Dynamic Traffic Conditions**: Conventional systems cannot adapt in real-time to accidents, road works or sudden increases in vehicle density.
- **Environmental Impact**: Vehicles stuck in traffic produce higher emissions of CO_2, NOx & particulate matter contributing to urban air pollution.
- **Urban Sustainability**: For cities aspiring to become "smart cities" integration of intelligent traffic systems is essential for achieving sustainable urban mobility goals.
- **Efficiency in Resource Use**: Instead of continuously expanding roads STMS utilize existing infrastructure more efficiently through real-time management.

1.3 Core Components of Smart Traffic Management Systems

A Smart Traffic Management System (STMS) is not a single technology but an integration of multiple interconnected components that work together to optimize traffic flow. Major components are as follows:

1. **IoT-based Sensors and Detectors**

   IoT devices as inductive loop sensors, GPS trackers, CCTV cameras & RFID readers provide real-time data on vehicle density, speed & flow. These sensors act as "nervous system" of STMS feeding live information into central control platform.

2. **Adaptive Signal Control Mechanisms**

   Unlike fixed-time traffic lights, adaptive signals use real-time data to adjust green, yellow & red phases dynamically. During peak hours, longer green times can be allocated to high-traffic lanes while off-peak times can allow smoother cross-direction movement.

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3. **AI-driven Predictive Analytics**

Machine learning & AI models analyze historical & real-time traffic data to predict congestion patterns. These models allow proactive interventions as rerouting vehicles adjusting signal priorities before bottlenecks develop.

4. **Cloud-based Centralized Platforms**

Cloud technology enables large-scale storage, processing & visualization of traffic data. Authorities can monitor traffic conditions citywide from centralized control rooms ensuring quick decision-making in emergencies as accidents, flooding or road closures.

5. **Vehicle-to-Infrastructure (V2I) Communication**

In advanced systems connected vehicles can communicate directly with traffic signals, warning systems or control centers. This helps in smoother navigation reduced waiting times & enhanced road safety.

These components make STMS not only responsive but also predictive & proactive in managing traffic. They represent the transition from manual supervision to autonomous data-driven decision-making which is vital for future urban mobility.

Table 1: Comparative Analysis of Smart Traffic Systems Worldwide

Country/City	Technology Used	Impact on Congestion	Remarks
Singapore	AI-based traffic prediction, IoT sensors	Reduced peak-hour congestion by 25%	Highly successful
London	Congestion pricing + adaptive	Traffic reduced by	Revenue reinvested in

	signals	30%	public transport
Los Angeles	Adaptive Signal Control Technology	Travel times reduced by 12%	Covers 400+ intersections
New Delhi	IoT traffic monitoring	Pilot studies show 20% reduction in delays	Implementation expanding

Table 2: Benefits versus challenges in deploying Smart Traffic Management Systems

Dimension	Benefits	Challenges
Mobility	Reduced delay/stops; improved reliability; better throughput	Complex tuning; heterogeneous fleets; demand variability
Safety	Smoother flow; emergency VRU detection	False positive in CV; mixed traffic edge cases
Environment	Lower idling emissions; exposure reduction	Measurement uncertainty; rebound effects
Economics	Travel time savings; fuel savings	Capex/Opex; vendor lock-in; maintenance
Governance	Data-informed decisions; transparency via dashboards	Privacy, cybersecurity, data sharing agreements

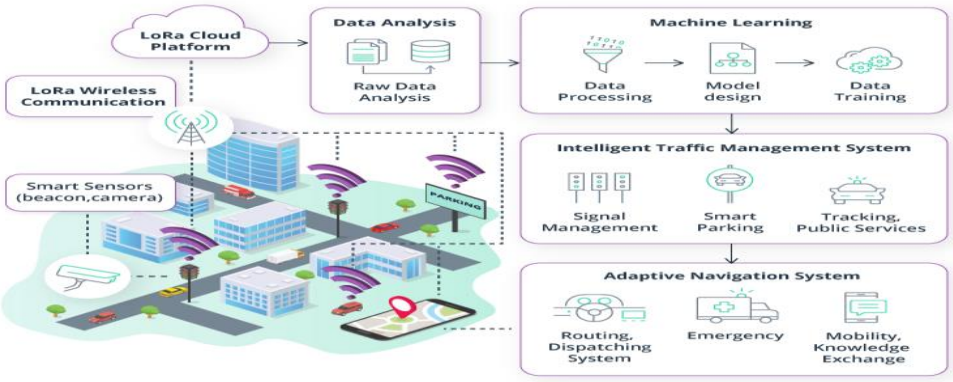

Figure 1 Diagram of a Smart City

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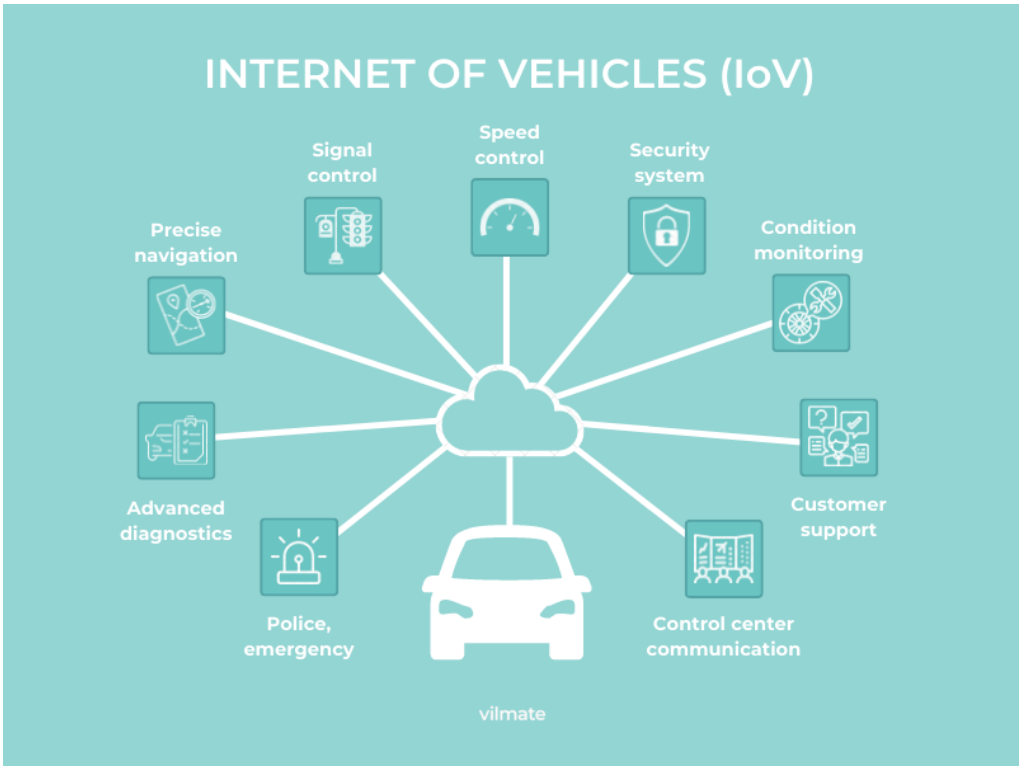

Figure 2 Diagram of Internet of Vehicles

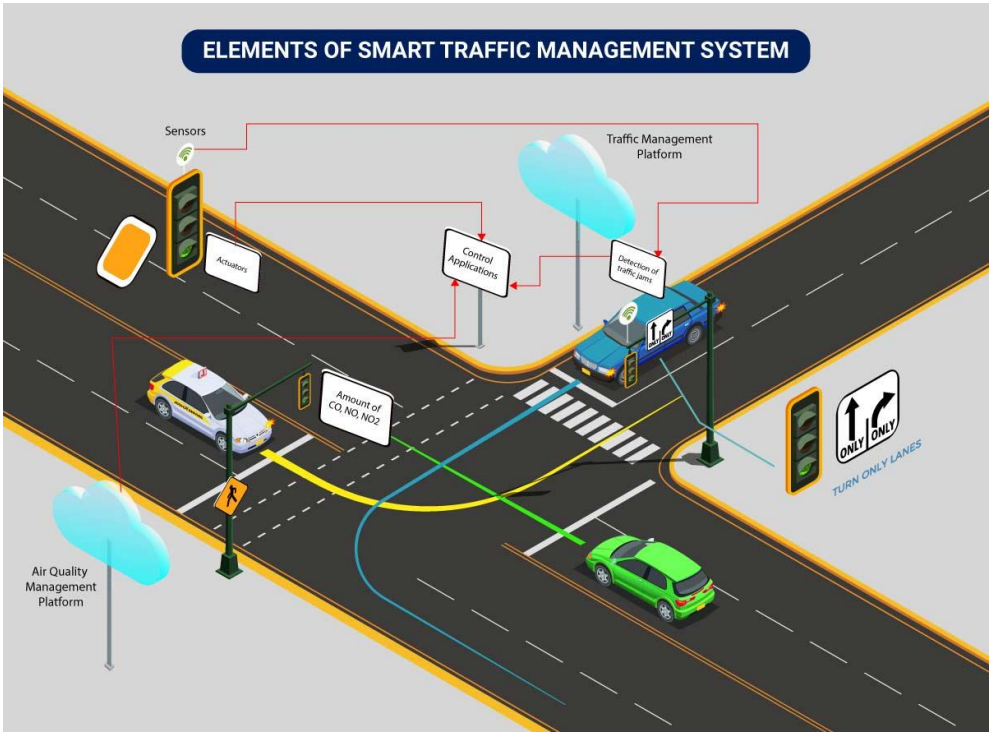

Figure 3 Diagram of Elements of Smart Traffic Management System

1.4 Impact of Smart Traffic Management Systems (STMS)

Implementation of Smart Traffic Management Systems has shown transformative impacts on urban mobility across globe. By leveraging real-time data analytics & adaptive decision-making STMS significantly improve both traffic efficiency & environmental sustainability.

1.4.1 Reduction in Congestion

One of most direct impacts of STMS is measurable reduction in congestion. Case studies from cities like Singapore, London & Los Angeles have demonstrated that adaptive traffic signal control can reduce average waiting times at intersections by 20–30%. This leads to smoother vehicular flow & shorter travel times for commuters.

1.4.2 Environmental Benefits

Traffic congestion is a major contributor to greenhouse gas emissions. Vehicles idling at intersections consume more fuel & emit higher concentrations of pollutants. STMS minimize idling and unnecessary acceleration-deceleration cycles thereby reducing CO_2 & NOx emissions. This aligns with global sustainability goals as Paris Climate Agreement & United Nations Sustainable Development Goals (SDGs).

1.4.3 Enhanced Road Safety

By monitoring traffic in real time STMS can detect unusual traffic patterns, accidents or hazardous road conditions & alert authorities instantly. Integration of AI-driven video analytics also assists in detection of violations reducing chances of collisions at intersections.

1.4.4 Economic Productivity

Traffic delays cause billions in economic losses annually due to

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wasted fuel, lost working hours & delayed goods delivery. World Economic Forum estimates that effective smart traffic systems could save up to 15–20% of these losses thus enhancing urban economic competitiveness.

1.4.5 Citizen Experience & Smart City Integration

From perspective of urban residents STMS not only reduce travel stress but also contribute to a better quality of life when integrated with smart parking, public transport & mobility-as-a-service (MaaS) platforms, STMS form backbone of smart city ecosystems.

1.5 Challenges in Implementing STMS

Despite their numerous benefits deployments of STMS is not without significant challenges. These challenges need to be critically examined to ensure effective policy-making & system design.

1.5.1 High Implementation Costs

Installation of advanced IoT sensors, cameras, AI systems & cloud infrastructure requires substantial initial investment. Developing countries often face budgetary constraints that limit large-scale deployment.

1.5.2 Data Privacy & Security Concerns

Since STMS rely on continuous data collection from vehicles, cameras & mobile devices privacy concerns emerge regarding misuse of personal & locational data. Cybersecurity risks as hacking into traffic systems can also disrupt entire city networks.

1.5.3 Technological Interoperability

Different vendors provide varying hardware & software platforms. Ensuring interoperability among devices, communication protocols & platforms remains a challenge in building cohesive STMS.

1.5.4 Maintenance & Reliability

IoT devices & sensors installed in outdoor environments are prone to failures due to weather conditions, vandalism, wear & tear. Ensuring reliable operation with minimal downtime is a critical challenge.

1.5.5 Policy & Governance Issues

Success of STMS requires effective coordination among municipal authorities, transport departments & private technology providers. Inadequate governance frameworks often delay decision-making & implementation.

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Chapter 7

A Systematic Review of Artificial Intelligence Integration in Outcomes- Based Education

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Abstract

Artificial Intelligence (AI) incorporated into the education domain lead to transformational possibilities for personalized, adaptive, and competency-based education. Concurrently, the Outcomes- Based Education (OBE) model emerged, giving rise to strategic approaches based on defined learning outcomes, learner-cantered pedagogical practice, and the ongoing assessment of performance. The incorporation of AI in education has reinvented pedagogical frameworks, especially when conjoined with OBE. This review articulates the way in which AI technologies Deep Learning (DL), Reinforcement Learning (RL), Personalized Learning (PL), Natural Language Processing (NLP), Gamification, and Learning Analytics align with educational outcomes in cognitive and affective domains. Higher education institutions utilizing AI augmented OBE

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frameworks develop learner centered environments, personalize learner learning pathways, promote appropriate summative assessment strategies, adopt ethical competencies, and apply problem-solving skills, understanding that these elements are needed for a workforce competent in AI. The paper identifies current limitations including scale, issues with standardization, and the absence of comprehensive theoretical models or articulation linking AI with OBE practices in education. In summary, the review highlights the potential for a shift to AI based OBE and potential deficiencies, and subsequent recommendations for effective and ethical AI in education.

Keywords: Artificial Intelligence; Outcomes-Based Education; Deep Learning; Reinforcement Learning; Personalized Learning;

1. Introduction

The COVID-19 pandemic has triggered a major shift in the education system worldwide, as both school systems and other higher education institutions have hastily moved to an online or hybrid instructional model [1]. The drastic move from face-to-face to a digital delivery model fuelled innovative teaching and learning practices, as digital technologies expanded in education. Within these advancements is an emergence of AI development, which significantly altered the ways in which knowledge is delivered, assessed, and the way student learning experience is personalized [2]. Higher education institutions around the world are now deploying AI technologies to facilitate not only flexibility in instruction but to also establish learner-cantered environments that emphasize creativity, collaboration, and curiosity qualities that needed to develop global citizens in a borderless digital environment [3]. AI in education has many possibilities, in OBE

intelligent tutoring systems, and efficient workflow improvements in administrative processes. As AI tools continue to develop educational stakeholders including government, higher education and technology developers all invest in AI learning systems to improve access and equity in education [4-5]. Nonetheless, with AI tools being adopted rapidly, the deployment of these technologies often lacks a larger conceptual theory or design model of education. Although usage of AI tools in educational settings is increasing, there is little evidence that they are being systematically integrated into educational structures or teaching practices [6-7]. Consequently, in addition to producing educational content, educators and educational institutions continue for producing a generation of individuals to possess the digital competencies and skills required in the modern workforce [8]. The Framework of OBE Outcome Domains is shown in Figure 1, which shows learning outcomes are categorized into cognitive, and affective, domains that inform instructional strategies, curriculum design, and assessment techniques.

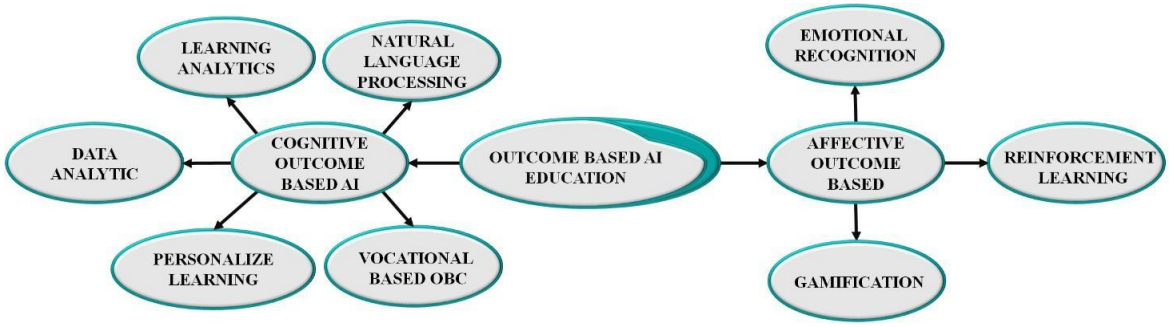

Figure. 1: Framework of OBE in AI technology Outcome Domains

Alongside the advancement of these technologies, OBE has emerged as an educational model that is grounded in defining and achieving clear, measurable learning outcomes. The framework of OBE emphasizes demonstrating students' knowledge, skills, and attitudes by organizing curriculum, instruction, and assessment around

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competencies in industry-specific contexts [9]. OBE ensures that graduates are equipped with attributes to align with the evolving and iterative demands of the workforce, especially in fields driven by the digital or AI revolution [10]. However, although it has promise, AI in education is still in its early stages, with adoption lagging in real institutional contexts and lacking an educational foundation for theoretical concepts. In addition, existing studies are often lacking a comprehensive educational framework to connect AI innovations and established educational frameworks like OBE [11]. This lack of comprehensive educational frameworks to ground existing research constrains the practical effect of AI technologies on curriculum design, learning analytics, and valuation. This survey article summarises the use of AI technologies which include DL, RL, PL, NLP, Gamification, data analytics, learning analytics in OBE and its impact on cognitive, affective and skill-based outcomes, while also indicating gaps in current research and recommending future opportunities.

2. Review of Outcomes-Based AI Education

OBE is a learner-cantered approach that emphasizes identified outcomes across cognitive, affective, and psychomotor expectations. Cognitive outcomes address knowledge, the acquisition of knowledge, understanding, and critical-thinking skills; the affective learning outcomes address motivation to learn, values, and attitudes. These technologies support the alignment of curriculum and assessments and assure institutional attention to student performance indicator and improvement on reachable qualitative competencies.

2.1. Cognitive Outcomes-Based AI Education

Cognitive outcomes relate to knowledge and understanding, and skills of thinking. Through adapting content, tracking progression,

and supporting skills of critical thinking, technology such as like DL, NLP, PL, Data analytics and learning alanytics enhance student's cognitive outcomes, providing deeper learning experiences and ultimately better performance in an OBE model.

2.1.1 Deep learning based OBE

OBE system grounded in DL, with personalized anticipations for learning recommendations and classroom quality assessments. This is a significant improvement over the traditional teaching delivery methods, which are limited in their evaluation approach. The system is based on a content-based recommendation algorithm using Convolutional Neural Networks (CNNs) which takes historical learner profiles and past preliminary knowledge, in multimodal formats, and utilizes DL models to identify highly accurate, individualized learning pathways. The CNN is fundamental when training the recommendation model and uses the text content from the learning resources as input data. The following is a mathematical representation of the feature extraction process:

$$ci = (w * xi + b) \quad (1)$$

The convolution operation produce new generation at;

$$a = (w * b + b) \qquad (2)$$

The objective function of the model is, implicit factors. The regularization factor is used to balance the strength of the constraint and fidelity terms in the objective function. The assessment data is transmitted by the $i - th$ learner to the $j - th$ learning resource. This technology supports an impartial, documenting, real-time attendance measure and feedback during the entire academic process. Nevertheless, constraints, such as lack of standardization, data scarcity, and challenges of scalability diminish the validity and

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effectiveness of these systems in different twist learning environments.

2.1.2 Natural Learning Processing

NLP improves OBE by mapping Course Learning Outcomes (CLOs) to Program Learning Outcomes (PLOs) using automation. This NLP system uses tokenization, vectorization, and cosine similarity to detect semantic relationships between CLOs and PLOs while significantly reducing human error and increasing accuracy. This NLP framework enables accurate evaluations of educational programs in ways that align with accreditation standards. One of the issues with the application of NLP in educational settings includes challenges in appropriate parsing of context related terms or the obscured variation of instructional text, leading to unreliable linking or feedback.

2.1.3 Personalized Learning

In AI-based education systems, personalized learning aims to adapt instructional content to a specific learner profile. These systems utilize a learner's data (e.g., academic progress, prior knowledge, interaction patterns) to supply content individualized to the learner. Personalization through the use of predictive analytics incorporates adaptive learning, deep learning, and knowledge tracing to better tailor content as it implicit factors.

$$J(U.\ V) = \Sigma$$

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The U matrix shows the association between users and implicit variables, while V indicates the correlation between learning resources and needs. AI-based personalized learning enables learners to achieve cognitive outcomes by structuring understanding, demonstrating mastery concepts and achieving improved academic outcomes. Recommender systems introduce education learners with a sequence of learning resources organized around prescribed cognitive goals framed in terminology congruent with OBE principles. The complex challenge of personalization lies in the observed identification of beneficial and preferred learner models in real- time which takes us to sophisticated data collection, and considerable computational resources.

2.1.6 Vocational education based on OBE

AI-supported vocational education framework based on OBE to satisfy the industry workforce requirements. The framework demonstrated two models, the Creative Vocational Education Model (CVEM) which demonstrated the stages of OBE in application, and the Performance Vocational Education Model (PVEM) which demonstrated outcome performance. Using Structure Equation Modelling (SEM) the study established a significant effect on AI capabilities to both models, and CVEM's influence on PVEM. The research supports the role AI has to offer in assisting creativity and performance in an OBE- based vocational education. However, the study had limitations as the data collected from vocational institutions in only the capital region, and therefore it cannot be generalized. Various institutions may use various approaches and

policies to implement AI and OBE. The research did not take account the components relevant the initial processes of the AI implementation and the internal decision making of organizations. Nonetheless, an important negative of vocational OBE models is the limited ability to generalize across different institutional contexts [16].

2.1.7 Data Analytics

Data analytics emphasizes equipping students with the practical skills, analytical thinking, and decision-making abilities required to extract meaningful insights from data using AI techniques. AI, which provides insights into student performance, learning trends, and areas for improvement, assists educators in making data- driven choices by analysing massive quantities of educational data. This approach focuses on clearly defined learning outcomes, such as the ability to clean, process, and visualize data and interpret results to solve real-world problems. By integrating AI tools like Python, and data visualization platforms with an outcomes-based framework, students gain hands-on experience in predictive modeling, and intelligent automation. Securing data privacy and compliance with regulations in a world of large-scale educational data is an important challenge.

2.1.8 Learning Analytics

Learning Analytics focuses on using AI-driven data analysis to enhance educational effectiveness and ensure that students achieve clearly defined learning outcomes. In order to inform instructional strategies and customize the learning experience, learning analytics entails gathering and evaluating data on student behavior, performance, and engagement. In an outcomes-based framework, this approach helps educators monitor progress toward specific

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cognitive, technical, and affective goals. By applying AI techniques such as pattern recognition, predictive modeling, and clustering, institutions can identify at-risk students, optimize curriculum delivery, and improve assessment design. Data quality, ignoring or losing contextual considerations, or being poorly informed on the possible conclusions to be drawn limit the meanings of learning analytics.

2.2. Affective Outcomes-Based AI Education

It focuses on shaping students' attitudes, values, and ethical understanding in the application of artificial intelligence. This approach goes beyond technical proficiency by emphasizing the responsible and human-centered use of AI technologies. Learners are encouraged to critically reflect on the societal, cultural, and moral implications of AI systems, such as fairness, transparency, privacy, and bias. Educational activities often include case studies, ethical debates, policy analysis, and reflection-based assessments to cultivate empathy, social responsibility, and ethical decision-making. Emphasizes theoretical understanding of AI concepts like Gamification, Reinforcement Learning.

