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International Conference on Innovations in Science for Sustainable Development (Sustainable & Innovative Materials in Chemical, Physical and Biological Sciences)

ICISSD-2025

20th March 2025

Organized By

Smt. Narsamma Hirayya Shaikshanik Trust's
Smt. Narsamma Arts Commerce and Science College, Amravati
Research Committee and Department of Chemistry
In Collaboration with
Association of Chemistry Teachers (ACT), Mumbai, Maharashtra, India

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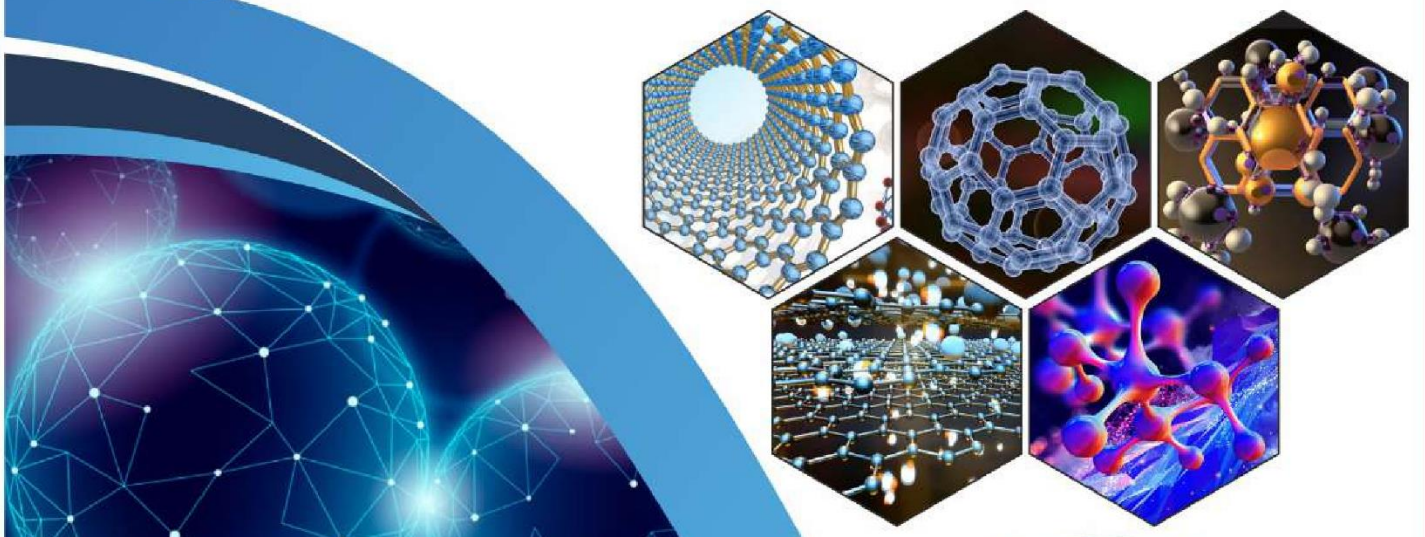

DATE

19 - 20

MARCH, 2025

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Smt. Narsamma Arts, Commerce and Science College, Amravati

Our College began its UG classes in the year 1995 with small rented building. Geographical location of our campus caters to lower income localities in the town. So, most of our students come from socially and economically disadvantaged background. Around 1700 students of primary school, Junior College, Undergraduate and Postgraduate courses studied in our campus. Despite having their entry-level percentage very low, many of our students have done exceptionally well in the fields of academics, sports as well as performing arts. Our college has accredited by National Assessment and Accreditation Council with CGPA of 2.58 (B+) on four-point scale. We have now 10.25 acres of campus. The college started with a vision to bring this economically underdeveloped region into current flow of modern era. In the universally notorious establishments and government organizations, our number of students has been placed in leading positions. The College has 13 departments spread through three faculties of Arts, Commerce and Science. The college has recognised research centres for Ph.D. programs. Many research scholars are working for their Ph.D. in these laboratories and centres.