2.2.1 Reinforcement learning

RL to support the improvement of students' CLOs within an OBE model. A student-CLO matrix constructed, and the student representations grouped using bi-clustering (Bi-bit algorithm) to identify students with similar patterns of performance. Each bi-cluster mapped to a 2D grid representing the RL environment, where the agent begins its navigation based on the cosine similarity between the student and bi-cluster vectors. The agent provides recommendations for targeted learning resources e.g., articles, videos,

tutorials, or books to improve deficient CLOs. The learning use cosine similarity to determine initial state as, the psychological effects of constant monitoring. The learning outcomes focus on fostering values such as empathy, accountability, and respect for individual rights. Students are expected not only to understand facial recognition systems function but also to appreciate the moral responsibility that comes with designing and implementing such technologies. The ethical implications of using facial recognition in education include privacy violations, potential bias, and the risk of emotional misreading.

2.2.3 Gamification

The principles of outcome-focused education with game-based learning strategies to enhance student engagement, motivation, and achievement in artificial intelligence education. In the gamification, it is presented to allow students to

$$sinCosine = \quad \Sigma i \epsilon CM\ (st,).M(bic,i)$$

Organically explore and use AI algorithms through

$$(st,bic)$$

$$\sqrt{\ } \Sigma\, i \epsilon C(st,i)\ \sqrt{\ } \Sigma\, i \epsilon C \qquad 2$$

$$M(bic,i)$$

Cooperative and competitive events.

Here, C represents a set of common CLOs shared by student st, bi-cluster bic, and i represents an individual CLO in C. (st,i) represents student st's CLO attainment marks in CLO i, whereas $M(bic,i)$ represents the column-wise average CLO attainment marks of i in bicluster bic. The RL model requires precise state representation and

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tuned reward but also the ability to accommodate complex, noisy, and sparse data present in educational contexts.

2.2.2 Emotional Recognition Systems

In the Emotional recognition systems emphasizes cultivating students' ethical awareness, social responsibility, and emotional intelligence in the development and application of facial recognition technologies. This approach encourages learners to critically examine the societal implications of deploying AI-based facial recognition, particularly concerning privacy, surveillance, discrimination, and consent. Through activities like ethical case analyses, role-playing debates, and reflective writing, students explore real-world issues such as racial bias in facial recognition algorithms, misuse in authoritarian regimes, and approach, game elements such as points, badges, leader boards, challenges, and interactive simulations are integrated into the AI curriculum to support the mastery of clearly defined learning outcomes. These outcomes may include understanding AI concepts, applying machine learning algorithms, solving real-world problems, and demonstrating ethical decision-making. Gamification encourages active learning and persistence by making complex AI topics more accessible and enjoyable. It also provides immediate feedback and progress tracking, helping students visualize their learning journey and stay focused on achieving specific competencies. By blending AI education with gamification techniques, educators can foster deeper understanding, collaborative learning, and long-term skill retention in a dynamic, student- centered environment. Gamification could lead to a focus on extrinsic rather than intrinsic rewards, reducing intrinsic motivation, and potentially leading students away from deeper conceptual understanding.

3. Goals and Challenges

This section examines the outcomes of implementing the OBE ecosystem and its goals, challenges, and some recommendations to manage these challenges.

3.1. Goals

3.1.1 Develop Industry-Relevant AI Skills

Equip students with technical competencies such as data analysis, machine learning, deep learning, and AI model development aligned with real- world demands.

3.1.2 Ensure Mastery of Learning Outcomes

Focus on measurable achievements in cognitive, skills, and affective domains to ensure holistic development.

3.1.3 Enhance Problem-Solving and Critical Thinking

Train learners to analyze complex problems, design intelligent systems, and make informed decisions using AI.

3.1.4 Encourage Lifelong Learning and Adaptability

Prepare students to continuously learn and adapt to evolving AI technologies, tools, and professional practices.

3.2. Challenges

3.2.1 Rapid Technological Advancements

Constant evolution in AI tools, algorithms, and applications makes it difficult to keep learning outcomes and course content up to date. Challenging to create measurable, clear, and specific outcomes for higher-order skills such as ethical decision-making and real-world problem- solving.

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3.2.2 Shortage of Skilled Faculty

Limited number of educators who have both AI expertise and experience in designing and delivering outcomes-based curricula. It requires continuous, performance-based assessments which are more demanding than traditional exams.

3.2.3 Evaluation of Affective Outcomes

Assessing students' ethical reasoning, social responsibility, and professional attitudes is subjective and requires innovative assessment tools.

4. Conclusion

This study highlights the synergistic potential of combining OBE with emerging AI technology for creating effective, learner-centered educational experiences. By organizing curriculum and assessment around explicitly specified cognitive and affective learning outcomes, AI-enhanced OBE assures that students gain theoretical knowledge, practical skills, ethical awareness, and adaptive thinking. The utilization of tools like DL, PL systems, Gamification learning environments, learning analytics, and RL helps students achieve academic success, and prepares students to face challenging real-world challenges. As AI evolves, this framework provides a roadmap to developing inclusive, sustainable, and industry-relevant training models that prepare professionals for the future digital economy.

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Chapter 8

Power Edge Domination Number on Mycielskian of Certain Special Graphs

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Abstract

A dominating set of a graph G is a set S of vertices of G such that any vertex in $V - S$ is adjacent to a vertex in S. For a graph $G = (V, E)$, a subset F of E is called an Edge Dominating set of G if every edge not in F is adjacent to some edge in F. The edge domination number $\gamma(G)$ of G is the minimum cardinality taken over all edge dominating set of G. For a graph $G(V, E)$ with size n, and for any edge $f \in E$, a set $S' - E$ is said to be an power edge dominating set of graph G if each edge $g \in E - S'$ is dominated by the following rules: (i) an edge f in E is in power edge dominating set (in short PEDS), then it dominates itself and dominates all the adjacent edges of f (ii) an observed edge h in E has $m > 1$ adjacent edges and if $m - 1$ of these edges are observed earlier, then the remaining non-observed edge is also observed by $h \in E$. The minimum cardinality of a power edge domination number of G is denoted by $\gamma'_{ped}(G)$. In this project we are determine about power edge domination on Mycielskian of some special graphs.

Keywords: Domination Number, Edge Domination Number, Power Domination Number, Power Edge Domination Number.

1. Introduction

Graph theory has witnessed significant progress in the study of domination since the 20th century. Domination concepts, introduced by Ore in 1962, focus on subsets of vertices or edges that control the structure of a graph. Power domination, formally defined in the late 1990s, has applications in electrical networks, while edge domination extends the notion to edge-based monitoring. The Mycielskian construction, introduced in 1955, allows the generation of triangle free graphs and has been studied in relation to domination. This paper investigates power edge domination in Mycielskian graphs of certain special graphs, providing results and comparisons with classical power domination. Domination in graphs has been widely studied, with variations such as total domination, independent domination, and power domination receiving attention for their theoretical and practical significance. Mycielskian graphs have been employed to study chromatic numbers and domination properties. Research has established formulas and bounds for power domination numbers in cycles, complete graphs, and bipartite graphs. Studies on edge domination have further extended the field by examining middle graphs, total graphs, and shadow graphs. The convergence of Mycielskian transformations and power domination offers fertile ground for exploring new domination parameters. The study focuses on analyzing the power edge domination number for Mycielskian graphs derived from paths, cycles, and comb graphs. For each graph class, we construct the Mycielskian, apply domination definitions, and compute the corresponding values. We establish general formulas supported by illustrative examples. Results are compared with classical power domination numbers to evaluate efficiency.

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1.1. Mycielskian Graph

For a graph $G = (V, E)$, the Mycielskian of G is the graph $\mu(G)$ with vertex set $V \cup V' \cup \{u\}$, where $V' = \{x' : x \in V\}$ and edge set $E \cup \{xy' : xy \in E\} \cup \{y'u : y' \in V'\}$. The vertex x' is called the twin of the vertex x (and x the twin of x') and the vertex u is called the root of $\mu(G)$. For $n \geq 2$, $\mu^n(G)$ is defined iteratively by setting $\mu^n(G) = \mu(\mu^{n-1}(G))$.

2. Main Results on Power Edge Domination Number

2.1 Theorem

For a path P_n , $\gamma'_{ped}(\mu(P_n)) = \left\lfloor \frac{n}{2} \right\rfloor, n \geq 2$

Proof:

Let P_n be the path with vertex set $V = \{v_1, v_2, \ldots v_n\}$ and the edge set $= \{e_1, e_2, \ldots e_{n-1}\}$. To draw Mycielskian graph of path P_n denoted by $\mu(P_n)$) by introducing the shadow vertex set $\{v_1', \ldots, v_n'\}$ and a root vertex u. In order to obtain the power edge dominating set S'. Let us use an illustration.

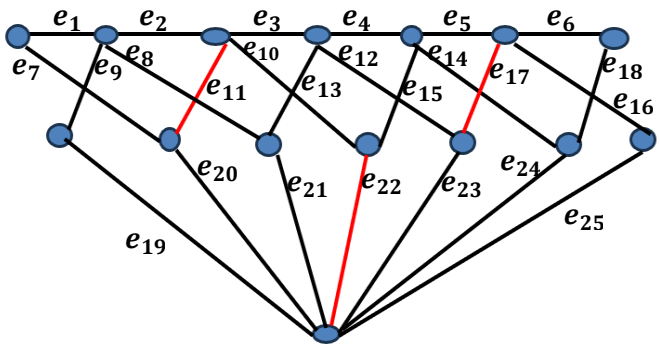

Figure. 1: Mycielskian of path P_7

Choose e_{11} to be in S' then e_{11} dominates $e_2, e_3, e_9, e_{10}, e_{20}$. Now e_8 is the only one non-observed edge for e_{13}, then e_{13} observes e_8, also e_8

observes e_1 and e_1 observes e_7. Since there are no more edges to be observed, we have to choose another edge in S'. Let e_{22} be another edge in S' then e_{22} dominates $e_{13}, e_{15}, e_{19}, e_{20}, e_{21}, e_{22}, e_{23}, e_{24}, e_{25}$. Now e_4 is the only one non-observed edge for e_{12}, then e_{12} observes e_4, also e_6 observes e_{18}. Let e_{17} be another edge in S' then e_{17} dominates $e_{14}, e_{15}, e_{16}, e_{12}$. Thus $\gamma'_{ped}(\mu(P_7))$=3. Proceedings in this way, we get for $n \geq 2$, $\gamma'_{ced}(\mu(P_n)) = \left\lfloor \frac{n}{2} \right\rfloor$.

2.2 Theorem

For a cycle C_n ,$\gamma'_{ped}(\mu(C_n)) = n - 2,\ n \geq 3$.

Proof

Let C_n *b*e the cycle on $n \geq 3$ vertices. Let $V = \{v_1, v_2, \ldots . v_n\}$ be the vertex set and $E = \{e_1, e_2 \ldots e_k\}$ be the edge set. The Mycielskian of a cycle C_n, denoted by $\mu(C_n)$ is obtained using the definition. To obtain the power edge dominating set' of $\mu(C_n)$ let us use an illustration of $\mu(C_5)$.

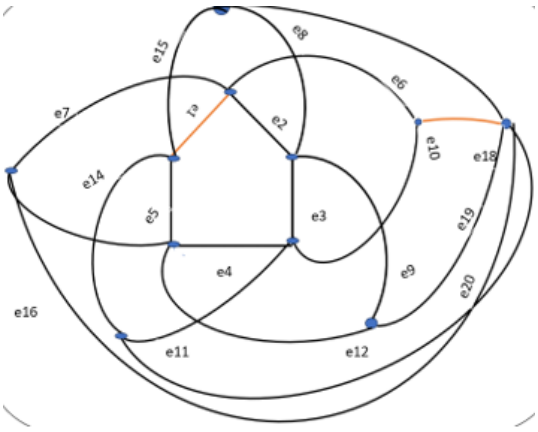

Figure. 2: Mycielskian of Cycle C_5

Let e_{18} to be in the set S', then e18 dominates $e_6, e_{10}, e_{16}, e_{17}, e_{19}, e_{20}$. Since there is no more edges to be observed , we have choose another edge to be in S',then e_1 dominates $e_2, e_6, e_7, e_5, e_{14}, e_{15}$. Next, we have to

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choose another edge to be in S'. Then e_4 dominates $e_3, e_{11}, e_{12}, e_{13}$. Now e_9 is the only one non-observed edge for e_{15}, then e_{15} observes e_8. Thus $\gamma'_{ped}(\mu(C_n))$ =2. Proceeding in this way we get, for ≥ 3, $\gamma'_{ped}(\mu(C_n)) = n - 2$.

2.3 Theorem

let P_n^+be a comb graph, then

$$\gamma'_{ped(\mu(P_n^+))} = \begin{cases} \left(\frac{n}{2}\right) + 1, & for\ n\ is\ \ even \\ \left[\frac{n}{2}\right], & for\ \ n\ is\ \ odd \end{cases}$$

Proof

Let P_n^+ be a comb graph with vertex set $V = \{ v_1, v_2, v_3 \ldots . v_n\}$ and edge set $E = \{e_1, e_2, \ldots e_{n-1}\}$. The Mycielskian of a comb graph $\mu(P_n^+)$is obtained using the definition. To obtain the power edge dominating set S′ of $\mu(P_n^+)$. Let us use an illustration of $\mu(P_2^+)$.

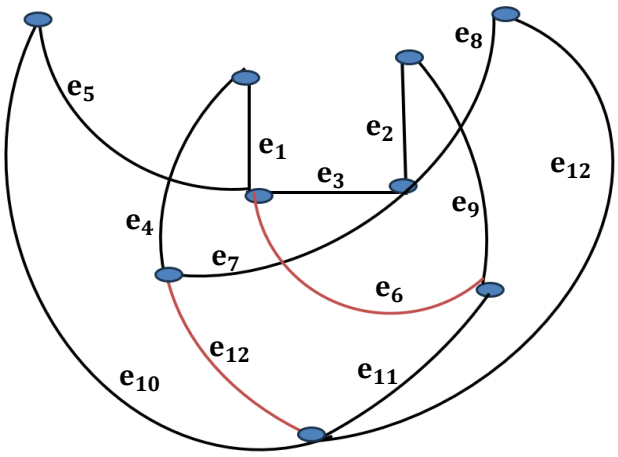

Figure. 3: Mycielskian of Comb P_2^+

Let to be in the set S′, then e_6 dominates $e_1, e_3, e_5, e_9, e_{13}$. Since there are no more edges for domination, we have to choose other edges to

be in S′, then e_{12} dominates e_4, e_7, e_{10}, e_{11}. Now e_8 is the only one observed edge for e_{11}, thus e_{11} observes e_8, thus $\gamma'_{ped(\mu(P_2^+))} = 2$. Proceeding in this way we get

$$\gamma'_{ped(\mu(P_n^+))} = \begin{cases} \left(\frac{n}{2}\right) + 1, \ for\ n\ is\ \ even \\ \left[\frac{n}{2}\right], for\ \ \ n\ is\ \ \ odd \end{cases}$$

3. Comparison Study of Power Domination Number with Power Edge Domination Number

S. No	Graph	Power Domination Number	Power Edge Domination Number
1.	Path	$n-1$	$n-3$
2.	Cycle	$n-1$	$n-2$
3.	Comb	$n-1$	$n-2$

From the above table we could conclude that the power edge domination number is less than the power domination number.

4. Conclusion

This paper examined power edge domination in Mycielskian graphs of paths, cycles, and comb graphs. The results highlight that power edge domination often requires fewer dominating elements than classical power domination, making it a promising tool for efficient network monitoring and optimization. Future work may extend this analysis to other classes of graphs and explore practical applications in communication and power systems.

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Chapter 9

Solvability of Peg Solitaire on Octahedral Graph

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Abstract

Peg solitaire is a single-player board game that involves removing pegs from a board, usually leaving just one peg in the end. In the traditional game, jumps were only allowed to occur in a linear fashion. In this paper the jumps are allowed to occur in any direction since the layout of any graph in graph theory is arbitrary. In order to completely solve board, or graph, these jumps must continue until only one peg remains. This Chapter obtains Peg Solitaire game is solvable, freely solvable on an octahedral graph. Deriving the result of playing Peg Solitaire on these graphs involve finding the optimal sequence of moves that allows to remove all but one peg from the graph, following the game rules. As the game proceeds the goal is to minimize the number of pegs remaining on the board at the end. For derive the result of the game, strategies and logical thinking to plan the moves are required.

Keywords: Solvability; Peg Solitaire; Octahedral graph.

1. Introduction

Peg solitaire is a single-player board game that involves removing pegs from a board, usually leaving just one peg in the end. The game is typically played on a board with holes arranged in a pattern, such

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as a triangular, square, or cross-shaped grid. Each hole initially contains a peg, except for one designated empty hole. The objective of peg solitaire varies depending on the specific version being played, but the most common objective is to remove pegs by "jumping" over them with other pegs, similar to the mechanics of checkers. The rules for jumping vary, but typically, a peg can jump over an adjacent peg, either horizontally or vertically, to land in an empty hole, removing the jumped peg from the board. The jumped peg is then taken off the board. Converting the game concept of Peg Solitaire into graph theory involves representing the game board and its possible moves as a graph. Each position on the Peg Solitaire board can be represented as a node in a graph. The connections between nodes represent legal moves from one position to another. Each node in the graph represents a configuration of the board, with pegs placed in certain positions. Edges in the graph represent valid moves from one board configuration to another. For example, if a peg can be moved from position A to position B in the game, there will be an edge between the corresponding nodes in the graph. This Chapter uses graph theory concepts to optimize Peg Solitaire solutions, such as finding the shortest path to a winning configuration or minimizing the number of moves required to solve a puzzle. It considers the peg solitaire game on octahedral graph and analyses the optimal strategies and explore the complexity of the game on its specific graph structures.

2. Peg Solitaire on Octahedral Graph

An octahedral graph is a specific type of graph that is formed from the octahedron, one of the five Platonic solids. The octahedron is a polyhedron with eight faces, each of which is an equilateral triangle.

The octahedral graph is closely related to the octahedron in that its vertices correspond to the vertices of the octahedron, and its edges correspond to the edges of the octahedron. The following Figure1 shows an octahedral graph with six vertices and 12 edges. The vertices are marked as v_1 , v_2 , v_3, v_4 , v_5 and v_6. All the vertices are having degrees 4.

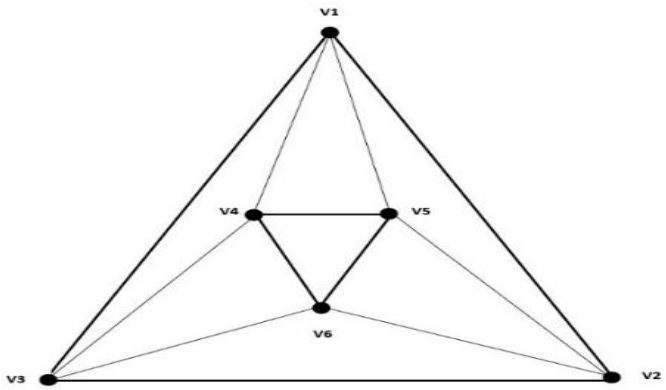

Figure.1: Octahedral Graph

Theorem 2.1

For an octahedral graph *G (V ,E)* with 6 vertices and 12 edges, then peg solitaire is freely solvable for *G*.

Proof.

Let the vertex set V be V=$\{ v_1 , v_2 , v_3, v_4 , v_5, v_6\}$ and the set of edges E be E=$\{e_1 , e_2 , e_3, e_4 , e_5, e_6, e_7 , e_8 , e_9, e_{10} , e_{11}, e_{12}\}$ (Refer Figure1).

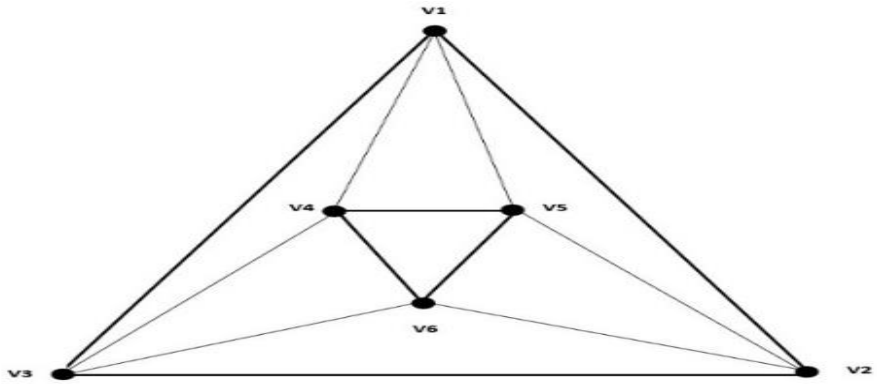

Figure.2

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Here the initial hole is in vertex v_1, the first move can be made from v_3 to v_1 through v_4 by creating a hole in the vertex v_4 and we can continue the game until only one peg remain in the graph. By using the strategic moves the peg solitaire can be solved in an Octahedral Graph.

Case i: Suppose the initial hole in v_1, the vertex in the outer boundary of the graph. The possible moves to solve the game are:

- v_2 to v_1 over v_5
- v_3 to v_5 over v_4
- v_1 to v_2 over v_5
- v_2 to v_3 over v_6

In the final step, only one peg was left out in the graph. Hence, we can say the peg solitaire can be solved in the octahedral graph when the initial hole is in v_1.Similarly, if the initial hole is in v_2 or v_3 which is in the outer boundary can be solved.

Case ii:

Now let's consider the initial hole is in the inner vertex v_4,

So, the possible moves are:

- v_3 to v_4 through v_1 holes in v_3 and v_1.
- v_5 to v_1 through v_4 holes in v_5 and v_4.
- v_1 to v_5 through v_2 , holes in v_1 and v_2.
- The final jump from v_5 to v_4 through v_6 resulting only one peg in v_4. So, the game is solved.

Similarly when the initial hole is in v_5 or v_6,the peg solitaire can be solved.

From the above two cases we can conclude that peg solitaire can be freely solvable in an octahedral graph (i.e. it can be solved from any starting position).

3. Conclusion

The octahedral graph is of interest in graph theory and combinatorics due to its symmetrical structure and its connections to the octahedron and other geometric shapes. It appears in various contexts, including as a configuration space for certain types of molecules in chemistry and as a model for studying the properties of symmetric graphs. For an octahedral graph G (V,E) with 6 vertices and 12 edges, then peg solitaire is freely solvable for G.

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Chapter 10

Harmonious Chromatic Number of At Least One Degree of Vertices in Some Graphs

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Abstract

A harmonious coloring is a proper vertex coloring such that every pair of colors occurs not more than single edge, the smallest quantity of colors in harmonious coloring is a harmonious chromatic number and it is denoted by $\chi_H(G)$. This paper shows that the harmonious chromatic number of at least one degree of vertices in certain graphs like the Hurdle graph Hd_n, Bull graph $B(G)$ and the complement of the Bull graph. Each graph of the vertices has degree at least one, i.e., $d(v_i) \geq 1$, for every vertex $v \in V(G)$ of degree at least 1, the neighbors of v receive distinct colors and also different color pair of vertices.

Keywords: Harmonious coloring; Hurdle graph; Bull graph.

1. Introduction

A graph coloring concept involves in the assignment of colors for the applications of scheduling and resource allocations. A harmonious coloring is a proper vertex coloring, every pair of colors look like together on not exceeding one edge, the least number of colors in

harmonious coloring is a harmonious chromatic number and it is denoted by $\chi_H(G)$ [5][7][10][12][14]. In 1982, Frank Harary and M. J. Plantholt [5] was published the first paper on harmonious coloring. The hurdle graphs and biregular rooted trees in Radio labeling is investigated [10]. The Bull graph was introduced by Weisstein [15]. Graph theory is a rapid growth in recent years can be attributed to its role as a foundational framework supporting modern areas of computer science combinatorial optimization, and operations research [1-6]. Graph - Coloring is an exclusive a part of graph, referred as a color to essentials of a graph subject to specific requirements. Harmonious coloring is distinctive form of graph coloring, every edge has allocated different color pair i.e., the colors orange, green in one edge of its connected vertices, then edges cannot have the same color pair {orange, green} [14]. Harmonious coloring has a potential application in network analysis, telecommunication, airspace, medical research centers and radio navigation systems tell that bad weather conditions and clustering [8, 9,11].

Hurdle graph

A graph attained from a path P_n by appending pendent edges to each internal vertex of a path. It is denoted by $Hd_{n.}$ and it is called Hurdle graph [13] with *(n-2)* hurdles.

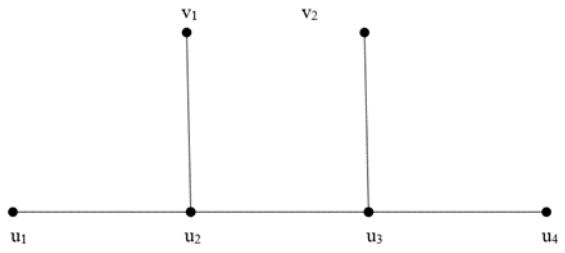

Figure. 1: Hurdle Graph Hd_4

Bull graph

A triangle with two disjoint pendant edges in the graph with *five*

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vertices and *five* edges is the Bull graph *B (G)* [15].

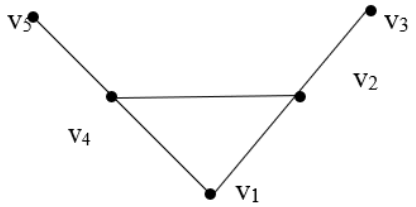


Figure. 2: Bull graph *B (G)*

2. MAIN RESULTS

In this section, it describes a Harmonious Coloring of Hurdle graph and Bull graph, and also its complement.

Theorem 2.1 For a Hurdle Graph, the harmonious coloring of hurdle Graph is n also $\chi_H(Hd_n) \geq 1 + \Delta(Hd_n)$ for $n \geq 4$.

Proof: Let us consider $(2n-2)$ vertices and $(2n-3)$ edges be the hurdle graph.

Assign $(Hd_n) = \{u_i, v_j : 1 \leq i \leq n \text{ and } 1 \leq j \leq n-2\}$ and $E(Hd_n) = \{u_i u_{i+1} : 1 \leq i \leq n-1\} \cup \{u_{i+1} v_i : 1 \leq i \leq n-2\}$.

By the definition of harmonious coloring, same color pairs should not repeat in the graph also no two adjacent vertices having the same colors in the graph.

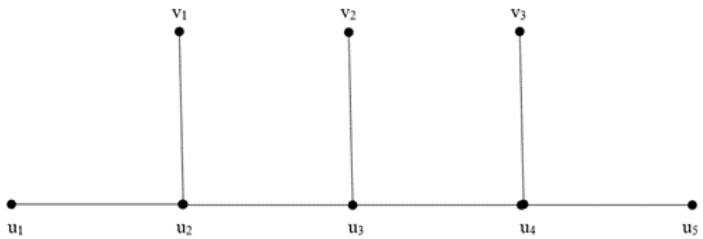


Figure. 3: Hurdle Graph Hd_5.

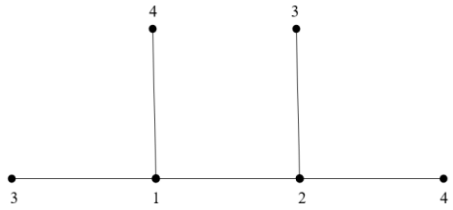
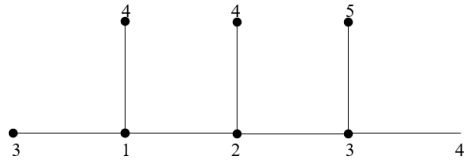
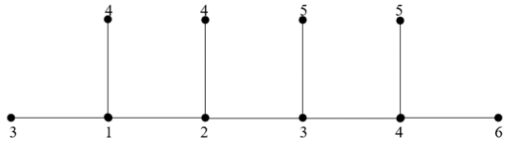
Maximum degree of the Hurdle Graph $\Delta(Hd_n)$ is 3 for $n \geq 4$.

Minimum degree of the Hurdle Graph $\delta((Hd_n)$ is 1 for $n \geq 4$.

Here the vertices take degrees 1, 2, 3 only. We need to assign colors to the vertices in the Hurdle Graph for finding the harmonious

coloring. If we allocate color to the vertex as same color pairs then it's a contradiction to our definition, Hence, the harmonious chromatic number of Hurdle Graph is $\chi_H(Hd_n) = n$, for $n \geq 4$.

Table 1: The harmonious coloring of Hurdle graph.

S.NO.	HURDLE GRAPH	GRAPH	$\chi_H(Hd_n)$
1.	*n=4,*		4
2.	*n=5,*		5
3.	*n=6,*		6

Therefore $\chi_H(Hd_n) \geq 1 + \Delta(Hd_n)$.

Theorem 2.2 For a Bull graph *B (G),* the harmonious chromatic number of Bull graph and harmonious chromatic number of Complement of the Bull Graph *B (G)* is same as *n-1*.

Proof. Let us consider the Bull Graph *B (G)* with *five* vertices and *five* edges. Assign vertices of Bull Graph are $\{v_1, v_2, v_3, v_4, v_5\}$.

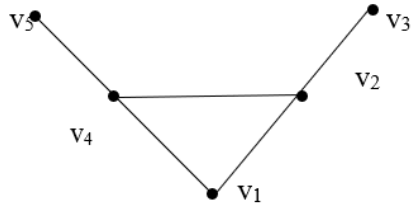


Figure. 4: Bull Graph *B (G)*

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Here $\{v_2, v_4\}$ *two* vertices take degree 3 and $\{v_3, v_5\}$ *two* vertices have degree 1, v_1 have vertex takes degree 2.

Maximum degree *B (G) is 3.* Minimum degree *B (G) is 1.* By the definition of harmonious coloring, same color pairs should not repeat in the graph also no two adjacent vertices having the same colors in the graph.

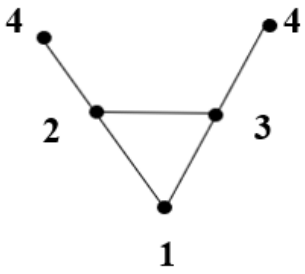

Figure.5: Harmonious chromatic number of Bull Graph χ_H *((B(G)))* = *n-1.*

By the definition of complement of graph, the two vertices have degree *3* and the two vertices has degree *one* and the only one vertex has degree *two*. Each adjacent vertex has assigned different colors. i.e., the harmonious chromatic number on complement of Bull Graph is *n-1*.

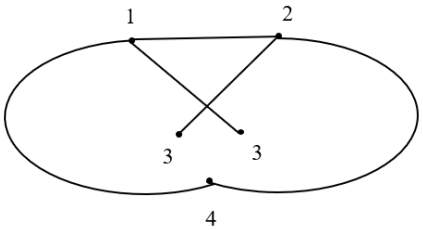

Figure. 6: Complement of Bull Graph *B (G).*

Harmonious chromatic number of Bull Graph = Harmonious chromatic number of Complement of Bull Graph.

3. CONCLUSION

This paper described that the harmonious chromatic number on the Hurdle graph, Bull graph and its complement of bull graph. The

future work will be equipped to extend with the other graphs and also explore its applications.

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Chapter 11

Krill Herd Algorithm-Based Approach for Combined Economic and Emission Dispatch Optimization

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Abstract

This paper addresses the multi-objective economic load dispatch (ELD) problem by simultaneously considering fuel cost and environmental emission functions. The Krill Herd Algorithm (KHA) is employed to obtain optimal solutions for this multi-objective optimization task. The effectiveness of the proposed approach is validated using a six-unit power system. The results demonstrate the algorithm's strong performance in terms of rapid convergence and solution quality.

Keywords: Economic Load Dispatch; Krill Herd Algorithm; Multi-objective Optimization; Emission Reduction;

1. Introduction

In recent times, the planning and operation of power systems have become increasingly challenging for power engineers due to system

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complexity and the growing demand for reliable and continuous electricity supply. A primary objective in power system operation is to deliver this service at the lowest possible cost while maintaining system reliability.

The application of soft computing techniques has significantly impacted the field of power systems, particularly in solving complex optimization problems, owing to their robustness, fast convergence, and reliability [1]. Among these challenges, the Economic Load Dispatch (ELD) problem stands out as a critical non-linear optimization task. It involves minimizing the total fuel cost of generation units over a specific time period, ensuring optimal power allocation while satisfying load demand and adhering to operational constraints, such as ramp rate limits and prohibited operating zones [2].

Several approaches have been proposed to address the ELD problem. S.K. Dash [3] introduced a method combining radial basis function neural networks with heuristic rule-based search and Hopfield neural networks to manage multiple fuel options. Dr. G. Srinivasan et al. [4] utilized a particle swarm optimization (PSO) technique incorporating chaotic sequences and crossover operations to enhance global search performance and prevent premature convergence. Radhakrishnan Anandhakumar et al. [5] proposed a non-iterative Direct Composite Cost Function method for economic dispatch with reduced computational time. Umamaheswari Krishnasamy et al. [6] presented a Refined Teaching–Learning-Based Optimization (RTLBO) algorithm for dynamic economic dispatch integrated with wind power and multiple fuel sources. Additionally, R. Balamurugan et al. [7] developed a self-adaptive mechanism to adjust control parameters during the optimization process for better handling of valve-point

effects and multi-fuel options.

In this study, the Combined Economic and Emission Dispatch (CEED) problem is addressed using the Krill Herd Algorithm (KHA), a nature-inspired metaheuristic optimization technique. The algorithm's performance is evaluated using a standard test system. Furthermore, the self-tuning of KHA parameters is explored, as these parameters play a crucial role in directing the search process and significantly influence the convergence behavior and solution quality.

2. Problem Formulation

2.1. Mathematical Model of Objective Function and Constraints

In this paper two objective functions were considered. First objective is to minimize the total generation cost of generating power plant and the second objective is to minimize the environmental emission of the generating plants.

2.2. Objective I

Economic Generation Cost Function Generation quadratic fuel cost characteristic of generating power plant is formulated as follows:

$$F_T = \text{Min } f(FC) \quad (1)$$

$$f(FC) = \sum_{i=1}^{N} a_i P_i^2 + b_i P_i + c_i$$

2.3. *Objective* II

Emission Objective Function In this paper environmental emission was evaluated with consideration of NO*x* gas. A typical NO*x* emission at thermal power plants can be formulated as shown . Consider the

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following:

$$E_T \text{ Min } \sum_{i=1}^{N} f(E_i(P_i)) \quad (2)$$

$$E_i(P_i) = (\propto_i + \beta_i P_i + \gamma_i P_i^2) + \varepsilon_i \sin(\lambda_i P_i) \quad (3)$$

Now both objectives may be combined in a single objective as given in (4), (5), and (6). The generation cost of each generator was evaluated at its maximum output:

$$F_i(P_{i\,max}) = (a_i P_{i\,max}^2 + b_i P_{i\,max} + c_i) \quad (4)$$

NOx emission of each generator at its maximum output was evaluated:

$$E_i(P_{i\,max}) = (\alpha_i + \beta_i P_{i\,max} + \gamma_i P_{i\,max}^2) \quad (5)$$

By (4) and (5) get

$$\frac{F_i(P_{i\,max})}{E_i(P_{i\,max})} = k_i \quad (6)$$

So the final objective incorporated total generation cost and environmental emission generation which is given as

$$F_{final\_object} = F_T + k_i(E_T) \quad (7)$$

2.4. Power Balance Constraints

The total generated power should be equal to the sum of total load demand and line loss. It can be formulated as (8). Consider the following:

$$\sum_{i=1}^{n} P_i = P_D + P_L \quad (8)$$

$$P_L = \sum_{i=1}^{n} \sum_{j=1}^{n} P_i B_{ij} P_j \quad (9)$$

2.5. Generator Limits Constraint

Generating output of each generating unit should lie between the maximum and minimum limits as given in

$$P_i^{min} \leq P_i \leq P_i^{max} \quad (10)$$

2.6. Lagrangian Formulation for Krill Herd Movement Dynamics

Predation in nature reduces the number of individuals in a krill swarm, thereby decreasing the average krill density and increasing the swarm's distance from the food source. This natural phenomenon is conceptually aligned with the initialization phase of the Krill Herd (KH) algorithm. In the biological system, an individual krill's fitness is influenced by both its proximity to the food source and its position relative to the densest region of the swarm. In the KH algorithm, this fitness is represented by the objective function value, interpreted as an "imaginary distance." The position of each krill over time, on a two-dimensional surface, is dynamically updated based on three key behaviors:

- Movement induced by other krill individuals
- Foraging behavior
- Random diffusion

These three mechanisms collectively guide the swarm's search process toward optimal solutions.

It is known that an optimization algorithm should be capable of searching spaces of arbitrary dimensionality. Therefore, the following Lagrangian model is generalized to an n dimensional decision space:

$$\frac{dX_i}{dt} = N_i + F_i + D_i \quad (11)$$

where Ni is the motion induced by other krill individuals; Fi is the

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foraging motion, and Di is the physical diffusion of the ith krill individuals.

3. Motion induced by other krill individuals

According to theoretical arguments, the krill individuals try to maintain a high density and move due to their mutual effects. The direction of motion induced is estimated from the local swarm density (local effect), a target swarm density (target effect), and a repulsive swarm density (repulsive effect) . For a krill individual, this movement can be defined as:

$$N_i^{new} = N^{max}\alpha_i + \omega_n N_i^{old} \quad (12)$$

where,

$$\alpha_i = \alpha_i^{local} + \alpha_i^{target} \quad (13)$$

and Nmax is the maximum induced speed, xn is the inertia weight of the motion induced in the range [0, 1], N_i^{old} is the last motion induced, a local i is the local effect provided by the neighbors and a target i is the target direction effect provided by the best krill individual. According to the measured values of the maximum induced speed , it is taken 0.01 (ms). The effect of the neighbors can be assumed as an attractive/repulsive tendency between the individuals for a local search. In this study, the effect of the neighbors in a krill movement individual is determined as follows:

$$\alpha_i^{local} = \sum_{j=1}^{NN} \hat{K}_{i,j}\,\hat{X}_{i,j} \quad (14)$$

$$\hat{X}_{i,j} = \frac{X_j - X_i}{\|X_j - X_i\| + \xi} \quad (15)$$

$$\hat{K}_{i,j} = \frac{K_i - K_j}{K^{worst} - K^{best}} \quad (16)$$

where $K^{worst}$and $K^{best}$are the best and the worst fitness values of the krill individuals so far; Ki represents the fitness or the objective function value of the ith krill individual; Kj is the fitness of jth (j = 1,2,. . .,NN) neighbor; X represents the related positions; and NN is the number of the neighbors. For avoiding the singularities, a small positive number, e, is added to the denominator. The right sides of Eqs. contain some unit vectors and some normalized fitness values. The vectors show the induced directions by different neighbors and each value presents the effect of a neighbor. The neighbors' vector can be attractive or repulsive since the normalized value can be negative or positive. For choosing the neighbor, different strategies can be used. For instance, a neighborhood ratio can be simply defined to find the number of the closest krill individuals. Using the actual behavior of the krill individuals, a sensing distance (ds) should be determined around a krill individual (as shown in Fig. 1) and the neighbors should be found. The sensing distance for each krill individual can be determined using different heuristic methods. Here, it is determined using the following formula for each iteration:

$$d_{s,i} = \frac{1}{5N}\sum_{j=1}^{N}\left\|X_i - X_j\right\| \qquad (17)$$

Where, ds,i is the sensing distance for the ith krill individual and N is the number of the krill individuals. The factor 5 in the denominator is empirically obtained. Using Eq. (17), if the distance of two krill individuals is less than the defined sensing distance, they are neighbors.

The known target vector of each krill individual is the lowest fitness of an individual krill. The effect of the individual krill with the best fitness on the ith individual krill is taken into account using Eq. (18).

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This level leads it to the global optima and is formulated as:

$$\alpha_i^{target} = C^{best}\hat{K}_{i,best}\hat{X}_{i,best} \quad (18)$$

where, C^{best} is the effective coefficient of the krill individual with the best fitness to the ith krill individual. This coefficient is defined since a target i leads the solution to the global optima and it should be more effective than other krill individuals such as neighbors. Here in, the value of C^{best} is defined as:

$$C^{best} = 2\left(rand + \frac{I}{I_{max}}\right) \quad (19)$$

where rand is a random values between 0 and 1 and it is for enhancing exploration, I is the actual iteration number and I_{max} is the maximum number of iterations.

3.1. Foraging motion

The foraging motion is formulated in terms of two main effective parameters. The first one is the food location and the second one is the previous experience about the food location. This motion can be expressed for the ith krill individual as follows:

$$F_i = V_f\beta_i + \omega_f F_i^{old} \quad (20)$$

where

$$\beta_i = \beta_i^{food} + \beta_i^{best} \quad (21)$$

and V_f is the foraging speed, ω_f is the inertia weight of the foraging motion in the range [0, 1], is the last foraging motion, $\beta_i^{food}$is the food attractive and β_i^{best} is the effect of the best fitness of the ith krill so far. According to the measured values of the foraging speed , it is taken 0.02 (ms-1). The food effect is defined in terms of its location. The center of food should be found at first and then try to formulate

food attraction. This cannot be determined but can be estimated. In this study, the virtual center of food concentration is estimated according to the fitness distribution of the krill individuals, which is inspired from "center of mass". The center of food for each iteration is formulated as:

$$X^{food} = \frac{\sum_{i=1}^{N} \frac{1}{K_i} X_i}{\sum_{i=1}^{N} \frac{1}{K_i}} \qquad (22)$$

Therefore, the food attraction for the ith krill individual can be determined as follows:

$$\beta_i^{food} = C^{food} \widehat{K}_{i,food} \widehat{X}_{i,food} \qquad (23)$$

where C^{food} is the food coefficient. Because the effect of food in the krill herding decreases during the time, the food coefficient is determined as:

$$C^{food} = 2\left(1 - \frac{I}{I_{max}}\right) \qquad (24)$$

The food attraction is defined to possibly attract the krill swarm to the global optima. Based on this definition, the krill individuals normally herd around the global optima after some iteration. This can be considered as an efficient global optimization strategy which helps improving the globality of the KH algorithm. The effect of the best fitness of the ith krill individual is also handled using the following equation:

$$\beta_i^{best} = C^{best} \widehat{K}_{i,ibest} \widehat{X}_{i,ibest} \qquad (25)$$

where Kibest is the best previously visited position of the ith krill individual.

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3.2. Physical diffusion

The physical diffusion of the krill individuals is considered to be a random process. This motion can be express in terms of a maximum diffusion speed and a random directional vector. It can be formulated as follows:

$$D_i = D^{max}\delta \tag{26}$$

$$D_i = D^{max}\left(1 - \frac{I}{I_{max}}\right)\delta \tag{27}$$

3.3. Motion Process of the KH Algorithm

The physical diffusion performs a random search in the proposed method. Using different effective parameters of the motion during the time, the position vector of a krill individual during the interval t to t + Δt is given by the following equation:

$$X_i(t + \Delta t) = X_i(t) + \Delta t\frac{dX_i}{dt} \tag{28}$$

It should be noted that Δt is one of the most important constants and should be carefully set according to the optimization problem. This is because this parameter works as a scale factor of the speed vector. Δt t completely depends on the search space and it seems it can be simply obtained from the following formula:

$$\Delta t = C_t\sum_{j=1}^{Nv}\left(UB_j - LB_j\right) \tag{29}$$

where NV is the total number of variables, and LBj and UBj are lower and upper bounds of the jth variables (j = 1,2,. . .,NV), respectively. Therefore, the absolute of their subtraction shows the search space. It is empirically found that Ct is a constant number between [0, 2]. It is also obvious that low values of Ct let the krill individuals to search

the space carefully.

3.4. Genetic operators

To improve the performance of the algorithm, genetic reproduction mechanisms are incorporated into the algorithm. The introduced adaptive genetic reproduction mechanisms are crossover and mutation which are inspired from the classical DE algorithm.

3.5. Crossover

The crossover operator is first used in GA as an effective strategy for global optimization. A vectorized version of the crossover is also used in DE which can be considered as a further development to GA. In this study, an adaptive vectorized crossover scheme is employed. The crossover is controlled by a crossover probability, Cr, and actual crossover can be performed in two ways: (1) binomial and (2) exponential. The binomial scheme performs crossover on each of the d components or variables/parameters. By generating a uniformly distributed random number between 0 and 1, the mth component of Xi ,Xi,m, is manipulated as:

$$X_{i,m} = \begin{cases} X_{r,m} & \text{rand}_{i,m} < C_r \\ X_{i,m} & \text{else} \end{cases} \quad (30)$$

$$C_r = 0.2\widehat{K}_{i,best} \quad (31)$$

3.6. Mutation

The mutation plays an important role in evolutionary algorithms such as ES and DE. The mutation is controlled by a mutation probability (Mu). The adaptive mutation scheme used herein is formulated as:

$$X_{i,m} = \begin{cases} X_{gbes,m} + \mu(X_{p,m} - X_{q,m}) & \text{rand}_{i,m} < Mu \\ X_{i,m} & \text{else} \end{cases} \quad (32)$$

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$$\text{Mu} = {}^{0.05}\Big/_{\widehat{\text{K}}_{\text{i,best}}} \tag{33}$$

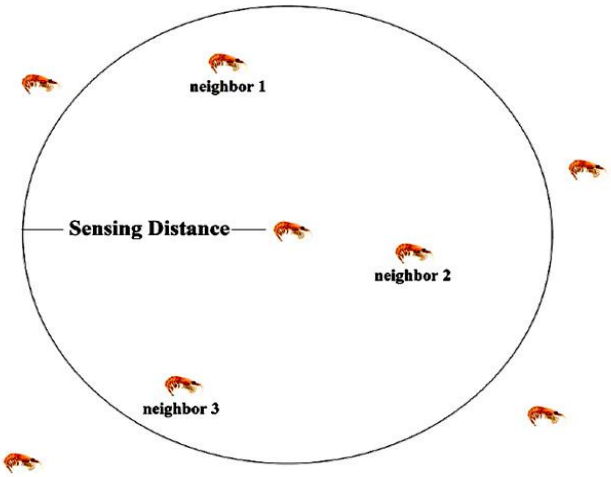

Figure. 1: Schematic representation of Sensing Distance around a krill individual

4. Methodology of the KH algorithm

Various krill-inspired algorithms can be developed by idealizing the motion characteristics of the krill individuals. Generally,the KH algorithm can be introduced by the following steps:

I. Data Structures: Define the simple bounds, determination of algorithm parameter(s) and etc.

II. Initialization: Randomly create the initial population in the search space.

III. Fitness evaluation: Evaluation of each krill individual according to its position.

IV. Motion calculation:

- Motion induced by the presence of other individuals,
- Foraging motion
- Physical diffusion

V. Implement the genetic operators

VI. Updating: updating the krill individual position in the search space.

VII. Repeating: go to step III until the stop criteria is reached.

VIII. End

5. Result

In this study, the Krill Herd Algorithm (KHA) is applied to solve the Combined Economic and Emission Dispatch (CEED) problem for the IEEE 30-bus test system with a total load demand of 283.4 MW. The simulation results, are given in table-1

Table1: Results of IEEE 30 bus systems for the load of 283.4MWwith line loss

Unit power output	**CPSO [20]**	**WIPSO [20]**	**MRPSO [20]**	**Proposed KHA with minimum Emission**	**Proposed KHA with minimum Fuel cost**
*P*1 (MW)	146.034	147.581	145.7801	146.564	146.0885
*P*2 (MW)	46.0732	46.889	43.0912	42.0854	46.836
*P*5 (MW)	34.0742	47.0705	43.07654	42.1506	34.084
*P*8 (MW)	26.0198	16.7863	24.0763	25.3844	25.0125
*P*11 (MW)	24.108	24.7219	23.1732	24.3856	24.8
*P*13 (MW)	26.0911	19.8925	23.0453	22.1458	25.248
Loss (MW)	19.0003	19.5407	18.8468	18.584	18.352
Fuel cost($/h)	2607622	2661327	2575426	2607638	2575419
Total power output	302.4	302.940	302.2468	302.7191	302.0092
Emission (Ton/h)	162228.5	167729	162153.6	162145.1	163338.9

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6. Conclusion

In this paper, the Krill Herd Algorithm (KHA) is applied to solve the combined economic and emission dispatch problem using a six-unit system as a test case. The results obtained are compared with those from other soft computing techniques. The comparison demonstrates that KHA delivers superior performance, exhibiting faster and more stable convergence behavior. Key advantages of the algorithm include high-quality solutions, consistent convergence characteristics, and strong computational efficiency. These findings suggest that KHA is a promising and effective approach for addressing complex optimization problems in power system operations.