Association of Chemistry Teachers

The Association of Chemistry Teachers (ACT) was formed in 2000 to serve as an apex National Body of Chemistry Educators to promote exvellence in Chemistry Education. The idea of formulating ACT was conceptualized by Homi Bhabha Centre for Science Education (TIFR), Mumbai. Since its inception, ACT has been striving tirelessly to strengthen chemistry education in India and to motivate students to pursue chemicstry as a career through its manifold activities-National and International conferences, training workshops, research convention, Concept Test in Chemistry for B. Sc. Students, newsletter, Celebration of National Chemistry Day and National Science Day and organization of Chemistry competitions for school and college students. The association plays a pivital role in the organization of National National Standard Examination in Chemistry (NSEC) which is the first stage examination leading to participation in the Indian National and International Chemistry Olympiads. ACT forges a synergistic relationship between academia, industry and research centres for mutual benfit and seeks collaboration with International Science Teachers organization for joint activities. ACT has a large network of active life members and institutional members spread across the country. The leading Chemical scientists of India are Honorary embers of ACT and provide valuable guidance and support.

The Conference

The Conference on Innovations in Science for Sustainable Development is a premier gathering of researchers, scientists, policymakers, and industry experts dedicated to exploring innovative scientific solutions for a sustainable future. This conference serves as a dynamic platform for knowledge exchange, fostering discussions on cutting-edge advancements in various scientific fields, including renewable energy, environmental conservation, biotechnology, sustainable agriculture, and digital transformation. As global challenges such as climate change, resource depletion, and environmental degradation continue to rise, science and technology play a crucial role in driving sustainable solutions. This conference aims to highlight ground breaking research, innovative methodologies, and practical applications that contribute to achieving sustainable development goals. Participants will have the opportunity to collaborate, share insights, and develop strategies that integrate science with sustainable practices. The event encourages interdisciplinary dialogue, fostering partnerships between academia, industry, and governmental organizations to create a more sustainable and resilient world.

Invitation

The Organizing Committee cordially invites you to participate in the International Conference on Innovations in Science for Sustainable Development (ICISSD-2025) going to be held at Smt. Narsamma Arts, Commerce and Science College, Kiran Nagar, Amravati, India from 19th to 20th March 2025 in hybrid mode (only inauguration in offline mode and remaining all sessions in online mode). The scientific programme includes keynote addresses, Invited talks, online presentations on the theme of conference. Prizes will be given for best presentations.

Call for Abstract/Papers

Authors should submit an abstract in the form of oral and poster presentation under various topics of Innovations in Sciences for Sustainable Development. All those presenting a paper in the conference are requested to submit one page abstract along with the completed registration form and send to the e-mail: atishkmaldhure@yahoo.co.in

Abstract for oral and poster presentations should be in Times New Roman and A4 format leaving 2.5 cm in the top and bottom and 3.00 cm, as left and right side margin. The title(font size 14) should be bold followed by authors name(s) and affiliation (Both in font size 12). This should follow the e-mail(font size 10) in italics of the presenting author and should be underlined. The text should follow the title as single space with font size 12. References should be placed at the bottom. All the accepted research papers after Peer Review may be published in journals having ISSN number (UGC Care listed, Springer Proceeding, Elsevier Scopus indexed Journals). Research Papers (Selected) will be published in Scopus, UGC and SCI with Additional Cost.

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Study of Variation in Viscometric and Ultrasonic Behaviour of Derivatives of Bisthiourea at Varying Temperature

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ABSTRACT

The present study is deals with the study of intermolecular interactions in terms of relative viscosity, specific viscosity, ultrasonic velocity and related parameters such as adiabatic compressibility, apparent molar compressibility, Intermolecular free length, Relative association, Specific acoustic impedance and apparent molar volume of substituted bisthiourea in different percentage and temperature of dioxane-water mixture. It has been prepared by change in the volume of solvent and keeping the volume of ligand fixed. The data obtained has been used to compute relative viscosity and thermodynamic parameters for viscous flow. The viscosities and ultrasonic parameters of 0.01M solutions of ligand 1-phenyl bisthiourea, has been found out in 75%, 80%, 85% and 90% 1,4-dioxane-water mixture at different temperature (298K, 300K, 302K and 304K).