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Chapter 12

A Flower Pollination Algorithm Approach or Optimal Reactive Power Dispatch

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Abstract

This paper proposes an effective and robust evolutionary optimization technique, known as the Flower Pollination Algorithm (FPA), to address the Optimal Reactive Power Dispatch (ORPD) problem in power systems. The performance of the proposed FPA is evaluated using the standard IEEE 30-bus test system, where control variables include bus voltages, transformer tap settings, and reactive power sources. The objective functions considered are the minimization of active power transmission losses, total voltage deviation, and enhancement of the voltage stability index. The results obtained using FPA are compared with those from other recently developed evolutionary algorithms reported in the literature. Simulation outcomes demonstrate that FPA provides superior performance in terms of solution quality, effectiveness, and convergence speed, making it a promising tool for solving the ORPD problem.

Keywords Optimal Reactive Power Dispatch; Flower Pollination

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Algorithm; Loss Minimization; Voltage Stability; ORPD;

1. Introduction

The Optimal Reactive Power Dispatch (ORPD) problem is recognized as one of the more challenging optimization tasks in power system operation. Reactive power sources include generators, synchronous condensers, capacitor banks, static compensators, and tap-changing transformers. The primary goal in reactive power optimization is to determine the appropriate levels of reactive power generation at various locations in the system to optimize a given objective function.

In essence, the ORPD problem involves the efficient utilization of generator voltage magnitudes, transformer tap settings, and reactive power source outputs to minimize transmission losses and enhance the system's voltage stability. This results in a complex, nonlinear optimization problem.

Historically, several mathematical methods have been applied to address this issue, including the gradient method [1–2], Newton's method [3], and linear programming approaches [4–7]. However, these conventional techniques often encounter limitations, particularly in handling inequality constraints and maintaining accuracy. For instance, the gradient and Newton methods struggle with constraint handling, while linear programming requires linear approximation of nonlinear relationships, which may lead to reduced accuracy.

To overcome these limitations, global optimization techniques such as Genetic Algorithms (GAs) have been explored [8–9]. GAs, inspired by the process of natural selection, are stochastic search methods that have been effectively applied to solve the voltage-constrained reactive power dispatch problem. These algorithms determine the

optimal settings of generator voltages, transformer taps, and reactive source outputs, aiming to reduce transmission losses and improve voltage stability. Test results using the IEEE 30-bus system have shown that GAs can achieve near-optimal solutions with lower computational burden and consistent performance [10].

In the present study, the Flower Pollination Algorithm (FPA) is employed to solve the ORPD problem with a focus on improving computational efficiency and convergence behavior. The algorithm is tested on the IEEE 30-bus standard power system. The performance of the proposed FPA approach is benchmarked against other computational intelligence techniques, and the simulation results demonstrate its superior performance in terms of convergence speed and solution quality.

2. Problem Formulation

ORPD problem is, mainly, concerned with either minimisation of PLoss or that of TVD or improvement of VSI, satisfying various equality and inequality constraints.

2.1. Minimisation of Ploss

The general formulation of Ploss minimisation problem may be expressed as follows

$$\text{minimize } J_1(x_1, x_2)$$

$$= \text{minimize } P_{loss}$$

$$= \sum_{K=1}^{NL} \left[G_k \left(V_p^2 + V_q^2 - 2V_p V_q \cos\delta_{pq} \right) \right] \quad (1)$$

subject to

$$\begin{Bmatrix} g(X_1, X_2 = 0) \\ h(X_1, X_2 \leq 0) \end{Bmatrix} \quad (2)$$

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where $J_1(x_1, x_2)$ is the active power transmission loss minimisation function, X_1 is the vector of dependent variables consisting of load voltages $(V_{L1}, \ldots, V_{LN_{PQ}})$ generators' reactive powers $(Q_{G1}, \ldots, Q_{GN_{PV}})$ and transmission line loadings $(S_{L1}, \ldots, V_{LN_L})$ X_2 is the vector of control variables consisting of generators' voltages $(V_{G1}, \ldots, V_{GN_{PV}})$ transformers' tap settings $(T_1, \ldots, T_{N_T})$ and reactive power injections $(Q_{C1}, \ldots, Q_{CN_C})$, G_k is the conductance of branch k, V_p, V_q are voltages of the pth and the qth buses, respectively and δ_{pq} is the voltage angle difference between buses p and q. Therefore X_1 and X_2 may be expressed as

$$X_1 = [V_{L1}, \ldots \ldots V_{LN_{PQ}}, Q_{G1}, \ldots\ldots Q_{GN_{PV}}, S_{L1} \ldots\ldots, S_{LN_L} \quad (3)$$

$$X_2 = [V_{G1}, \ldots\ldots V_{GN_{PV}}, T_1, \ldots\ldots T_{N_T}, Q_{C1} \ldots\ldots Q_{CN_C}] \quad (4)$$

where NPV is the number of generator buses, NPQ is the number of load buses, NL is the number of transmission lines, NT is the number of tap setting transformer branches and NC is the number of capacitor banks.

2.2. Minimisation of TVD

The general formulation of TVD minimisation objective may be stated as in (5)

$$\text{minimize } J_2(x_1, x_2) = \text{ minimize TVD} = \sum_{P=1}^{N_{PQ}} \left| V_P - V_P^{ref} \right| \quad (5)$$

where J2(x1, x2) is the TVD minimisation objective function, Vp is the voltage at bus p and V_P^{ref} is the desired value of the voltage magnitude of the pth bus, taken as 1 pu.

2.3. Improvement of VSI

The general objective of VSI improvement problem may be stated as in (6)

Minimise $J_3(X_1, X_2)$ = Minimise (Lmax)

$$= \min[\ \max(LK)], \quad K=1,2\ N\ P\ Q \tag{6}$$

where Lk is the voltage stability indicator (L-index) of the kth node. The value of Lk may be written as

$$L_k = \left|1 - \sum_{P=1}^{NPV} m_{qp} \frac{Vp}{Vq} < \{\lambda pq + (\theta_p - \theta_q)\}\right| \tag{7}$$

where Mqp are the (p, q)th components of the sub-matrices obtained from partial inversion of Ybus matrix.

The value of Mqp is given by (8)

$$M_{qp} = -[Y_{qq}]^{-1}[Y_{qp}] \tag{8}$$

where λpq is the phase angle of Mqp, θp, θq are phase angles of the pth and the qth bus voltages, respectively, Yqq is the self-admittance term of the qth bus and Yqp is the mutual admittance between the qth and pth buses.

2.4. Equality constraints

Constraints representing the load flow equations given by (9)

$$\begin{cases} P_{G_P} - P_{L_P} = \sum_{q=1}^{NB} V_p\ ||V_q(G_{pq}\cos\delta_{pq} + B_{Pq}\sin\delta_{pq}) \\ Q_{G_P} - Q_{L_P} = \sum_{q=1}^{NB} Vp||Vq(\ G_{pq}\sin\delta_{pq} - B_{pq}\cos\delta_{pq} \end{cases} \tag{09}$$

where PGp, QGp are injected active and reactive powers, at the pth bus, respectively, PLp , QLp are active and reactive power demands,

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at the pth bus, respectively, Gpq, Bpq are transfer conductance and susceptance, between the pth and the qth buses, respectively and NB is the number of buses.

3. Inequality constraints

3.1. Generator constraints

For all the generator voltages (including slack bus), real and reactive power outputs (including slack bus) must be restricted within their lower and upper limits as stated in (10)

$$\begin{cases} V_{G_P}^{Min} \leq V_{G_P} \leq V_{G_P}^{Max}, p = 1,2, \dots \dots . N_{PV} \\ V_{G_P}^{min} \leq Q_{G_P} \leq Q_{G_P}^{max}, P = 1,2 \dots \dots \dots N_{PV} \end{cases} \quad (10)$$

3.2. Transformer constraints

Transformer tap settings must be within their specified lower and upper limits as presented in (11)

$$T_{G_P}^{min} \leq Q_{G_P} \leq Q_{G_P}^{max}, p = 1,2 \dots \dots . . N_T \quad (11)$$

3.3. Shunt VAR compensator constraints

Reactive power outputs of shunt VAR compensators must be restricted within their lower and upper limits as written in (12)

$$Q_{C_P}^{min} \leq Q_{C_P} \leq Q_{C_P}^{max} \; p = 1,2 \dots \dots N_C \quad (12)$$

3.4. Security constraints

These include the constraints on voltages at load buses and transmission line loadings. Each of these constraints must be within their lower and upper operating limits, as expressed in (13) and (14), respectively

$$V_{L_P}^{min} \leq \mathrm{V}_{L_P} \leq V_{L_P}^{max}, p = 1,2 \ldots \ldots \ldots, N_{PQ} \quad (13)$$

$$S_{L_P} \leq S_{L_P}^{max}, p = 1,2 \ldots \ldots \ldots N_L \quad (14)$$

4. Nature-inspired Flower Pollination Algorithm

The flower reproduction is ultimately through pollination. Flower pollination is connected with the transfer of pollen, and such transfer of pollen is related with pollinators such as insects, birds, animals etc. some type of flowers depend only on specific type of insects or birds for successful pollination. Two main forms of pollination are A-biotic and biotic pollination. 90% of flowering plants are belonging to biotic pollination process. That is, the way of transferring the pollen through insects and animals. 10% of pollination takes A-biotic method, which doesn't need any pollinators. Through Wind and diffusion help pollination of such flowering plants and a good example of A-biotic pollination is Grass [10, 11]. A good example of pollinator is Honey bees, and they have also developed the so-called flower constancy. These pollinators tend to visit exclusively only certain flower species and bypass other flower species. Such type of flower reliability may have evolutionary advantages because this will maximize the transfer of flower pollen .Such type of flower constancy may be advantageous for pollinators also , because they will be sure that nectar supply is available with their some degree of memory and minimum cost of learning, switching or exploring. Rather than focusing on some random, but potentially more satisfying on new flower species, and flower dependability may require minimum investment cost and more likely definite intake of nectar [12]. In the world of flowering plants, pollination can be achieved by self-pollination or crosspollination. Cross-pollination means the

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pollination can occur from pollen of a flower of a different plant, and self-pollination is the fertilization of one flower, such as peach flowers, from pollen of the same flower or different flowers of the same plant, which often occurs when there is no dependable pollinator existing.

Biotic, crosspollination may occur at long distance, by the pollinators like bees, bats, birds and flies can fly a long distance. Bees and Birds may behave as Levy flight behaviour [13], with jump or fly distance steps obeying a Levy allotment. Flower fidelity can be considered as an increment step using the resemblance or difference of two flowers. The biological evolution point of view, the objective of the flower pollination is the survival of the fittest and the optimal reproduction of plants in terms of numbers as well as the largely fittest. The flower reproduction is done through pollination process. Flower pollination is connected with the relocation of pollen and such transfer of pollen is related with pollinators such as insects, birds, animals etc.

The major two pollination are A-biotic and biotic pollination. 90% of flowering plants are belonging to biotic pollination process. That is, the way of transferring the pollen through insects and animals. 10% of pollination takes Abiotic method, which doesn't need any pollinators. . Through Wind and diffusion help pollination of such flowering plants and a good example of A-biotic pollination is Grass. A very good example of pollinator is Honey bees, and they have also developed the so-called flower constancy. These pollinators tend to visit exclusively only certain flower species and bypass other flower species. Such type of flower reliability may have evolutionary advantages because this will maximize the transfer of flower pollen .

4.1. Rules for Flower Pollination Algorithm

1. Biotic and cross-pollination is considered as global pollination

process with pollen- carrying pollinators performing Levy flights.

2. Abiotic and self-pollination are considered as local pollination.

3. Flower constancy can be considered as the reproduction probability is proportional to the similarity of two flowers involved.

4. Local pollination and global pollination is controlled by a switch probability Pa∈ [0, 1]. Due to the physical proximity and other factors such as wind, local pollination can have a significant fraction pa in the overall pollination activities.

4.2. Mathematical representation of Flower Pollination Algorithm

The first rule plus flower constancy can be represented mathematically as

$$x_i^{t+1} = X_i^t + L(X_i^t - g_*) \quad (15)$$

where X_i^t is the pollen i or solution vector X_i at iteration t, and g_* is the current best solution found among all solutions at the current generation/iteration.

4.3. Levy distribution is given by

$$L \sim \frac{\lambda \Gamma \sin\left(\frac{\pi\lambda}{2}\right)}{\pi} \frac{1}{S^{1+\lambda}}, (S \gg S_0 > 0) \quad (16)$$

where L is the strength of the pollination should be greater than zero, Γ(λ) is the gamma function and this distribution is valid for large steps s > 0.

The local pollination can be represented as

$$x_i^{t+1} = X_i^t + \varepsilon\left(X_j^t - X_k^t\right) \quad (17)$$

where, X_j^t and X_k^t are pollens from the different flowers of the same plant species. This essentially mimic the flower constancy in a limited

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neighbourhood. Mathematically, if X_j^t and X_k^t comes from the same species or selected from the same population, this become a local random walk if we draw from a uniform distribution in [0,1].

4.4. Switch probability or proximity probability (pa)

Most flower pollination activities can occur at both local and global scale. In practice, adjacent flower patches or flowers in the not-so-far-away neighbourhood are more likely to be pollinated by local flower pollens that those far away. For this, we use a switch probability (Rule 4) or proximity probability pa to switch between common global pollination to intensive local pollination. in this simulation we used pa=0.6 and pa=0.8 to analyse the simulation result.

4.5. Pseudo code of Flower Pollination Algorithm (FPA)

Objective min or max f(x), x = (x1, x2, …, xd)

Initialize a population of n flowers/pollen gametes with random solutions

Find the best solution g_* in the initial population

Define a switch probability Pa∈ [0, 1].

while (t <MaxGeneration)

for i = 1 n (all n flowers in the population)

if rand < pa,

Draw a (d-dimensional) step vector L which obeys a Levy distribution

Global pollination via $x_i^{t+1} = X_i^t + L(X_i^t - g_*)$

else

Draw ε from a uniform distribution in [0,1]

Randomly choose j and k among all the solutions

Do local pollination via $x_i^{t+1} = X_i^t + \varepsilon(X_j^t - X_k^t)$

end if

Evaluate new solutions

If new solutions are better, update them in the population

end for

Find the current best solution g_*

end while

5. Simulation Results

FPA based results of the ORPD problem for Ploss, TVD and L-index minimisation objective of this test system is presented in Table 1. These results are compared with those offered by the algorithms such as KHA and CKHA.

Table 1: Best control variable settings for power loss, TVD and L-index minimisation

Control variables	KHA [18]	CKHA [18]	Proposed FPA For Loss Minimization	Proposed FPA For TVD Minimization	Proposed FPA For L-index Minimization
V_{G1}	1.05	1.05	1.05	1.05	1.05
V_{G2}	1.0381	1.0473	1.0278	1.0256	1.02389
V_{G5}	1.011	1.0293	1.0293	1.0238	1.0229
V_{G8}	1.025	1.035	1.028	1.016	1.012
V_{G11}	1.05	1.05	1.05	1.05	1.05
V_{G13}	1.05	1.05	1.05	1.05	1.05
T_{11}	0.9541	0.9916	0.9686	0.9548	0.9489
T_{12}	1.0412	0.9538	1.9538	1.9486	1.9369
T_{15}	0.9514	0.9603	0.9331	0.9327	0.9347
T_{36}	0.9541	0.967	0.948	0.948	0.946
QC_{10}	0.0089	0.0092	0.0092	0.0091	0.0097
QC_{12}	0	0	0	0	0
QC_{15}	0.0141	0.0153	0.0148	0.0139	0.0127
QC_{17}	0.04989	0.0497	0.0495	0.0492	0.0492
QC_{20}	0.0314	0.0302	0.0301	0.03	0.03

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QC_{21}	0.0345	0.05	0.045	0.033	0.041
QC_{23}	0.0241	0.0134	0.0234	0.0231	0.0238
QC_{24}	0.05	0.05	0.05	0.05	0.04
QC_{29}	0.0107	0.0121	0.0111	0.0118	0.0116
Ploss, MW	3.65	3.24	3.21	3.52	3.71
TVD, pu	1.3415	1.3364	1.3856	1.3356	1.3589
L-index, pu	0.1425	0.1402	0.1416	0.1437	0.1376

6. Conclusion

In this paper, the Flower Pollination Algorithm (FPA) is proposed as a solution to the Optimal Reactive Power Dispatch (ORPD) problem in power systems characterized by varying levels of dimensionality and complexity. To evaluate the effectiveness and robustness of the proposed approach, it is applied to the standard IEEE 30-bus power system. The simulation results obtained using FPA are compared with those produced by other well-known techniques recently reported in the literature. The comparison clearly demonstrates that the proposed FPA offers improved efficiency, greater flexibility, and enhanced stability, making it a promising tool for solving complex ORPD problems.

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Chapter 13

Unveiling the Adjuvant Therapeutic Potential of Dabrafenib Derivatives in Lung Adenocarcinoma via in Silico Multi-Targeting of B-RAF, NEK11, AND S1K1

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Abstract

The most prevalent subtype of non-small cell lung cancer (NSCLC) is lung adenocarcinoma (LUAD), which is distinguished by a high prevalence, a high death rate, and few available treatment choices. Because of its intricate signalling network, LUAD necessitates multiple-targeted therapy. Here, we evaluate Dabrafenib's effectiveness as a novel B-RAF, NEK11, and S1K1 target drug in LUAD, exploring a repurposing possibility for this selective B-RAF inhibitor, already approved for malignant melanoma. Pharmacokinetic characteristics, molecular interactions, and toxicity profiles of dabrafenib were evaluated using in silico methods. SwissADME confirmed favourable drug-likeness, including compliance with Lipinski's Rule of Five. Dabrafenib derivatives showed high binding affinities against all three target proteins, according to CB-Dock simulations. The OH-derivative had the highest

binding affinity for NEK11 (−11.0 kcal/mol). ProTox-II predicted minimal cytotoxicity and mutagenicity, along with moderate organ-specific toxicities. These findings support the hypothesis that dabrafenib may serve as a novel adjuvant therapy to inhibit multiple LUAD-related kinases.

Keywords: Molecular Docking; Dabrafenib; B-Raf; SIK1; NEK11; Lung Adenocarcinoma

1. Introduction

Cancer is a group of disease characterized by the uncontrolled growth of cells and spread to the other parts of the body. It is a genetic disease caused by changes to genes that control the way our cell function. Lung cancer is a grave and potentially fatal disease marked by the unchecked proliferation of abnormal cells within the lungs, which are essential for facilitating the exchange of gases between the air we inhale and our bloodstream. Adenocarcinoma of the lung is a complex and multifaceted disease that presents unique challenges in diagnosis and treatment. Its prevalence among non-smokers, particularly women, sets it apart from other lung cancer subtypes and underscores the importance of considering factors beyond tobacco use in lung cancer screening and prevention strategies.

The disease's tendency to develop in the lung periphery can make early detection challenging, but its relatively slow progression provides a window of opportunity for intervention if caught early through routine imaging studies. In most non-smokers who develop adenocarcinoma, specific genetic mutations, such as alterations in the EGFR (epidermal growth factor receptor), ALK (anaplastic lymphoma kinase), or ROS1 genes, can be identified. These mutations can drive the initiation and progression of cancer,

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particularly in patients with no history of tobacco use. The pathogenesis of lung adenocarcinoma involves the transformation of normal epithelial cells into malignant ones through a series of genetic and molecular changes. These changes lead to uncontrolled cell growth, resistance to programmed cell death (apoptosis), and the ability to invade nearby tissues and spread to other organs.

Adenocarcinoma often forms glandular structures and can produce mucus, indicating its origin from glandular cells. It is characterized by early metastasis, frequently spreading to the lymph nodes, brain, liver, bones, and adrenal glands. The management of lung adenocarcinoma has evolved significantly in recent years, with the advent of targeted therapies and immunotherapies complementing traditional treatment modalities. These advancements have led to improved outcomes for many patients, especially those with specific genetic mutations that can be targeted by precision medicines. However, the heterogeneity of adenocarcinoma means that treatment must be tailored to each individual case, considering factors such as tumor stage, molecular profile, and overall patient health. Despite progress in treatment options, ongoing research is crucial to further improve survival rates and quality of life for patients with this common form of lung cancer.

2. Materials and Methods

CBDOCK 2 tools is designed to predict the binding of small molecules with known target protein. In the active sites of target protein, binding energies of the small molecules are determined based on their binding mechanism. Biovia Discovery studio visualizer are used to visualize the ligand position in the enzyme binding site. To know the binding nature and for the development of potential drug molecules it is very

useful. ADME, molecular properties and toxicity of title compounds were also evaluated by the online tool in the organic portal.

2.1. Software Required

CB dock and discovery studio were downloaded. Chemsketch for sketching and chem 3D pro for energy minimization and convert chemsketch into sdf format.

2.2. Predictions of physiochemical properties and ADMET

In the drug discovery process, physicochemical properties by 5-Lipinski's rule observed for predicting the bioactive drug in oral route. In pharmacokinetic studies, screening of ADME properties evaluated for understanding their bioavailability. Additionally, molecular properties and toxicity were evaluated by the online tool in the organic portal web of SwissADME, Protox 3.0 & ADMET.

2.3. Molecular Docking

Computer Aided drug design is one of the tools which plays a vital role in understanding the structure activity relationship, binding energy, interaction between the protein and ligand, binding affinity etc. On this program, CB dock was widely used in evaluating the binding studies of our ligand with our target enzymes. This program helps us to predict how these small molecules of synthesized derivatives may bind with the targeted enzyme BRAF, Nek11, SIK1. . rcsb.org/ pdb (RCSB Protein Data Bank (PDB) database) and drug bank was used to retrieve the targeted enzyme.