Keywords: Substituted Bisthiourea, Relative viscosity, Specific viscosity, Ultrasonic velocity, Ultrasonic parameters

Introduction:

Viscosity is a very significant basic property of fluid, which essential for fluid transport, mixing, heat transfer and mass transfer process [1], [2]. The viscosity of some fluids is slightly exposed by temperature, and quietly affected due to variation in temperature. In general, it is seen that on increase temperature, viscosity of fluid decreases because the movement of fluid particles increases and the amount of time required to reach with their closure particles decreases. Thus, as temperature increases, the average intermolecular forces between fluid particles decreases. The understanding about viscosity is very crucial in designing some equipment such as equipment for storage, pumping or injection of fluids at required temperature. There is number of different techniques by which fluids resistance to flow are measured. Viscosity data is of great importance in many chemical engineering disciplines such as simulation of processes or the design of chemical equipment. Viscosity is also important in many commercial applications, such as consumer products like shampoo, and viscometers are used extensively in quality control [3]. In viscometric studies, the measurement and analysis of viscosity of

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fluid is very important for industrial and scientific area to check product quality, to study properties of material and innovation in technology. Its study is important in selection of lubricant for machine parts, in pharmaceutical industry to check purity of product, in polymer science as well as in food industries. The viscosity of fluid particularly depends on intermolecular forces of attraction of their molecules. The strong intermolecular force of attraction means high viscous fluid while weak force indicates less viscous fluid.

It may be due to the force of friction between two layers of a fluid moving speedily one another with different velocities. Literature survey shows that several workers have measured viscosity in fluid and used viscosity data to study the molecular interactions. Viscosity measurements like other transport properties of electrolyte provide useful information about solute-solute and solute-solvent interactions.

The present work also studies on the measurement of ultrasonic velocities, densities and viscosities of binary mixtures to understand the intra and intermolecular interactions between the molecules of components. The successful application of acoustical methods to physio-chemical investigation of solutions has become possible after the development of adequate theoretical approaches and methods for precise ultrasonic velocity measurements.

So, in the present study, we report experimental results of ligand, 1-phenyl bisthiourea on the viscosity and ultrasonic velocity for the binary liquid mixtures of dioxane + water in varying proportions at different temperatures.

Method and Experimental Technique:

Viscometrical studies of ligand 1-phenyl bisthiourea

The 0.01 M solutions of ligand 1-phenyl bisthiourea were prepared in 75%, 80%, 85% and 90% dioxane-water mixture. These solutions along with pure distilled water were kept inside a water thermostat to maintain the constant temperature, 305K. The Ostwald's viscometer was cleaned, dried and then mounted inside the thermostat vertically. 10 ml solution was filled into the viscometer through the wider limb. The viscometer and the solution were kept inside the thermostat for 15-20 minutes to attain the thermal equilibrium. After achieving the thermal equilibrium, the solution was sucked through rubber tube fixed at the other end (narrow limb) till the lower meniscus of the liquid crosses the upper fiducial mark on the limb containing capillary tube. The liquid was then allowed to flow down till it touches the lower fiducial mark and the flow time 't' for the flow of liquid from upper to lower fiducial mark, was measured by stopwatch. The process was repeated for three times and the mean value of the flow time was taken for calculation.

Viscometrical parameters

Study of viscosity shows the relation and the effect of temperature on solution.

These parameters are used in different types of industries such as oil, organic, inorganic, daily life, food processing plants, hopper level switches, tank level indicators etc.

The viscosity of each solution is determined by the following empirical formula

$\eta_2 = \eta_1 \times d_2t_2 / d_1t_1$ ---------- (1)

Where, η_2 = viscosity of ligand solution

η_1 = viscosity of solvent

d_1 and d_2 = densities of solvent and ligand respectively

t_1 and t_2 = time of flow for solvent and ligand respectively

$\eta_r = \eta_2/\eta_1 = d_2t_2 / d_1t_1$ ---------- (2)

Where, η_r = relative viscosity

Ultrasonic studies of ligand 1-phenyl bisthiourea

In an ultrasonic interferometer, the ultrasonic waves are produced by the piezoelectric method. In a fixed frequency variable path interferometer, the wavelength of the sound in an experimental liquid medium is measured, and from this, one can calculate its velocity through that medium. The apparatus consists of an ultrasonic cell, which is a double walled brass cell with chromium plated surfaces having a capacity of 10ml. The double wall allows water circulation around the experimental medium to maintain it at a known constant temperature.