2.4. Preparation of protein

Before starting the molecular docking, the water molecules were removed from the respective proteins. The selected enzymes from protein data bank were subjected to Molegro viewer by which those

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enzymes were refined.

2.5 Preparation of homology model

Homology modelling, a comparative protein structure prediction method, constructs a 3D model for a target protein based on the experimentally determined structure of one or more homologous proteins (templates). This process involves template identification, sequence alignment, model building using spatial restraints from the template, loop modelling, side-chain refinement, and model evaluation to generate a plausible structure for functional studies.

2.5 Preparation of ligand

The structures of ligands were drawn using Chem sketch software. Protein file (pdb) was being further optimized by adding hydrogen atoms and removing water molecules. The end up with all these procedures, the protein and ligand were well prepared for docking.

2.6. Docking

CB-Dock2 is a tool for molecular docking. It uses the Cavity-Based Docking method. First, upload the protein structure in PDB format and the ligand structure in PDB or MOL2 format. CB-Dock2 then predicts where the ligand might bind on the protein. It finds up to five possible binding spots, called cavities, on the protein surface. These spots are marked in the Vina software by making docking boxes around them. Then, the AutoDock Vina algorithm runs docking simulations. The ligand can fit into each cavity, and the software calculates how well it binds. More negative numbers mean stronger binding. The results show the docking scores, a 3D view of the protein-ligand complex, and files you can download. Biovia Discovery studio visualizer was used to visualize the intermolecular interactions with the targets.

3. Results and Discussion

3.1. In-silico Predictions of Molecular Properties and ADME

Pharmacokinetic studies of test derivatives were estimated using online Swiss ADME tool were predicted and presented. The results depicted that all the derivatives satisfied and obey the Lipinski five rule.

3.2. Toxicity predictions

Toxicology studies were performed using Protox 3.0 and ADMET. The results depicts that the derivatives of dabrafenib shows positive or negative toxicity. The toxicology performed using Protox 3.0 was

1. Ames Test Mutagenicity
2. Carcinogenicity
3. Cytotoxicity
4. Hepatotoxicity
5. Nephrotoxicity
6. Neurotoxicity
7. Respiratory toxicity

In the drug discovery process, the physicochemical properties, pharmacokinetics and toxicity studies of tested drugs are essential for qualifying in clinical trials. On this aspect, the molecular properties of the synthesized derivatives were predicted in molinspiration online tools. Based on the Lipinski rule, molecular weight, hydrogen donor/acceptor, and non-rotational bonds of the synthesized motifs produced their affordable result towards their molecular properties. Additionally, polar surface area was also showed significant value, which is accountable for their oral

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bioavailability.

Transport characteristics of molecules like blood-brain barrier penetration and intestinal absorption were determined from molecular volume. Based on the existing literature, these afforded values were referred. Based on the results of Lipinski rule and ADMET the synthesized motifs were optimized for further studies. In any case, the presence of good drug score in this part of the molecule was very effective for the activity.

3.3. Molecular Docking Study

From the targeted molecular simulations, it was found that the title analogues produced significant results in all tested targets and the obtained. The docking score for dabrafenib derivatives on **BRAF, Nek11, and SiK1** produced significant result. The binding affinity towards the targeted enzyme by hydrophilic and hydrophobic interactions were showed in the figures.

NEK11, involved in cell cycle arrest and DNA damage response, showed the strongest binding affinity among all three targets, especially with the OH derivative. The high docking score indicates that Dabrafenib derivatives can effectively occupy the kinase binding site of NEK11, potentially disrupting its activity.Hydrogen bonding with polar residues (e.g., Ser, Lys) and van der Waals interactions further stabilized the ligand within the pocket. This opens new avenues for NEK11 inhibition, which has not been extensively targeted pharmacologically.

Although the binding affinity was comparatively weaker for S1K1, the docking results still indicated moderate-to-strong interactions. S1K1 is a metabolic and stress-response kinase implicated in tumor adaptation. The COCL-POSITION derivative formed hydrophobic

interactions and a few polar contacts with the active site.This suggests that while Dabrafenib is less optimized for S1K1, certain derivatives can still engage the protein effectively, warranting further optimization for better selectivity.

4. Discussion

The Insilico evaluation of Dabrafenib and its derivatives has revealed a compelling rationale for its repurposing as a multi-target therapeutic agent in lung adenocarcinoma. The docking analysis demonstrated strong binding affinities between Dabrafenib derivatives and three critical oncogenic targets BRAF, NEK11, and S1K1. Notably, the OH-substituted derivative exhibited the highest affinity for NEK11 (−11.0 kcal/mol), followed closely by the $CONH_2$ derivative for BRAF (−10.8 kcal/mol) and the COCL-position derivative for S1K1 (−8.9 kcal/mol). These values indicate that the derivatives are capable of forming stable and energetic interactions within the ATP-binding pockets of the kinase domains, predominantly through hydrogen bonding, van der Waals forces, and hydrophobic interactions. These strong binding scores support the concept of multi-target inhibition, which is particularly advantageous in heterogeneous diseases like lung adenocarcinoma where multiple signalling pathways are simultaneously dysregulated.

SwissADME predictions suggest that all derivatives conform to Lipinski's Rule of Five, signifying acceptable drug-likeness. However, the predicted low gastrointestinal absorption and lack of blood-brain barrier (BBB) penetration may limit oral bioavailability, although these limitations are not necessarily detrimental for a drug intended for systemic or targeted delivery in lung tissues. Moreover, the absence of BBB penetration is beneficial in minimizing potential

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neurotoxicity. Bioavailability scores of 0.55 for all compounds indicate a moderate level of systemic absorption, which could be optimized through appropriate formulation strategies such as nano-formulations or co-administration with absorption enhancers.

Toxicity profiling using ProTox-II presented a nuanced safety profile. While the compounds were predominantly non-mutagenic and non-cytotoxic both essential attributes for a therapeutic candidate, the predicted nephrotoxicity and respiratory toxicity across all derivatives highlight potential safety concerns. The presence of certain functional groups may contribute to off-target toxicity, and therefore structural modifications aimed at mitigating these effects are warranted. Despite this, the LD_{50} values, ranging from 300 to 4000 mg/kg, place most derivatives in WHO Toxicity Classes III to V, which are considered moderately to practically non-toxic, supporting their further consideration in preclinical development.

Thus, Dabrafenib derivatives possess the essential molecular, pharmacokinetic, and safety attributes needed for advancement as lung adenocarcinoma therapeutics. The multi-target binding profile not only enhances therapeutic efficacy but may also help circumvent resistance mechanisms commonly encountered with monotherapies. Further experimental validation, including in vitro cell-based assays and in vivo efficacy and toxicity studies, will be crucial in translating these computational predictions into clinical insights. Additionally, refining the lead structures to improve selectivity and reduce organ-specific toxicities will be a key step toward the rational design of next-generation lung adenocarcinoma therapeutics.

5. Conclusion

The present in silico study aimed to evaluate the potential of

Dabrafenib, a clinically approved B-RAF inhibitor, as a multi-target adjuvant therapeutic agent in lung adenocarcinoma by assessing its interaction with three key kinases BRAF, NEK11, and S1K1. Through computational modelling, including molecular docking, pharmacokinetic profiling, and toxicity prediction, this research provides strong preliminary evidence supporting the repurposing potential of Dabrafenib and its structural derivatives.

Molecular docking results revealed high binding affinities across all three target proteins, with the OH derivative exhibiting the strongest interaction with NEK11 (−11.0 kcal/mol) and the $CONH_2$ derivative showing optimal binding to BRAF (−10.8 kcal/mol). These values suggest that Dabrafenib derivatives can effectively engage multiple signalling pathways involved in lung adenocarcinoma progression, thereby offering a potential multi-targeted therapeutic approach. Pharmacokinetic analysis using SwissADME confirmed favourable drug-likeness and oral bioavailability profiles, although low intestinal absorption remains a limitation to be addressed in future formulation strategies.

Toxicity predictions via ProTox-II identified the compounds as largely non-mutagenic and non-cytotoxic, with acceptable LD_{50} values. However, consistent nephrotoxicity and respiratory toxicity across all derivatives warrant cautious interpretation and further optimization. Despite these limitations, the overall safety profile remains within acceptable margins for further preclinical development.

The hypothesis of Dabrafenib can be repositioned as an effective adjuvant therapy for lung adenocarcinoma, particularly due to its ability to target multiple cancer-associated kinases. This study underscores the value of Insilico methods in early-stage drug

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discovery and provides a solid foundation for subsequent experimental validation.

A library of 10 Dabrafenib compounds was analyzed for their pharmacokinetic properties, toxicity, physicochemical properties, and binding scores with BRAF, Nek11, SIK1. -The results revealed that the compound with an OH group exhibited a higher binding score of -11.0 against Nek11 kinase, followed by $CONH_2$ with a binding score of -10.8 against Braf and COCL with a binding score of -8.9 against SIK1 demonstrating promising inhibitory potential.

The OH & $CONH_2$ group has good binding score, lower toxicity and favourable physicochemical properties. Based on these findings, the OH and $CONH_2$ groups were selected for further in vitro and in vivo studies due to their high binding scores and reduced toxicity profiles. The identification of Dabrafenib derivatives with improved binding scores and reduced toxicity profiles may lead to the development of novel therapeutic agents targeting Nek11 kinase & BRAF kinase. Further studies will be necessary to validate the efficacy and safety of these compounds.

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Chapter 14

Structure Based Drug Design of Shikimic Acid as a Putative Drug Target for BRCA via Insilico Method

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Abstract

Cancer is a type of tumor that exhibits aberrant cell proliferation and has the capacity to infiltrate or spread from its original organ (the "site") to other body parts. Breast cancer is heterogenous disease which may due to both genetic and environmental factors. Breast cancer accounts for 23% of all cancer fatalities in postmenopausal women, making it one of the top causes of death in this population. The "shikimate pathway," also referred to as the "shikimic acid pathway," is a metabolic route comprising seven steps, employed by a range of organisms such as plants, bacteria, algae, fungi, and some protozoans, for the biosynthesis of folates and aromatic amino acids. Molecular docking simulations were performed to investigate the binding interactions between shikimic acid and the target proteins BRCA1 and BRCA2, and the resulting interactions, such as hydrogen bonds, hydrophobic contacts, and electrostatic forces, were analyzed. Docking studies of shikimic acid and Niraparib with BRCA1 and BRCA2 were performed, considering the Lipinski rule, rerank score,

and MolDock score. In vitro experiments – DPPH free-radical scavenging and nitric oxide radical inhibition assays – were also carried out to connect these findings with anticancer potency. The shikimic acid and niraparib have a good interaction in holding the molecule in place (binding) of the active site, and docking investigations have been carried out using Molegro Virtual Docker (MVD).

Keywords Shikimic acid pathway; BRCA1; BRCA2; Breast Cancer; Lipinski rule; DPPH method;

1. Introduction

Breast cancer is the most often diagnosed cancer in the world. Breast cancer is the transformation of breast cells into malignant cells that multiply and form tumors. A breast consists of three key parts lobules (glands responsible for milk production), ducts (tubes conveying milk to the nipple), and connective tissue (fat and fibrous material encompassing and connecting all parts). Invasive breast cancer, which accounts for about 80% of cases, can spread beyond the breast to other parts of the body. The BRCA1 and BRCA2 genes create proteins involved in DNA repair.

The "shikimate pathway," also known as the "shikimic acid pathway," is a metabolic route consisting of seven steps, utilized by organisms including plants, bacteria, algae, fungi, and some protozoans, for the production of folates and aromatic amino acids. This pathway is absent in mammals. It involves seven distinct enzymes chorismite synthase, 3-dehydroquinate synthase, DAHP synthase kinase, DAHP synthase dehydrogenase, DAHP synthase dehydratase, and EPSP synthase. The process begins with phosphoryl pyruvate and

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erythrose-4-phosphate as initial substrates, ultimately producing chorismite, which contains three aromatic amino acids.

In the shikimate pathway, the fifth enzyme, Shikimate kinase facilitates the ATP-dependent phosphorylation of shikimate, resulting in the production of shikimate 3-phosphate. Subsequently, 5-enolpyruvylshikimate-3-phosphate (EPSP) synthase mediates the combination of shikimate 3-phosphate and phosphoenolpyruvate. Glyphosate, the primary ingredient in the herbicide Roundup, functions as a competitive inhibitor of EPSP synthase. Through a transition state comparison, it exhibits a greater binding affinity for the EPSPS-S3P complex than phosphoenolpyruvate (PEP), effectively blocking the shikimate pathway (1).

2. Materials and Methods

Auto Dock methods predict how small molecules bind to known target proteins. The binding energy of these molecules is determined by their attachment process to the active sites of target proteins. The Biovia Discovery Studio visualizer is used to picture the ligand's location within the enzyme's active site. This application is especially useful for inspecting binding mechanisms and designing prospective medicinal agents. Additionally, an online tool on the organic portal was leveraged to determine the ADME (absorption, distribution, metabolism, and excretion) characteristics, molecular attributes, and harmfulness of the relevant compounds (2).

2.1 Software Used

AutoDock 4.2 and MGL (Molecular Graphics Laboratory) tools were available for download from the Scripps website. Chemdraw Ultra serves as a sketching tool, while Chem 3D Pro is utilized for energy minimization and transforming Chemdraw files into pdb format.

Molegro Molecular Viewer () facilitates protein preparation, analysis of binding site interactions, and exploration of docked complexes (3).

2.2 Predicting Physiochemical Properties and ADMET

Drug developers use physicochemical characteristics to identify bioactive substances suitable for oral administration, applying the 5-Lipinski's rule. ADME properties are evaluated through pharmacokinetic studies to determine bioavailability. Additionally, the Molinspiration tool and the SwissADME organic portal web's online tool were used to evaluate toxicity and molecular properties (4).

2.3 Molecular Docking

Computational drug design is crucial for elucidating structure-activity relationships, binding energy, protein-ligand interactions, and binding strength. In this research, AutoDock was extensively employed to evaluate the binding capabilities of the ligands (shikimic acid and niraparib) with the target enzymes. This software aids in predicting the potential interaction of these small, synthetic derivative molecules with the targeted enzymes BRCA-1 (PDB ID 6GVW) and BRCA-2 (PDB ID 1IYJ). The targeted enzyme structures were obtained from the RCSB Protein Data Bank (PDB) database (5).

2.4 Preparation of Protein

The water molecules were extracted from the corresponding proteins prior to initiating the molecular docking. Molegro viewer was used to refine the enzymes that were chosen from the protein data database (6).

2.5 Preparation of Ligand

The software Chem Draw was used to illustrate the ligand structures. The addition of hydrogen atoms and the removal of water molecules

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improved the protein file (pdb). After going through all of these steps, the protein and ligand were finally ready to dock.

2.6 Grid box preparation and Docking

The docking investigation estimated cavity space for analogs within protein binding sites and converted files using Chem Draw Ultra. Co-crystallized inhibitory ligands were re-docked in order to verify accuracy and compare docking scores. The docking methodology explored the optimal conformational space with a population size of 150 individuals, obtaining comparable docking poses for each control ligand. By analyzing each ligand shape in every protein binding site, a guided docking technique was employed to improve docking efficiency. The lowest binding free energy indicated the most expected ligand/protein affinity. A scoring method was utilized to determine the best protein-ligand binding affinities. Certain intermolecular interactions with target molecules were observed utilizing the Biovia Discovery Studio visualizer (7).

2.7 In vitro Studies

Evaluation of DPPH Free Radical Scavenging Activity

The assessment of the antioxidant test chemicals' capacity to scavenge the stable radical forms the basis of this assay. The DPPH radical assay was used to test the SHIKIMIC ACID's capacity to scavenge free radicals in vitro. (9), (10)

$$\text{Inhibition (\%)} = (\text{Control sample})/\text{Control} * 100$$

2.8. Nitric Oxide Radical Inhibition Assay

The NO radical inhibition assay was used to test the SHIKIMIC ACID's capacity to scavenge free radicals in vitro (11).

2.9. Determination of Cytotoxicity by MTT Assay

A sterile 0.22 µ filter was used to filter a stock concentration of 5 mg/mL MTT that had been produced in PBS for the investigation.

3. Results and Discussion

3.1. In-silico Predictions of Molecular Properties and ADMET

In molinspiration toxicity was anticipated and shown, and pharmacokinetic studies of test compounds (Shikimic acid and Niraparib) were evaluated using the online Swiss ADME program (Table 1 and 2). According to the findings, every synthesized analog complied with and followed the Lipinski five rules.

Table 1 Physicochemical Properties

Niraparib	319.40	2.58	0.84	53.82	1	4	3

[a] Calculated octanol/water partition coefficient; [b] Molecular descriptor degree of hydrophocity; [c]Water partition coefficient; [d]Topological polar surface area; [e]Number of hydrogen-bond donors; [f]Number of hydrogen-bond acceptors; [g]Number of rotatable bonds.

Table 2 Toxicity Prediction

	Toxicity Prediction		
Compound	**Ames Test Mutagenicity**	**Mouse carcinogenicity**	**Rat Carcinogenicity**
Shikimic acid	Mutagen	Positive	Positive
Niraparib	Mutagen	Positive	Negative

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Table 3 ADME Properties

Compound code	BBB[a]	PgP[b]	HIA [c]	BS [d]	SA [e]
Shikimic acid	Yes	No	High	0.85	1.09
Niraparib	Yes	No	High	0.55	4.19

[a] Blood Brain Barrier penetration, [b] P-glycoprotein substrate, [c] Human Intestinal Absorption,

[d] Bioavailability, [e] Synthetic accessibility

3.2. Molecular Docking Study

The focused molecular simulations revealed noteworthy outcomes for the subject analogues across all evaluated targets, as illustrated in Table 4. For BRCA-1 (PDB ID 6GVW), the docking scores of synthetic derivatives (Shikimic acid and Niraparib) were substantial, ranging from -5.41 Kcal/mole to -6.63 Kcal/mole, as detailed in Table 4. Figures 1A and 1B depict the binding affinity of hydrophilic and hydrophobic interactions for the specified enzyme.

Table 4 Docking score of BRCA-1

Ligands	Docking score (kcal/mole) COX-1 BRCA-1
Shikimic acid	-5.41
Niraparib	-6.63

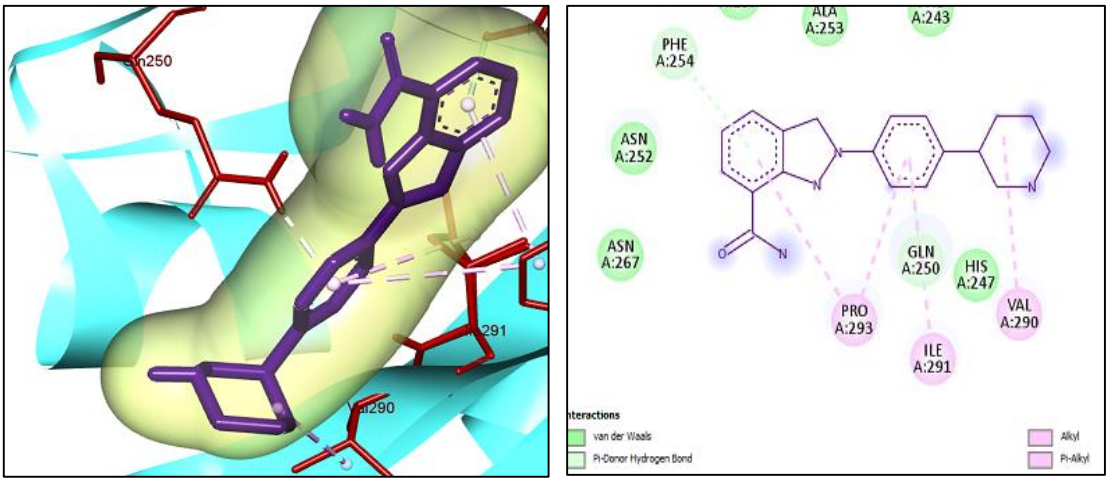
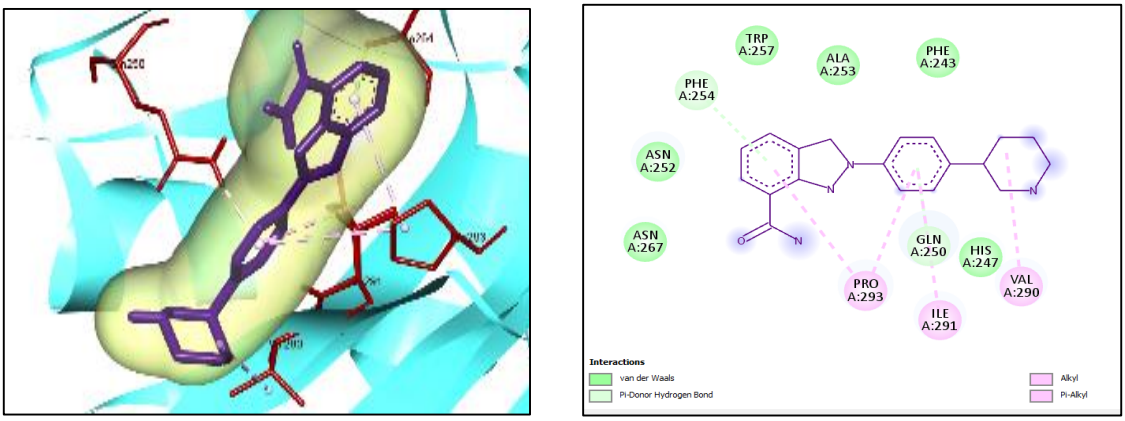


Figure. 1(A) Hydrogen bond interactions on Shikimic acid and BRCA-1 (green dashed lines) and Hydrophobic bonds (Pink dashed lines) and other amino acid residues.

Figure 1(B) Molecular interactions between shikimic acid and BRCA-1 by Biovia discovery studio visualiser



A **B**

A. Docked pose of Niraparib and BRCA-1 binding site.

B. Hydrogen bond interactions on Niraparib and BRCA-1 (green dashed lines) and hydrophobic bonds (Pink dashed lines) and other amino acid residues.

BRCA-2 serves as the second focus for the molecular docking study, with all examined compounds demonstrating strong binding to this

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receptor. As shown in Table 5, Shikimic acid and niraparib exhibited binding scores of -6.02 and -5.06 kcal/mole, respectively. Their binding configurations are illustrated in Figures 2A and 2B.

Table 5 Docking score of BRCA-2

Ligands	**Docking score (kcal/mole) BRCA-2**
Shikimic acid	-6.02
Niraparib	-5.06

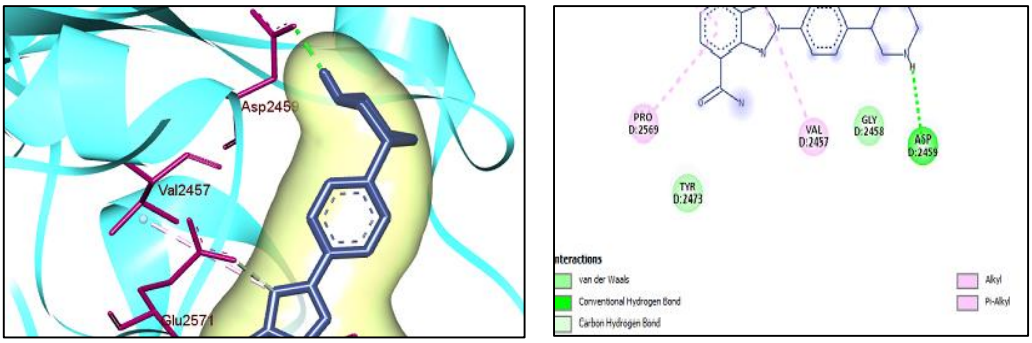
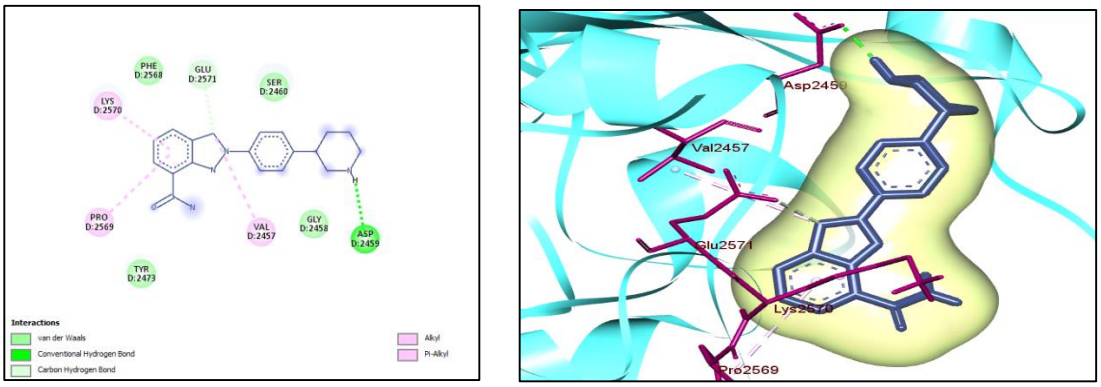


Figure. 2A Molecular interactions between Shikimic acid and BRCA-2 by Biovia discovery studio visualiser. Docked pose of Shikimic acid and BRCA-2 binding site.

Figure 2B. Molecular interactions between shikimic acid and BRCA-2 by Biovia discovery studio visualiser.



A **B**

A. Docked pose of Niraparib and BRCA-2 binding site

B. Hydrogen bond interactions on Niraparib and BRCA-1 (green dashed lines) and hydrophobic bonds (Pink dashed lines) and other amino acid residues.

BRCA1 is a 1,863 amino acid protein, is crucial for DNA repair, particularly in double-strand breaks, and maintaining genomic stability. It plays a key role in homologous recombination, a precise DNA repair mechanism that fixes double-strand breaks. Mutations in BRCA1 disrupt these repair processes, increasing the risk of cancer. Understanding BRCA1's function has led to targeted therapies, such as PARP inhibitors targeting cancer cells with BRCA mutations. BRCA2 is similar, with 3,418 amino acids and a central role in homologous recombination. Mutations in BRCA2 disrupt this process, leading to impaired DNA repair and increased genomic instability, potentially contributing to cancer development. The research assessed the anti-tumor potential of designed motifs on BRCA-1 and BRCA-2 via molecular docking approaches. Shikimic acid and niraparib exhibited high binding affinity towards both proteins, indicating their potential as potential cancer treatments.

3.3. Invitro Effect of Shikimic Acid

Table 6 In vitro effect of Shikimic Acid

S.No	**Tested material**	**DPPH method**	**Nitric oxide radical inhibition assay**
1	Shikimic acid	5.1 ± 1.04	4.26±0.84

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The study reveals that shikimic acid (SA) can inhibit neuro-inflammation, suggesting potential for Parkinson's disease treatment. It also suggests strategies to treat inflammation-related diseases by targeting neuro-inflammation. Plant-microbe interactions are crucial for plant health and agricultural sustainability. Certain banana varieties can resist pathogens by stimulating specific fungi in the rhizosphere, like Trichoderma and Penicillium, which can inhibit the Foc TR4 pathogen. This highlights the importance of recruiting pathogen-suppressive fungi for plant health improvement. This study also aimed to improve menaquinone-7 (MK-7) biosynthesis in *Bacillus natto*. The researchers found that supplementing with precursor compounds like pyruvate, shikimic acid, and sodium glutamate led to a two-fold elevation in MK-7 generation. Introduction of an innovative fermentation technique further boosted MK-7 production, reaching 63 mg/L. Furthermore, shikimic acid was observed to counteract increased serum creatinine concentrations and support recuperation in mice.

4. Conclusion

The interaction between proteins and ligands is important in structural drug design. The analysis of these dockings highlighted certain critical molecular interactions. The shikimic acid is essential for holding the molecule in place (binding) at the active site. These investigations are expected to provide useful insights into the effects of various substitution patterns on the shikimic acid derivative, as well as aid in the synthesis of more effective molecules.

In this study, we docked shikimic acid with BRCA 1 and BRCA 2 and compared it to common medications used to treat breast cancer. This research utilized commercial ADME/T methodologies to assess the

properties of shikimic acid derivatives, thereby reducing time and expenses in drug development. To determine anticancer efficacy, laboratory tests were conducted, including assessments of DPPH free-radical scavenging and nitric oxide radical inhibition. These findings suggest that certain modified natural compounds surpass currently available commercial drugs. Further experimental validation and clinical studies are necessary to establish shikimic acid derivatives or analogues as more effective treatments for breast cancer.

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Chapter 15

Stress and Coping Strategies among School Teachers in Varanasi: An Empirical Study

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Abstract

Teaching is widely acknowledged as a high-stress profession, yet research on stress among school teachers in India remains limited. This study investigates the prevalence, sources, and management of stress among teachers in the Varanasi region, aiming to highlight effective coping strategies and institutional interventions. A structured questionnaire was administered to 270 teachers across 18 schools, equally representing government, private-aided, and private-unaided institutions. Responses were analyzed using quantitative techniques, including rank-order scaling and descriptive statistics.

The findings indicate that while all respondents reported satisfaction with teaching as a profession, stress was still a significant concern. Student disengagement (43.7%), excessive workload (20.3%), and job insecurity (8.5%) emerged as the leading stressors. Psychological symptoms such as restlessness (29.3%) and persistent pressure (22.2%) were common, alongside physical health issues like headaches (43.3%) and back pain (21.1%). Although family (53.3%) and colleagues (17%) provided meaningful support, only 26.7% practiced yoga or meditation. School-level interventions were limited, with 57% of teachers reporting no management support. The study

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concludes that stress is strongly linked to classroom dynamics, workload, and lack of institutional support, rather than salary or school type. Recommendations include structured stress management programs, workload rationalization, and fostering supportive environments.

Keywords: *Teacher stress, coping strategies, occupational stress, school education, Varanasi*

1. Introduction

Occupational stress is increasingly recognized as one of the major challenges to workplace well-being. Defined as the body's psychological and physical response to external demands, stress can be both motivating (positive stress) and debilitating (negative stress). Within the teaching profession, prolonged exposure to stress often leads to burnout, absenteeism, low job satisfaction, and attrition.

Globally, studies have found that teachers face some of the highest levels of occupational stress compared to other professions. Contributing factors include large class sizes, student misbehavior, parental expectations, administrative demands, and inadequate resources (Kyriacou, 2001; Maslach et al., 2001). In countries such as the United States and the United Kingdom, teacher stress has been linked to teacher shortages and declining educational quality.

In India, while stress among secondary and higher education teachers has received some attention, educators remain under-researched. Yet, they face unique challenges: managing very young children, catering to diverse developmental needs, and navigating high parental expectations. The profession is also highly feminized, meaning teachers often balance professional stress with domestic responsibilities.

This study therefore seeks to fill the research gap by focusing on school teachers in Varanasi district, Uttar Pradesh. The city is both a cultural hub and a growing educational center, making it an ideal setting for such a study.

Objectives of the Study:

1. To investigate stress management practices employed by school teachers in the Varanasi region.
2. To categorize and analyze the types of occupational stress experienced.
3. To examine psychological and physiological indicators of stress.
4. To evaluate the effectiveness of coping strategies and stress management techniques.

By identifying stressors and coping strategies, the study provides insights that can guide school administrators, policymakers, and mental health professionals in supporting teacher well-being.

2. Literature Review

2.1 Teacher Stress: A Global Perspective

International research has consistently shown teaching to be a high-stress profession. Kyriacou (1987) described teacher stress as negative emotional responses triggered by job-related demands that threaten self-esteem or well-being. Maslach et al. (2001) emphasized the link between teacher stress and burnout, which manifests in emotional exhaustion and depersonalization.

Key global stressors include:

- Workload and time pressure (Fletcher & Payne, 1982)

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- Student misbehavior and classroom disruptions (Hargreaves, 1990)
- Administrative control and accountability pressures (Schwab & Iwanicki, 1982)
- Role ambiguity and poor working conditions (Trendall, 1989)

2.2 Teacher Stress in India

Indian studies highlight factors such as overcrowded classrooms, rigid curricula, and limited professional development (Gupta, 1981). Abosede (2004) emphasized that gender and marital status influence stress responses, with female teachers often experiencing additional domestic pressures. More recently, technological adoption and increased parental involvement have added to teacher workloads.

2.3 Coping and Stress Management

Coping mechanisms include both individual strategies (yoga, meditation, humor, hobbies) and institutional support systems (counseling services, workload reduction, training). Research suggests that while teachers may adopt informal coping methods, formal institutional mechanisms are often absent, particularly in developing countries (Love & Irani, 2007).

2.4 Research Gap

Although extensive studies exist on teacher stress globally, limited research addresses school teachers in India. Their unique role in shaping children's foundational years, combined with occupational and domestic pressures, makes them particularly vulnerable to stress. This study addresses this gap by empirically analyzing the experiences of 270 school teachers in Varanasi.

3. Methodology

3.1 Research Design

A descriptive survey design was employed to quantify stress levels, identify stressors, and analyze coping strategies.

3.2 Sample and Sampling Method

- Population: School teachers in Varanasi district, Uttar Pradesh.
- Sample size: 270 teachers.
- Schools: 18 (6 government, 6 private-aided, 6 private-unaided).
- Sampling method: Random sampling, ensuring proportional representation.
- Respondent profile: 92.6% female, majority aged 30–50, over half married with children.

3.3 Instrumentation

The questionnaire consisted of 26 items, divided into four sections:

1. Demographics.
2. Sources of stress (student behavior, workload, salary, school environment).
3. Health outcomes (physical and psychological symptoms).
4. Coping strategies and management support.

Question types included dichotomous items, rank-order scaling, and Likert-type ratings. A pilot study refined the instrument for clarity and reliability.

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3.4 Data Collection and Ethics

Data were collected between October–December 2024. Participation was voluntary, with assurances of confidentiality. Respondents provided informed consent.

3.5 Data Analysis

Responses were analyzed using descriptive statistics (percentages, frequency tables, bar charts, and pie charts). Cross-tabulation examined relationships between stress and demographic variables.

4. Results

4.1 Demographics

- Gender: 92.6% female, 7.4% male.
- Age: 40.7% aged 30–40, 35.2% aged 40–50, 13.7% aged 20–30, 10.4% over 50.
- Marital status: 58.1% married with children, 31.5% married without children, 10.4% single.

4.2 Sources of Stress

- Student disengagement: 43.7% identified lack of student interest as their primary stressor.
- Excessive workload: 20.3% cited workload as stressful.
- Job insecurity: 8.5%.
- Influence of social media: 76.3% believed student exposure to social media negatively impacted classroom discipline.
- Salary: Only 20.4% reported dissatisfaction, indicating it was not a major stressor.

4.3 Impact of Stress

- Psychological symptoms: Restlessness (29.3%), persistent pressure (22.2%), anger/frustration (17.8%).
- Physical symptoms: Headaches (43.3%), back pain (21.1%), migraines (10%).
- Absenteeism: Only 4.1% reported absenteeism due to stress.

4.4 Coping Mechanisms

- Social support: 53.3% shared stress with family, 20% with friends, 17% with colleagues.
- Lifestyle practices: Only 26.7% practiced yoga/meditation; hobbies (42.6%) and humor (59.2%) were more common.
- Medication: Rare (4%).

4.5 Institutional Support

- 57% reported no management support.
- 18.9% had access to counseling services.
- 13.3% reported workload reduction initiatives.

5. Discussion

The study reveals that student disengagement is the single largest contributor to teacher stress, overshadowing traditional concerns such as salary. This reflects the changing classroom environment, where digital distractions and social media shape student attitudes.

Workload was the second major stressor, particularly for teachers managing administrative duties in addition to teaching. Interestingly, marital status and school type had limited correlation with stress levels, contrasting with earlier studies (Abosede, 2004).

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Coping strategies leaned heavily on informal mechanisms such as family support, humor, and hobbies, while structured approaches like yoga or meditation were underutilized. The lack of management intervention is striking, with most schools offering no systematic support for stress management.

5.1 Practical Implications

- Schools must institutionalize stress management programs.
- Policymakers should consider teacher well-being as part of education reforms.
- Teacher training should include modules on psychological resilience and classroom management.

5.2 Limitations

- The study is limited to one district (Varanasi) and School teachers only.
- Self-reported data may understate absenteeism or health impacts due to stigma.
- Cross-sectional design limits causal inference.

5.3 Future Research

- Comparative studies across regions and school levels.
- Longitudinal studies on stress and teacher attrition.
- Evaluation of intervention programs such as mindfulness and digital detox initiatives.

6. Conclusion

This study confirms that stress among School teachers in Varanasi is widespread, driven largely by student disengagement, workload, and lack of institutional support. Despite strong intrinsic

motivation and job satisfaction, teachers continue to experience both psychological and physical symptoms of stress.

Addressing these challenges requires a dual approach:

1. Individual-level support: Encouraging yoga, meditation, hobbies, and peer networks.
2. Institutional-level interventions: Counseling services, workload rationalization, balanced teacher-student ratios, and professional training.

By prioritizing teacher well-being, schools can foster more resilient educators and improve the overall quality of early childhood education.

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Chapter 16

An Overview on Therapeutically Important 1,2,3-Triazoles

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Abstract

There are many heterocyclic ring structures, which have been designed in such a way that their binding efficiency with the receptor increases after structural modifications. One of the motifs is azoles, which have been explored widely and still have scope in the research field to achieve many advancements in medicinal chemistry. Therefore, most of the researchers showed their interest in the synthesis of drugs containing azole family due to its most bioactive nature. Azoles are one of the classes of heterocycles containing a five-membered heterocyclic aromatic ring having one or more than one nitrogen atom and at least one other non-carbon atom such as either nitrogen, sulphur or oxygen. Azoles are mostly acts as antifungal,

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antiviral, antibacterial, antibiotic, anti-inflammatory, antimalarial, antitubercular, antimicrobial, antitumor, anti-HIV, antidiabetic, herbicidal, insecticidal, fungicidal and antioxidant agents.

Keywords: Triazoles, therapeutic agents, bioactive heterocycles, drug design, pharmacological applications.

1. Introduction

Some of the prominent examples of aromatic heterocycles comes under the class azoles contains oxazole, imidazole, pyrazole, carbazole, isoxazole, isothiazole, oxadiazole, thiazole, 1,2,3-triazole, tetrazole, 1,2,4-triazole, pentazole, isoxazole and thiadiazole. The molecular structures of all these azoles are collectively shown in the following Figure 1.

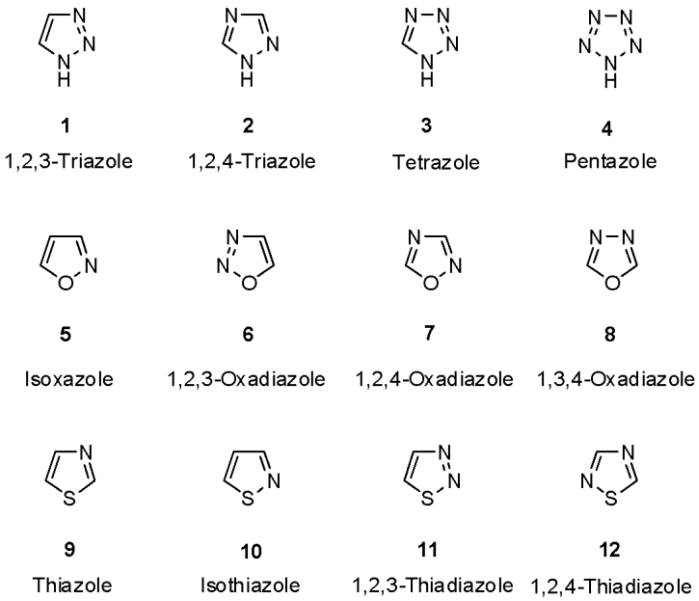

Figure 1. Some representative molecular structures of azoles

Among the class azoles, triazole is one of the widely used heterocycles in drug discovery. Triazoles are heterocyclic organic compounds containing five membered rings with three nitrogen and two carbon atoms. On the basis of the position of nitrogen atoms in the five membered ring, two types of triazoles exist namely 1,2,3-triazole and

1,2,4-triazole. If the triazole ring having three nitrogen atoms at 1,2,3 position then it is called as '1,2,3-triazole' whereas, if the triazole ring having three nitrogen atoms at 1,2,4 position then it is called as '1,2,4-triazole'. Both these types of triazoles with their different isomeric forms are depicted in Figure 2.

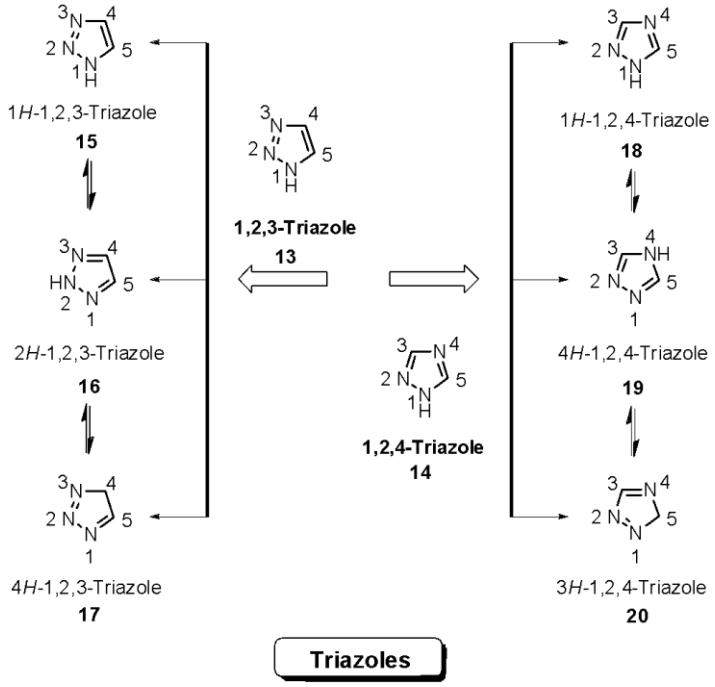

Figure 2. Isomeric forms of 1,2,3-triazole and 1,2,4-triazole

Both 1,2,3-triazoles and 1,2,4-triazoles are highly biologically active in nature and generally shows antileishmanial, antifungal antimicrobial, antibacterial, anticonvulsant, anti-inflammatory, antimalarial, antitubercular, antitumor, anti-HIV, antiviral, antihypertensive, herbicidal, fungicidal and insecticidal biological activities. Some representative clinically used drugs containing 1,2,3-triazolyl scaffold as well as 1,2,4-triazolyl scaffold are shown in Figure 3 and Figure 4, respectively.

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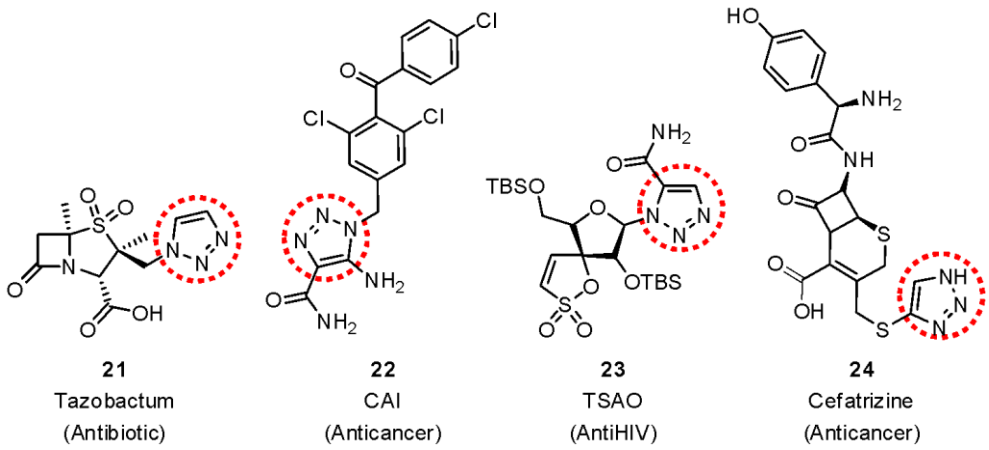

Figure 3. Clinically used drugs containing 1,2,3-triazolyl scaffold

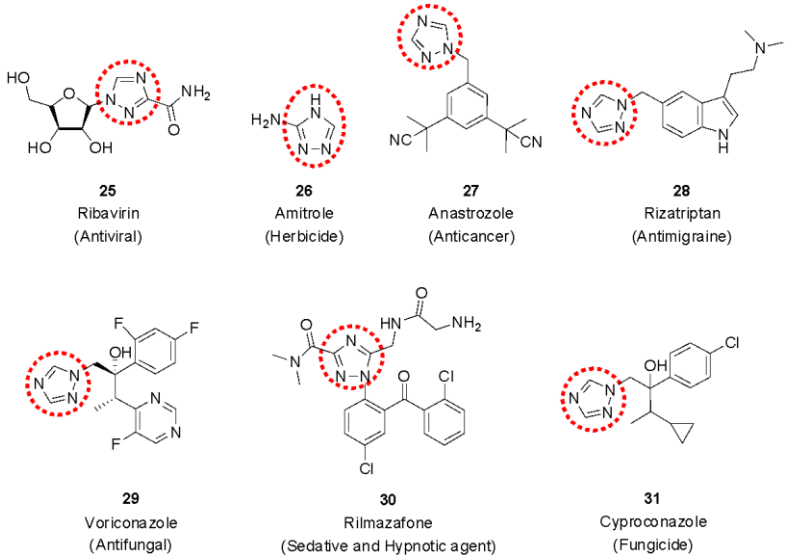

Figure 4. Clinically used drugs containing 1,2,4-triazolyl scaffold

The 1,2,3-triazoles acts as a bioisostere of amide bond due to the similarities observed between 1,2,3-triazoles and amide bond that is nothing but the peptide linkage present in the organism. As already discussed, 1,2,3-triazoles belong to a class of azoles. The 1,2,3-traizole structure contains five membered aromatic heterocyclic rings possessing three adjacent nitrogen atoms at 1, 2 and 3 positions with three available substitution sites at positions 1, 4 and 5 (Figure 5). Although the proton shown with nitrogen at the N1 position in the structure of 1H-1,2,3-triazole does not remain stationary. There are

three tautomeric forms of 1,2,3-triazoles, which are already shown in Figure 2.

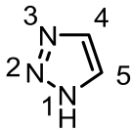

Figure 5. Structure of 1H-1,2,3-triazole

Nowadays, peptide-based drugs are becoming an important component of pharmaceutical drugs. Peptides generally have low bioavailability and metabolic stability. The natural peptide bonds also undergo proteolysis by various proteases. The disulfide bond usually stabilizes the secondary or tertiary structure in peptides and proteins. However, it is unstable in redox or thiol/disulfide exchange conditions. Therefore, natural peptides are not considered as good drug pharmacophores. In above cases, the replacement of unstable bonds with non-natural stable structures while maintaining the same biological activities can be useful for improving the drug ability.