The micrometre scale is marked in units of 0.01mm and has an overall length of 25mm. Ultrasonic waves of known frequency are produced by a quartz crystal which is fixed at the bottom of the cell. There is a movable metallic plate parallel to the quartz plate, which reflects the waves. The waves interfere with their reflections, and if the separation between the plates is exactly an integer multiple of half-wavelengths of sound, standing waves are produced in the liquid medium. Under these circumstances, acoustic resonance occurs. The resonant waves are a maximum in amplitude, causing a corresponding maximum in the anode current of the piezoelectric generator.

In the present investigation, a variable path ultrasonic interferometer (Mittal enterprises, New Delhi Model M-82) is used to measure the ultrasonic velocity in liquid mixtures and solutions. The working frequency of variable path ultrasonic interferometer is 2 MHz.

Ultrasonic Velocity Measurements

The ultrasonic velocities of substituted Bisthioureas were measured in the concentration of 0.01M. The cell of ultrasonic interferometer was filled fully with the solution and the needle of ammeter was adjusted in the range of 20 to 60 with the help of "Adj" knob. It was warmed for 10 minutes so that the range should remain steady. Micrometre reading was noted. Screw was moved anticlockwise to get maximum deflection of needle. Movement of screw was continued to get five deflections. After returning back of needle to original position, micrometre screw reading was noted. The difference between these two readings gave the distance travelled by the screw for getting five maxima. From this, distance required through which micrometre screw should move for one maxima was calculated just by dividing it by 5 and multiplying by 2. The same procedure was repeated many times.

Ultrasonic Parameter

Ultrasonic velocity and related parameters are adiabatic compressibility (β), apparent molar compressibility (ϕk), Intermolecular free length (Lf), Relative association (RA), Specific acoustic impedance (Z) and apparent molar volume (ϕv).

(i) Adiabatic compressibility (β)

The ultrasonic velocity and other molecular properties have been calculated theoretically by using number of equations. The variation in velocity due to mechanical disruption has been reflect on a basic property of liquids. By measuring ultrasonic velocity (U) and density (d) experimentally, the adiabatic compressibility (β) can be calculated mathematically by using Laplace's equation.

$\beta = 1/U^2d$

(ii) Apparent molar compressibility (ϕ_k)

It is an acoustic property which determined by taking the measurement of density and ultrasonic velocity that depends on the molarities of solution and molecular weight of the solute. It can be calculated by the relation,

$\Phi_k = 1000\ X\ [\beta sdo - \beta ods\ /m\ x\ ds\ x\ do] + [\beta s\ x\ M/\ ds]$

Where,

do = density of pure solvent

ds = density of solution

m = molarity of solution

M = molecular weight of solute

βo = adiabatic compressibility of pure solvent and

βs = adiabatic compressibility of solution.

(iii) Intermolecular free length (L_f)

It is also an acoustic property which helps to study the intermolecular interactions. Intermolecular free length has been determined from adiabatic compressibility (β) by Jacobson's formula,

$L_f = K\sqrt{\beta}$

Where, K is the temperature dependent constant known as Jacobson's constant and is independent of the nature of liquid. Examining very large number of liquids, Jacobson obtained values of K at various temperatures. In obtaining these values for 'K' Jacobson has taken sound velocity (U) in m/s, the density in g/cc and free length (Lf) in A^0.

(iv) Relative association (R_A)

It is a function of ultrasonic velocity and calculated by the equation,

$R_A = (dsdo) \times (UoUs)^{1/3}$

Where, Uo and Us are ultrasonic velocities in solvent and solution.

(v) Specific acoustic impedance (Z)

It is determined from the measurement of ultrasonic velocity and density by formula,

Z = Us x ds

The solute-solvent interactions may be interpreted in terms of acoustic impedance.

(iv) Apparent molar volume (ϕ_v)

This acoustic property depends on densities of solution and solvent, molecular weight of solute (M) and molarity of solution (m). Unlike above acoustic properties, it does not depend upon ultrasonic velocity. To calculate apparent molar volume, the following formula is used by measuring densities of solution and solvent, molecular weight of solute (M) and molarity of solution (m).