In the last decade, 1,2,3-triazoles have received much attention due to its physical and biological properties, as well as their excellent stability, recommending it as a promising drug core structure. As they are stable to reduction and oxidation in acidic and basic conditions, they possess high aromatic stabilization. They have also attracted increasing attention as a bioisostere of the amide bond linkage of peptides. Therefore, 1,2,3-triazoles can be potential surrogates of amide bonds for peptide modification to achieve more bioactive and physicochemically stable therapeutic leads for the potent drugs discovery. Some already existing biologically active molecules having 1,2,3-triazoles in their architectural framework are collectively shown in Figure 6.

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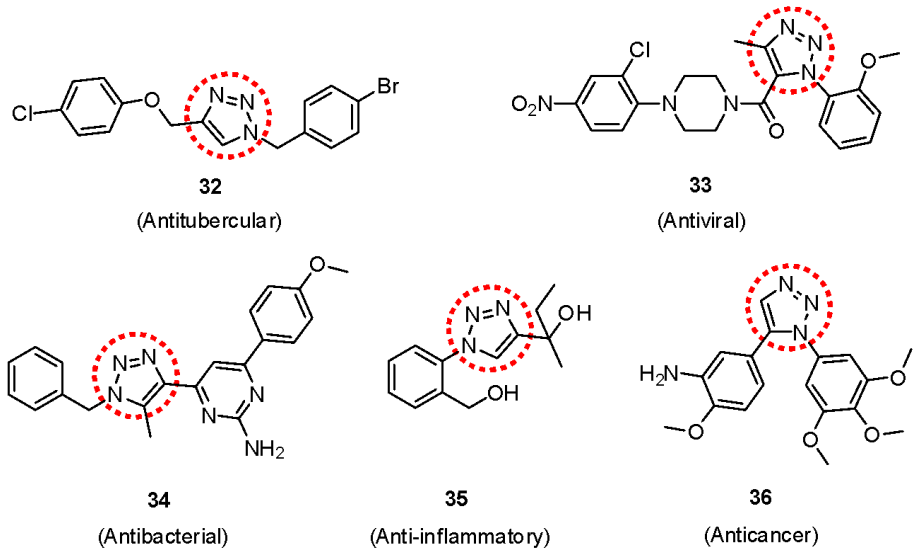

Figure 6. Some bioactive molecules containing 1,2,3-triazole Moiety

Aforementioned Figure 6 shows some heterocyclic compounds having 1,2,3-triazolyl unit in their molecular framework with various biological activities such as, antifungal, antimicrobial, anticonvulsant, antiproliferative, antioxidant, antimalarial, antitubercular, antiviral, antibacterial, anti-inflammatory, anticancer and anti-HIV. The 1,2,3-triazoles act as more stable and improved mimics of amides. It is also one of the most important significance of 1,2,3-triazole. The similarities in between 1,2,3-triazoles and amides are described in Figure 7.

These similarities can be clearly seen in terms of their sizes that is measured by the distances between substituents R1-R2, dipole moment, position of electrophilic carbons, H-bond acceptor and H-bond donor capacities.18 It is observed that the distances between substituents R1-R2 are 3.9 Å in trans-amides and 5.0 Å in 1,4-disubstituted 1,2,3-triazoles which are seems to be very close distances in both the moieties. Similarly, the distances between substituents R1-R2 are observed exactly the same in cis-amides as well as in 1,5-disubstituted 1,2,3-triazoles that is 2.4 Å. The other

one similarity is dipole moment and it is observed ~ 4 Debye and ~ 5 Debye in amides and 1,2,3-triazoles, respectively.

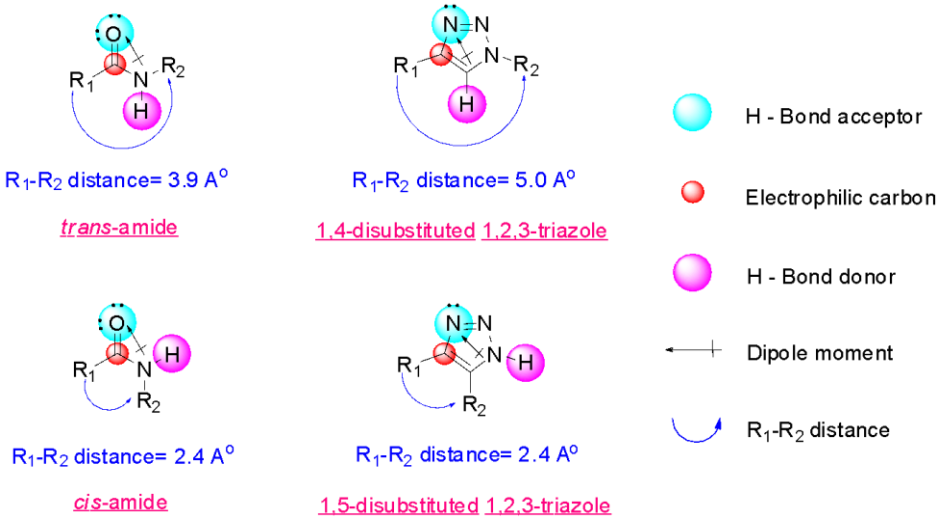

Figure 7. Similarities between 1,2,3-triazoles and amides

Because these similarities existed in between 1,2,3-triazoles and amides, it clearly indicates that the 1,2,3-triazoles acted as bioisosteres of amides. In this present study, we are interested in the synthesis of 1,4-disubstituted 1,2,3-triazoles as it shows bioisosteric effect on trans-amides as well as synthesizing easily by using a greener approach of click chemistry. It is a regioselective synthetic method that preferentially gives 1,4-disubstituted 1,2,3-triazoles without any side products.

2. Conclusion

In this chapter, we have presented a concise account on the azoles, triazoles, triazole containing marketed drugs, therapeutic importance of triazoles, click chemistry, 1,2,3- triazoles, 1,2,4-triazoles. Herein, we have also discussed the similarities between amide bond linkage and 1,2,3-triazoles, which might be responsible for the better binding affinity towards the targeted molecules as well as enhanced therapeutic activity. Therefore can conclude that the 1,2,3-triazoles

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bearing heterocyclic compounds will show potent bioactivity and can act as lead.

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Chapter 17

Artificial Intelligence in Drug Design: Machine Learning Models in Medicinal Chemistry

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Abstract

Artificial Intelligence (AI) and machine learning (ML) have transformed medicinal chemistry by offering rapid, data-driven insights that significantly reduce the time and cost associated with drug discovery. The integration of computational models enables accurate prediction of biological activity, toxicity, pharmacokinetic properties, and molecular interactions. This chapter provides a comprehensive examination of AI-driven approaches in modern drug design, including deep learning, generative models, molecular docking automation, and predictive modeling. Key challenges, emerging opportunities, and the future scope of AI-powered drug discovery pipelines are discussed. The chapter also highlights the Sustainable Development Goals (SDGs) supported through AI innovations in healthcare.

Keywords: *Machine Learning in Drug Discovery, Medicinal Chemistry Modeling, Artificial Intelligence Applications, Computational Drug Design, Predictive Pharmacology.*

1. Introduction

Drug discovery has long been recognized as an expensive and time-consuming endeavor, often requiring over ten years to progress from

initial target identification to final clinical approval. Medicinal chemistry plays a vital role in this journey, as it involves the identification, design, and optimization of potential therapeutic molecules. However, the sheer magnitude of chemical space—estimated to exceed 10^{60} possible compounds—makes traditional trial-and-error experimentation insufficient and inefficient. Exploring even a tiny fraction of this space requires enormous resources, leading to delays, high attrition rates, and significant financial burdens for pharmaceutical researchers.

Artificial Intelligence (AI), especially machine learning (ML), has emerged as a transformative solution. These computational techniques significantly reduce the workload of early-stage drug discovery by accurately predicting the biological activities, physicochemical properties, and toxicity of molecules before synthesis. Advances in computational power, algorithmic efficiency, and the availability of large-scale chemical and biological datasets have further accelerated this progress. Today, ML models support key activities such as virtual screening, quantitative structure–activity relationship (QSAR) modeling, toxicity forecasting, de novo molecular generation, and structure-based drug design. These innovations not only reduce time and cost but also greatly enhance the precision and success rate of modern drug discovery pipelines.

2. Materials and Methods

High-quality data forms the foundation of any successful machine learning model in drug design. Data sources typically include publicly available chemical and biological repositories such as PubChem, ChEMBL, and ZINC, which provide extensive information on molecular structures, physicochemical properties, and bioassay

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results. In addition, Protein Data Bank (PDB) serves as a crucial resource for structural information on protein targets, enabling structure-based modeling and docking studies. Pharmaceutical industries also rely heavily on proprietary datasets obtained from internal research and clinical studies, which often contain highly curated and domain-specific information. Furthermore, high-throughput screening (HTS) experiments generate massive volumes of activity data, offering valuable training samples for classification and regression models.

A wide range of computational tools is employed to preprocess data, perform molecular modeling, and develop predictive algorithms. Python has become the dominant programming language in this domain due to its versatility and availability of specialized libraries such as RDKit for cheminformatics, Scikit-learn for classical machine learning, and TensorFlow and PyTorch for deep learning architectures. To simulate protein–ligand interactions and perform docking studies, powerful molecular modeling software such as AutoDock, Schrodinger Suite, and related platforms are widely used. For handling large datasets efficiently, researchers adopt robust database management systems, including SQL-based relational databases and NoSQL frameworks, ensuring scalable data storage and retrieval.

Cloud computing technologies have further enhanced the capability to process, analyze, and model large-scale datasets. Platforms such as Amazon Web Services (AWS) and Google Cloud offer flexible and scalable computational environments where machine learning experiments can be executed efficiently. These platforms also provide access to preconfigured GPU instances, deep-learning frameworks, and storage solutions, allowing researchers to run intensive

simulations without maintaining physical hardware. Cloud-based pipelines improve collaboration, reproducibility, and accessibility across research teams and institutions.

To meet the demands of modern AI-driven drug discovery, advanced hardware configurations are essential. GPU-enabled workstations significantly accelerate the training of deep learning models, reducing computational time and improving overall productivity. For large-scale tasks such as molecular dynamics and docking simulations, researchers rely on high-performance computing (HPC) clusters, which support parallel processing and specialized applications. Additionally, cloud-based scalable instances provide on-demand computational power, enabling teams to expand resources whenever required. Together, these materials and methods ensure that machine learning applications in medicinal chemistry are supported by reliable data, powerful tools, and efficient computational infrastructure.

3. Methodology

3.1 Data Preprocessing

Data preprocessing is a critical first step in developing reliable machine learning models for drug design. One of the primary tasks involves molecular featurization, where chemical structures are converted into numerical representations. Commonly used molecular fingerprints include Extended Connectivity Fingerprints (ECFP) and MACCS keys, both of which capture structural patterns relevant to biological activity. In addition, physicochemical descriptor calculation—such as molecular weight, logP, hydrogen bond donors/acceptors, and topological indices—provides essential quantitative parameters for modeling. To improve data quality, outlier

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detection and normalization techniques are applied, ensuring that extreme values or inconsistencies do not negatively influence model performance. Finally, datasets are divided into training and testing sets, allowing models to be trained on one portion of the data while validating performance on unseen samples.

3.2 Predictive Modeling

Predictive modeling forms the core of AI-driven drug discovery, enabling the prediction of molecular properties, biological activities, and toxicity profiles. A variety of machine learning algorithms are employed based on the complexity and nature of the task. Random Forest (RF) models are widely used in QSAR studies due to their ability to handle nonlinear relationships and reduce overfitting. For classification tasks such as active vs. inactive molecule prediction, Support Vector Machines (SVM) provide high accuracy and robustness. Gradient Boosting algorithms, including XGBoost and LightGBM, are particularly effective for toxicity prediction and multi-parameter optimization. Meanwhile, Deep Neural Networks (DNNs) excel at modeling complex relationships in large datasets, offering superior performance in predicting biological activities and pharmacokinetic properties.

3.3 Structure-Based Drug Design (SBDD)

Structure-Based Drug Design integrates computational modeling with protein structural information to identify and optimize drug candidates. Advanced approaches incorporate Convolutional Neural Networks (CNNs) to analyze and predict protein–ligand interactions by learning spatial and structural features directly from 3D molecular conformations. These methods often assist in automatic scoring function optimization, improving the ranking of binding affinities

beyond traditional docking techniques. Computational tools perform docking simulations, which are further enhanced by ML-ranked predictions, allowing researchers to prioritize compounds with the highest likelihood of strong binding. This synergy between docking and machine learning significantly accelerates hit identification and lead optimization.

3.4 Generative Models for De Novo Design

Generative modeling represents a revolutionary approach in medicinal chemistry, enabling the creation of completely new molecules with desirable properties. Variational Autoencoders (VAEs) learn compressed molecular representations and generate novel chemical structures by sampling from latent spaces. Generative Adversarial Networks (GANs) provide another pathway by generating molecules optimized for drug-likeness, synthesizability, and activity. Additionally, Reinforcement Learning (RL) strategies fine-tune molecular structures to meet specific design objectives, such as target selectivity or improved ADMET characteristics. These generative tools not only expand chemical diversity but also automate the design process, reducing dependence on manual molecular modification.

3.5 Model Evaluation

Reliable evaluation is essential to ensure the accuracy and generalizability of machine learning models used in drug design. Classification models are often assessed using ROC–AUC (Receiver Operating Characteristic – Area Under Curve), which measures their ability to distinguish between active and inactive compounds. Regression models predicting continuous values—such as binding affinities—are evaluated using RMSE (Root Mean Square Error) and MAE (Mean Absolute Error). To ensure robustness, external test

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validation is performed using datasets not employed in training. Moreover, cross-validation techniques, such as k-fold validation, help reduce bias and assess model performance across multiple data subsets, ensuring consistency and reliability.

4. Discussion

Machine learning has significantly transformed the field of medicinal chemistry by enhancing the efficiency of compound screening and reducing the high attrition rates commonly observed in later clinical phases. Traditional drug discovery often involves synthesizing and testing large numbers of molecules, which is both time-consuming and expensive. ML-based predictive models enable researchers to evaluate molecular properties *in silico*, identifying promising candidates before physical synthesis. This capability not only accelerates early-stage discovery but also allows for more rational decision-making, ultimately saving substantial resources. Furthermore, deep learning models have shown exceptional strength in capturing nonlinear and complex relationships within chemical and biological datasets, improving the prediction of activity, toxicity, and pharmacokinetic behaviors.

In addition to predictive modeling, generative algorithms have introduced innovative pathways for automated drug design. Models such as VAEs, GANs, and reinforcement learning frameworks can generate novel chemical structures optimized for pharmacological relevance and ADMET characteristics. These generative approaches expand the accessible chemical space far beyond what is achievable through traditional intuition-driven design. Meanwhile, AI-powered Structure-Based Drug Design (SBDD) combines machine learning with protein structural data to improve the accuracy of binding site

prediction, identify interaction hotspots, and refine docking predictions. The integration of ML-enhanced scoring functions and docking workflows significantly accelerates hit discovery and lead optimization.

Despite these advancements, several important challenges remain. One major limitation is data scarcity—many biological targets have limited experimental data available, which can hinder the development of reliable models. Another concern is the interpretability of machine learning outputs, as deep learning models often function as "black boxes," making it difficult for chemists to understand the reasoning behind predictions. This lack of transparency can limit trust and adoption in regulatory or clinical contexts. Additionally, effective application of AI in drug design requires strong interdisciplinary collaboration between chemists, biologists, computational scientists, and data engineers.

Ethical considerations must also be addressed to ensure responsible deployment of AI systems in drug discovery. Issues such as data privacy, algorithmic bias, and reproducibility require careful attention. Validation protocols need to be robust, standardized, and transparent to guarantee the reliability of ML-driven predictions, especially when they influence costly or high-risk decisions. As the field evolves, addressing these challenges will be crucial for unlocking the full potential of artificial intelligence in medicinal chemistry.

5. Conclusion

The growing fusion of artificial intelligence and medicinal chemistry is revolutionizing the landscape of drug discovery by enhancing accuracy, speed, and cost-efficiency across all stages of development. Machine learning tools enable the rapid exploration of vast and

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previously unreachable chemical spaces, significantly improving the identification and optimization of potential drug candidates. As computational methods continue to advance, AI is poised to play an increasingly critical role in personalized medicine, high-throughput screening, and precision drug design, ultimately contributing to more effective therapies and accelerated healthcare innovation.

6. Future Scope

- Integration of quantum computing for molecular simulations
- Expansion of global collaborative AI drug discovery networks
- Improved explainable AI (XAI) models for better decision transparency
- Automated lab platforms using robotics and AI
- Personalized drug design based on patient-specific genetic data

Abbreviations

- AI: Artificial Intelligence
- ML: Machine Learning
- QSAR: Quantitative Structure–Activity Relationship
- DNN: Deep Neural Network
- SBDD: Structure-Based Drug Design
- ADMET: Absorption, Distribution, Metabolism, Excretion, and Toxicity
- VAE: Variational Autoencoder
- GAN: Generative Adversarial Network
- ROC-AUC: Receiver Operating Characteristic–Area Under Curve
- PDB: Protein Data Bank

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Chapter 18

Renewable Energy Resources towards Eco-Friendly Society

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Abstract:

Renewable energy resources are the primary candidate for sustainable, eco-friendly, and low-cost electricity generation. These resources not only reduce dependence on fossil fuels but also contribute to a healthier environment by lowering greenhouse gas emissions. As technology advances, the efficiency and accessibility of renewable energy are expected to improve even further, making it a vital part of our energy future. The International Energy Agency (IEA) states that depletion of fossil fuels has been producing the power since 2019. Therefore, intense research is being done to move towards increasing the efficiency of renewable energy resources in order to enhance their performance. Herein the main aim of this book chapter is understanding and exploring the available renewable energy technologies, including solar energy, hydro energy, bioenergy, wind energy, and geothermal energy.

1.1 Introduction

At present, renewable energy resources are gaining more attention in order to replace the conventional energy resources, including fossil fuels, due to demand in both developed and developing countries [1]. Fossil fuels are harmful to the environment, including causing climate change and global warming [2]. The greenhouse gas emission has rapidly increased into the atmosphere from power generation for the past few decades [3]. Therefore, renewable energy such as solar, wind, hydro, biomass, geothermal, and hydrogen energy was introduced in order to address the current environmental crisis [4]. The renewable resources' ability to produce power without atmospheric pollutants and their environmentally friendly nature leads to gaining more attention [5]. It not only gives sustainable energy but also helps to improve the economy due to it generating the electricity from natural and renewable resources [6]. Even though renewable energy resources are producing power, the majority of power production still relies on fossil fuels due to the high cost and intermittency of renewable energy [6]. For example, solar cells are only operating during the daytime, wind turbines could be working when there is sufficient air flow, and hydro turbines work when water flow is there and then only produced energy. Therefore, researchers are desperately working on improving renewable energy in order to address its limitations.

The aim of this book chapter is to represent the different renewable energy resources and their applications for electricity production and introduce the latest technologies proposed by researchers. In addition, addressing limitations of the latest renewable energy technologies. The following topics are elaborately discussed: the current status of energy division and contribution of renewable

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energy resources, and various energy resources and their development. Further, their limitations and challenges are briefly explained.

1.2 Current status of energy resources

In the 21st century, most countries rely on fossil fuel for the production of electricity due to a lack of technologies, atmospheric conditions, and limited resources. However, due to awareness of the environmental crisis, renewable energies are linearly increased for power production. The following figures represent the data analysis usage of fossil fuel, comparison of fossil fuels and generation of renewable energies, and different types of electricity production by renewable energy resources.

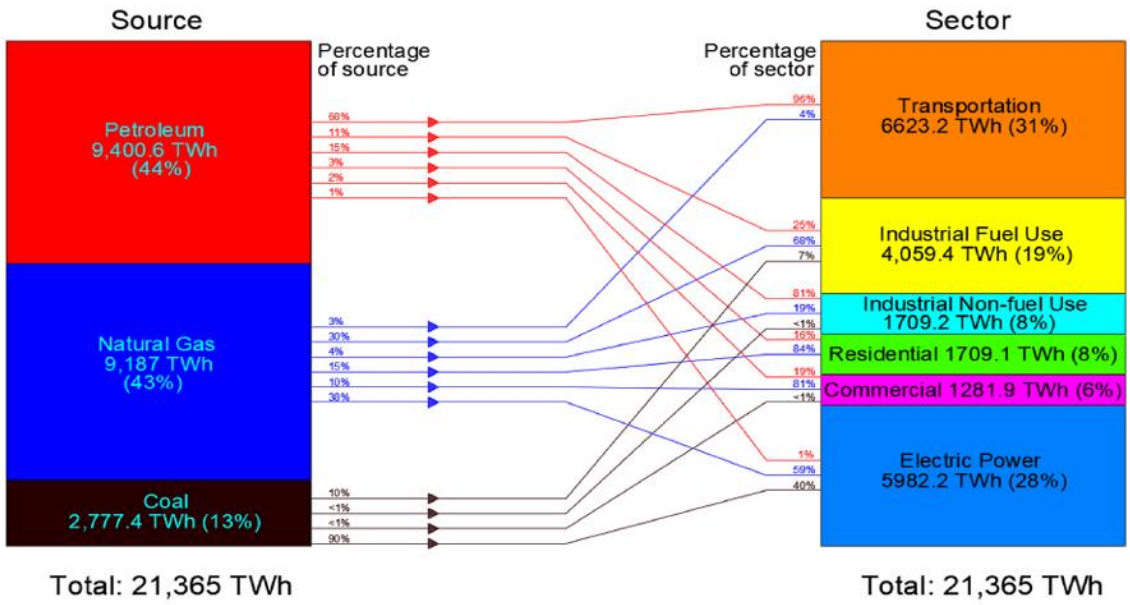

Figure:1. Usage of fossil fuel in different sectors in 2020 (U.S)

Figure 1 shows the usage of fossil fuels and the distribution of them in the United States (US) in 2020 [7]. Among them, petroleum contributed more, 44% out of 9400.6 TWh. Natural gas is provided 43%, which is 9187 TWh. 2777 TWh is used for coal, which is the

least usage for electricity generation. There are five sectors there to produce the power generation from fossil fuel resources. Most fossil fuels are used in transport sectors, which is 6623.2 TWh (31%) in 2020. Besides this, coal contributed 2392 TWh (90%) and natural gas 3529.5 TWh (36%) in 2020. Figures 2(a) and 2(b) show the comparison of generation power from fossil fuel and renewable sources from 2010 to 2019.

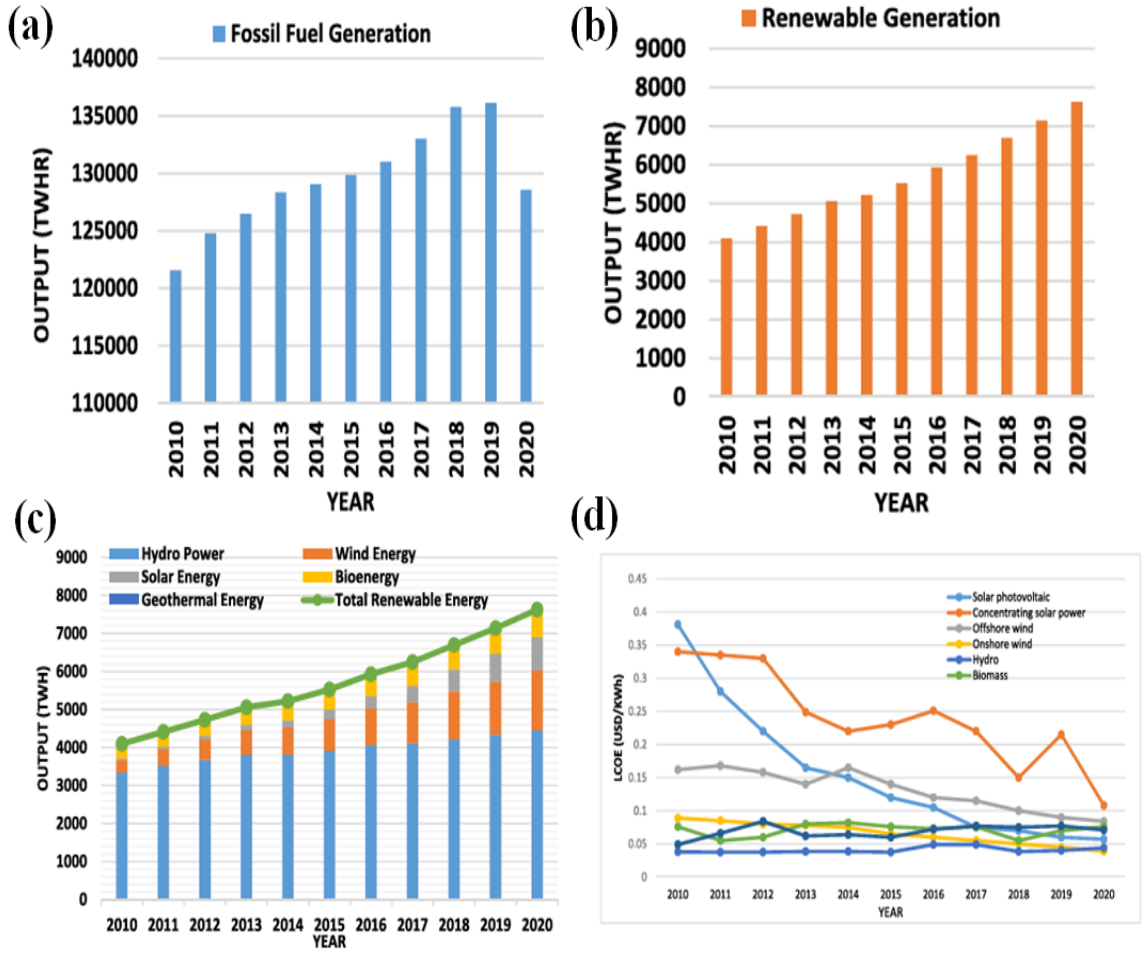

Figure:2. The comparison of (a) generation of fossil fuel, (b) the growth of renewable generation from 2010 to 2020, (c) usage of total renewable energy from 2010 to 2020, (d) Global weighted-average utility scale levelized cost of energy (LCOE) from 2010 to 2020.

The generation of fossil fuel is slightly decreased from 2010 to 2020.

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However, usage of electricity increased from 2010 (121,531 TWh) to 2019 (136,131 TWh) but after that decreased in 2020. Meanwhile, the renewable generation has increased linearly from 2010 (4098 TWh) to 2019 (7,140 TWh). The usage of total renewable energy for electricity production from 2010 to 2020 is shown in figure 2 (a), (b), (c) [8], [9], [10]. In 2021, according to IEA's global energy review, usage of renewable energy has significantly increased from 2010 (4,098 TWh) to 2020 (7,627 TWh). The largest portion of the electricity generated is hydropower with other renewable energies. On the other hand, the solar energy set the trend to produce the electricity due to solar energy technology, which is linearly developed and increasing the power conversion efficiency (PCE). Meanwhile, the wind energy also significantly generates the power, which also sets the trend.

Besides these three, bioenergy and geothermal energy have been rendering the lowest efficiency since 2010, due to the fact that they need specific locations to produce the power plant and also the process of generating power is complicated. Figure 2(d) shows the weighted-average levelized cost of energy (LCOE) from 2010 to 2020 around the world. In general, LCOE is known as the average cost of electricity per kWh for a generator, which considers all the costs from different renewable energies such as fuel, capital, electricity market prices, and maintenance. According to IRENA, the generating power cost of the solar energy system and wind system significantly decreased in LCOE from 2010 to 2020. Among all other renewable energy systems, solar systems have dropped the largest, by 85%, from 2010 to 2020. This happens due to increasing the solar technologies in order to control the economies of scale, developer experiences, and competitive supply. Meanwhile, bioenergy, hydro energy, and geothermal energy systems have limited contributions throughout

the year.

1.3 Renewable energy resources

Now a days, for generating the electricity, the renewable energy has gained more attention due to environmentally friendly and cost of production. There are five major renewable energy resources are solar energy, hydro energy, wind energy, bio energy and geothermal energy. The following sections are elaborately discussed all these energy resources.

1.3.1 Solar energy

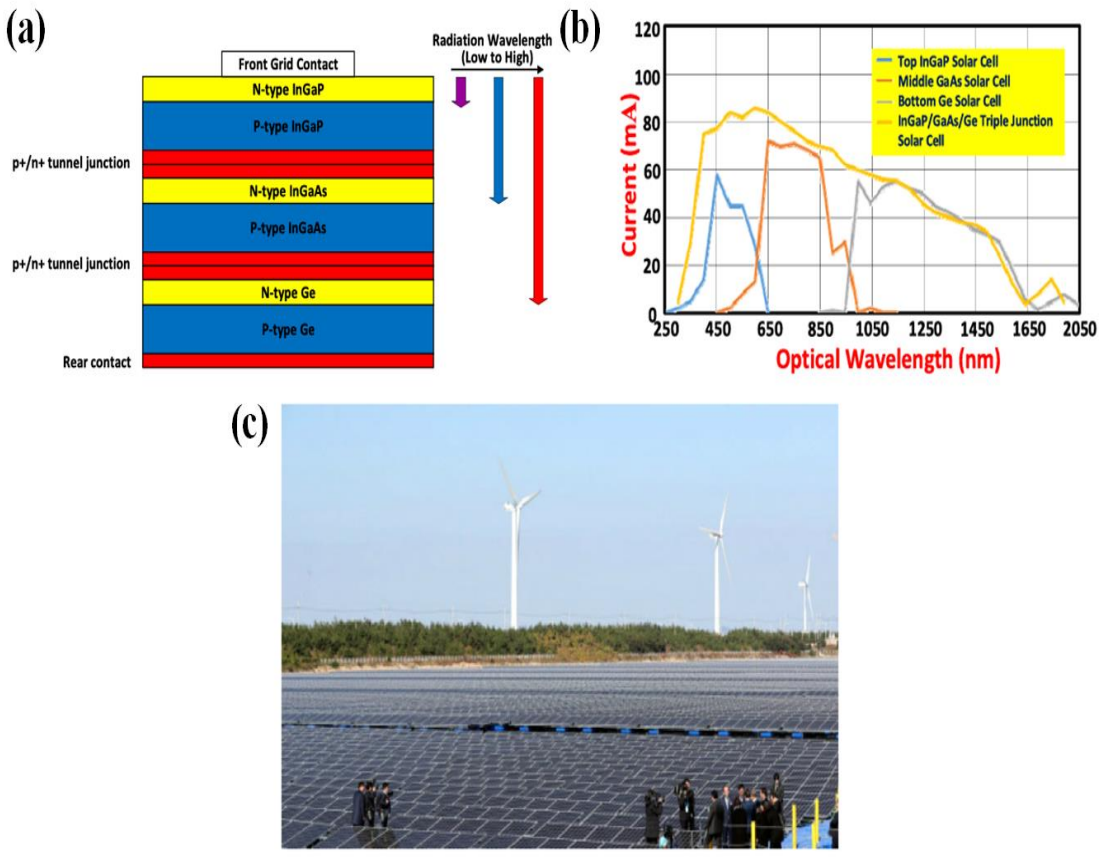

Figure: 3. (a) Structure of Multiple-junction (InGaP/GaAs/Ge) solar cells, (b) The spectral response curve between individual semiconductor solar cells, (c) The largest floating photovoltaic system in Korea.

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Solar energy is one promising green and clean energy resource, radiation emitted from the sun that can be utilized globally. The researchers are doing intense research in order to increase the power conversion efficiency (PCE) of solar energy by optimizing the design of the solar energy system and reducing the cost of production and environmental impacts. There are two crucial solar energy systems: (i) photovoltaic devices (PV) and (ii) solar thermal energy. Herein we discuss only photovoltaic devices.

1.3.1.2 Photovoltaic device

The solar cells, or photovoltaic devices, are one of the leading technologies in solar energy, which is a promising energy resource for the future. At present, only 7% of generating electricity all over worldwide. Schockley and Queisser have shown that conventional solar cells attain only about 31% of PCE, which is called the SQ limit. The researchers are exploring new designs and optimizing the advanced materials to enhance the PCE of photovoltaic devices. There are advanced technologies to increase the PCE, including (a) concentrator photovoltaic (CPV) system, (b) hot carrier converters, (c) multi-junction solar cells, and (d) floating photovoltaic device power generation. **(a) Concentrated Photovoltaic (CPV):** CPV is a method of focusing solar radiation by using concentrating optics on the solar cells. The aim of CPV is to collect solar radiation and scatter it, which is then concentrated on the photovoltaic device. There are three types of CPV: (i) (i) low concentration over the range of 1-40x, (ii) medium concentration over the range of 40-300x, and (iii) high concentration over the range of 300-2000x. The maximum PCE that can be obtained from CPV is 40%, according to IEA (International Energy Agency). **(b) Hot Carrier Converter:** It is one of the solar cells that convert excessive photons into electrons and generate the electricity. These

phenomena happen only in two different electronic states, which are known as conduction and valence bands, by means of absorbed photon energy. Nevertheless, the photo energy will be dissipated as heat at threshold energy gaps. Therefore, these converters help to improve the efficiency of solar energy via utilizing the excessive photon energy. The main aim of converters is to reduce the heat dissipation and stay longer so the carrier's energy can be utilized. As a result, the PCE of the hot carrier converter could be obtained around 65%, which is higher than that of a conventional solar cell.

(C) Multi-junction solar cells (MJSC): MJSC consists of stacking different semiconductors of p-n junctions, which are connected in series. This is called tandem solar cells, which effectively enhance the PCE of photovoltaic devices. The device structure of MJSC is shown in figure 3(a) [11], [12], [13]. In order to avoid the blockage of current flow, an interconnector will be installed between the subcells. This interconnector should have high optical transmission with low electrical resistance. The maximum obtained PCE of MJSC is 40.7%. The top cell materials are playing a major role in achieving the high PCE of MJSE. InGaP is a promising candidate as a top cell for Ga or GaAs subcells due to it having less oxidation reaction and a lower recombination rate with the best window layer material than AlGaAs. Figure 3(b) shows the spectral responses of subcells InGaP, GaAs, Ge, and MJSC of InGaP/InGaAs/Ge on optical wavelength. (d) Floating Photovoltaic (FPV): This type of photovoltaic device is installed on water surfaces such as pools, reservoirs, and lakes, which are supported by floating structures. FPV technology is mostly installed in Japan, the US, China, Italy, and Brazil. The purpose of this type of photovoltaic is to prevent heat in the PV arrays by a cooling effect, and the mechanism is similar to conventional photovoltaic devices.

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The cooling effect significantly contributes to the efficiency of photovoltaic devices for energy harvesting. Two benefits are in FPV: (i) (i) this system could reduce the rate of algal growth, and (ii) it decreases the water evaporation while rendering the cooling effect to the photovoltaic device, as a result significantly enhancing the efficiency of solar panels. Eventually, when FPV is installed on water storage like ponds, lakes, and reservoirs, it leads to positive solutions for environmental crises. In addition, it has faced no environmental issues like atmospheric pollutants and climate changes like fossil fuel energy resources. Figure 3(c) shows the largest floating photovoltaic technology is installed in Korea, which is 5 million solar cells over 30 km² and provides 2.1 GW of power.

1.3.2 Hydropower

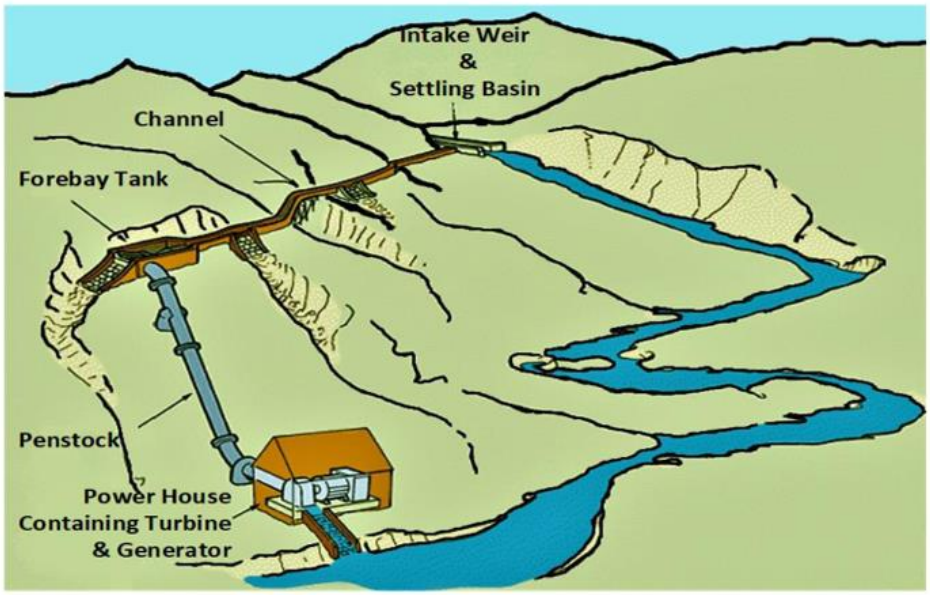

Figure: 4. The small hydropower system

Hydropower is one of the most cost-effective systems in renewable energy resources; the power is generated by flowing water from higher to lower elevations. Among other renewable energy resources, hydropower has a higher efficiency of about 90% to

produce electrical energy [14]. Worldwide, 20% of power is generated from hydropower. There are several types of hydropower, including small hydropower plants, cascaded reservoir hydropower plants, and pumped storage systems.

Figure 4 shows the small hydropower system is one of the cost-effective technologies, especially in rural areas, for generating electricity [15]. The mechanism of a small hydropower system is that the river water is split and collected by intake weirs, which are controlled by valves. When the small hydropower is not working, then the valve is turned off and water passes through the system. In order to prevent the hydro turbine from damage, there is one tank installed before the weir and settled down in the river. Therefore, it can be installed at any location that has low water output. This is one of the crucial systems due to its environmentally friendly and cost-effective nature compared to other renewable energy resources.

1.3.3 Wind energy

Wind energy is the most crucial resource in renewable energy for producing electrical power after hydropower owing to its facile process, low cost, and well-matured technology. By wind turbines, the wind energy is transferred into electricity[16]. Wind energy could be categorized into two types, such as onshore wind farms and offshore wind farms. The majority of wind systems are located onshore; the locations depend on the speed of wind, which might be sufficient to produce the electrical power. The wind turbines are categorized into two types, such as vertical axis and horizontal axis. Figure 5 shown the horizontal axis of inner structure which are most popular one among the renewable energy resources system [17]. It consists of a steel or concrete pole that turns in the direction of the

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wind and is connected between the nacelle and other parts, including the tower, gearboxes, and converter.

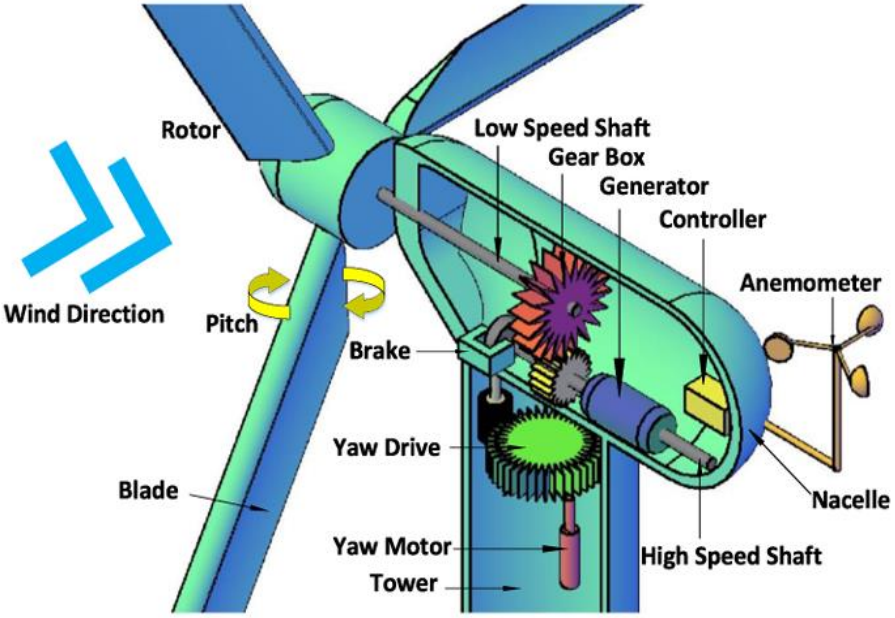

Figure: 5. The wind turbine system

1.3.4 Bio energy

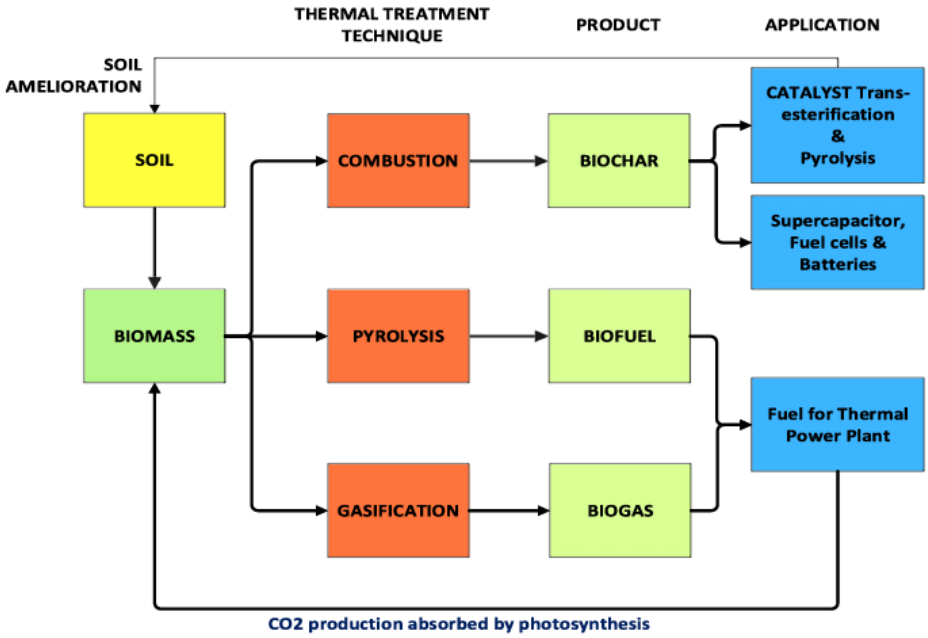

Figure: 6. Thermal treatment of biomass for bioenergy production

Bioenergy is one of the attractive resources due to its ability to help the heating and transport sector. It is an environmentally friendly power. The bioelectricity is produced from biological materials such as biomass. There are four types of biomass, including solid waste, energy crops, wood residues, and agricultural residues. The biomass contains low nitrogen and no sulfur, unlike coal, which leads to no effect on the environment, including ozone and acid rain. In addition, it released NOx and SOx to the environment with a low content of emission.

Figure 6 depicted the various thermal treatment of different biomass and obtained the products from them [18]. By using biomass, we can produce the biogas, biochar and biofuel.

1.3.5 Geothermal energy

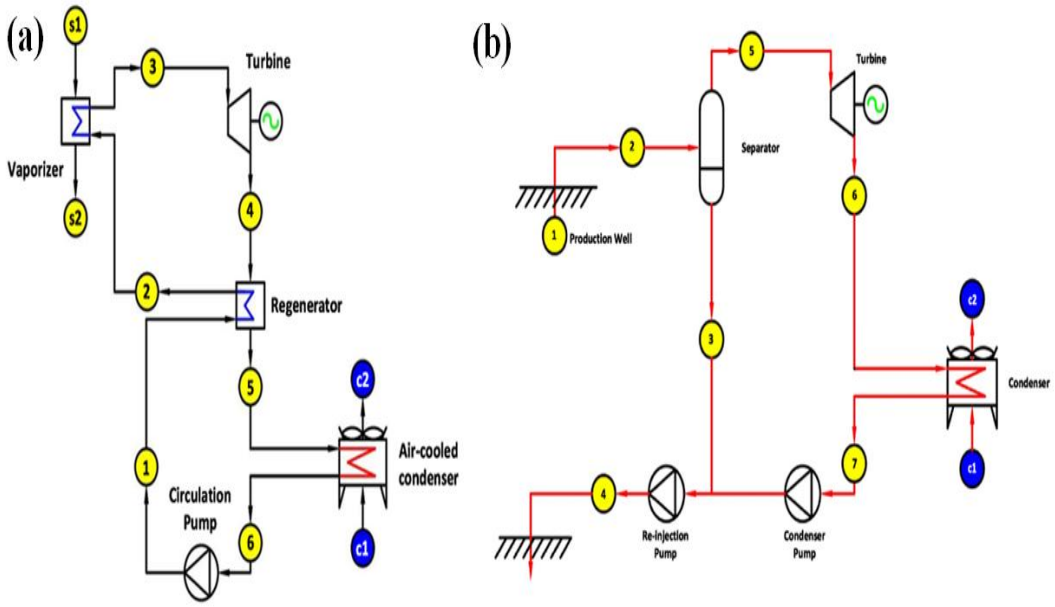

Figure: 7. (a) Schematic diagram of ORC cycle, (b) Flow chart of single flash cycle

The thermal energy will come from the radioactive decay of earth minerals, which are primitive structures of the planet [19].

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According to the depth of the earth, the geothermal gradient increased by 0.03 cm^{-1}, which confirms that 99% of the planet's temperature is higher than 1000°C. Among renewable energy resources, geothermal energy is highly enriched and inexhaustible. In addition, it is eco-friendly and has no emission of carbon dioxide (CO_2) to the environment. At present, 26 countries are using geothermal energy for producing electric power, including the US, Japan, Indonesia, Mexico, Iceland, the Philippines, and Italy.

Figure 7 shows the flow chart of the organic Rankine cycle (ORC) and single flash cycle [20]. ORC operates at low temperature, and it has low mechanical stress compared to others. In a single flash cycle, the fluid is collected at station 1, where it is boiled and transferred to station 2. After that the separator is transferred to station 3 and reinjected. Meanwhile, the steam is transferred to station 5. After that, steam is passed through a condenser, cools, and will collect. These flowcharts are shown in figure 7(b).

1.4. Summary

At present, the environmental crisis, including global warming, depletion of the ozone layer, and climate change, is severely devastating. In order to address these issues, all the countries, both developed and developing, take the initiative to use renewable energy technologies. The intense research and innovations are necessary in order to be carried out. New methodologies and new technologies are encountered to enhance the efficiency and reduce the cost of production. This book chapter is exploring the available renewable energy resources and new technologies. However, all resources have certain limitations; therefore, we have to overcome them in order to use them widely. Besides all these technologies, availability of

resources, cost of production, eco-friendliness, and awareness are necessary. Government and non-government are playing crucial roles in order to take the initiative. Furthermore, intense research is also mandatory to ensure the location and implementation process are based on renewable energy resources.

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Publicizing Research

Perspectives on Multidisciplinary Research in Science and Technology: Concepts and Statistical Approaches, September 2025

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