$\Phi v = [M/ds] \; X \; [(do–ds)x10^3]/[m \times ds \times do]$

Where,

M is molecular weight of solute and

m is molarity of solution

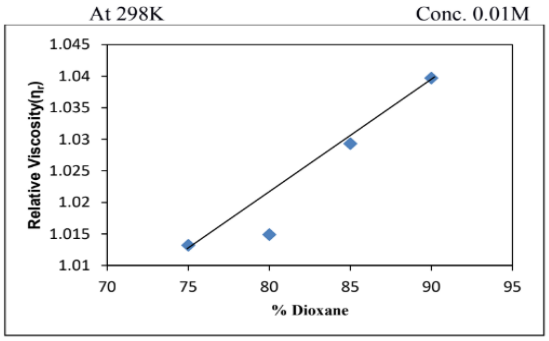
do and ds are densities of pure solvent and solution respectively.

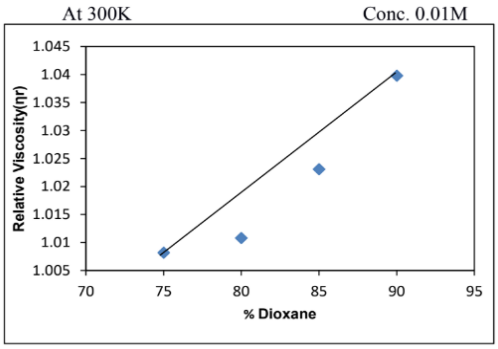
Results and Discussion

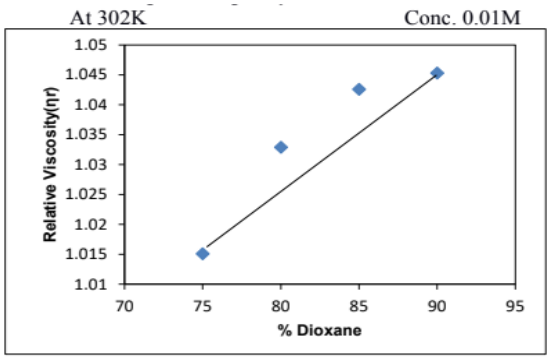
In the present study, viscosities of ligand 1-phenyl bisthiourea has been calculated by equations (1) and (2). The 0.01 M solutions of ligand was prepared in different percentage of dioxane-water mixture. From the values all parameters like relative viscosity and specific viscosities of solutions are calculated and listed in Table.

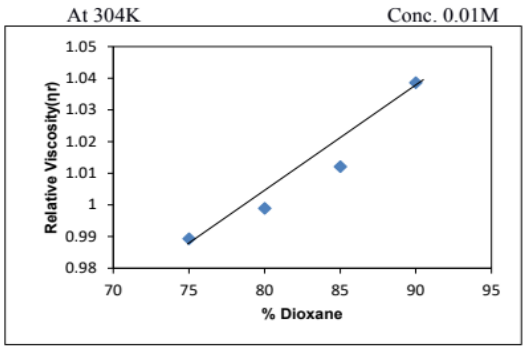
% Dioxane-water	√C mole$^{1/2}$/lit$^{1/2}$	Density (d)	Density d X 10^3 kgm^{-3}	Time flow 't' second	Relative viscosity (η_r)	Sp. Viscosity $\eta_{sp} = \frac{\eta r - 1}{\sqrt{C}}$
1-phenyl Bisthiourea (L)						
At 298 K						
75	0.01	0.9729	972.9	180.00	1.0132	0.1323

80	0.01	0.9711	971.1	173.00	1.0149	0.1492
85	0.01	0.9723	972.3	163.66	1.0293	0.2937
90	0.01	0.9624	962.4	140.66	1.0397	0.3974
At 300 K						
75	0.01	0.9882	988.2	176.33	1.0082	0.0823
80	0.01	0.9823	982.3	170.33	1.0108	0.1084
85	0.01	0.9823	982.3	161.00	1.0231	0.2311
90	0.01	0.9882	988.2	138.00	1.0398	0.3989
At 302 K						
75	0.01	0.9747	974.7	180.00	1.0151	0.1510
80	0.01	0.9752	975.2	175.33	1.0329	0.3293
85	0.01	0.9729	972.9	165.66	1.0426	0.4260
90	0.01	0.9700	970.0	141.33	1.0453	0.4536
At 304 K						
75	0.01	0.9941	994.1	172.00	0.9893	-0.1068
80	0.01	0.9882	988.2	167.33	0.9989	-0.0101
85	0.01	0.9882	988.2	158.33	1.0121	0.1217
90	0.01	0.9823	982.3	138.66	1.0386	0.3865









From table, it is seen that as the percentage of binary mixture (1,4 dioxane- water) increases, relative viscosity and specific viscosity also increases for all ligand solutions. At different percentage of solvent (1,4 dioxane-water mixture) the values of ηr and ηsp increases with increasing the percentage of solvent (75%, 80%, 85% and 90%).

For 1-phenyl Bisthiourea : Ligand shows positive values of specific viscosity at different percentage of Dioxane+water mixture at varying temperature i.e. it shows strong interaction with binary mixture.

It is observed that-

Ligand shows positive values of relative and specific viscosity at varying temperature.

If the solute has positive value of specific viscosity they are characterized as 'structure formers' and will impose a new order by reorientation of the adjacent water indicating strong solute-solvent interactions.

L1, shows strong interaction with binary mixture of 1,4 dioxane and water

The present work deals with the interaction of 1-phenyl bisthiourea in different % composition like 75, 80, 85 and 90 of Dioxane-water at different temperatures. Table and graphs show the values and variation according to temperature, concentration on substituted Bisthioureas

Acoustic Parameters at different percentages of 1,4 dioxane-water mixture

Temp. = 298K Conc.= 0.01M Ultrasonic Frequency: 1MHz

% Dioxane	U (m/sec)	ds x 10^3 ($Kg.m^{-3}$)	βs x 10^{-10} (pa^{-1})	Φ_k x 10^{-6} ($m^3mol^{-1}pa^{-1}$)	Φ_v x 10^{-5} (m^3mol^{-1})	R_A	L_f x 10^{-11} (m^{-1})	Z x 10^3 ($kg\ m^{-2}sec^{-1}$)
75	1491.888	0.9729	4.6180	-10.8101	1.0267	0.9788	4.4188	1451.457
80	1447.208	0.9711	4.9167	-7.7181	1.0288	0.9869	4.5594	1405.383
85	1442.376	0.9723	4.9435	-7.5195	1.0274	0.9892	4.5719	1402.422
90	1446.392	0.9694	4.9308	-7.4767	1.0308	0.9854	4.5660	1402.132

Temp. = 300K Conc.= 0.01M Ultrasonic Frequency: 1MHz

% Dioxane	U (m/sec)	ds x 10^3 ($Kg.m^{-3}$)	βs x 10^{-10} (pa^{-1})	Φ_k x 10^{-6} ($m^3mol^{-1}pa^{-1}$)	Φ_v x 10^{-5} (m^3mol^{-1})	R_A	L_f x 10^{-11} (m^{-1})	Z x 10^3 ($kg\ m^{-2}sec^{-1}$)
75	1453.592	0.9882	4.7892	-9.7891	1.0092	1.0042	4.5164	1436.439
80	1444.000	0.9823	4.8822	-8.5148	1.0158	1.0004	4.5600	1418.441
85	1438.408	0.9823	4.9203	-8.1344	1.0158	1.0017	4.5777	1412.948
90	1422.408	0.9882	5.0015	-7.6661	1.0092	1.0115	4.6154	1405.623

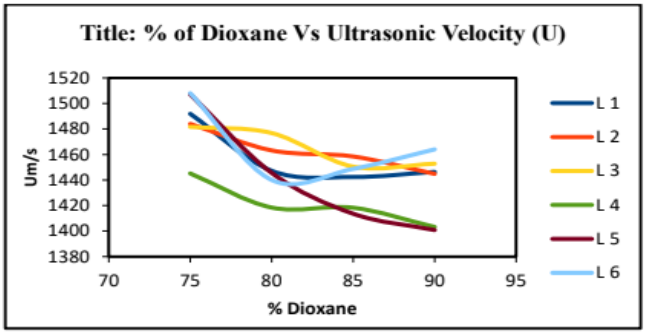
Temp. = 302K Conc.= 0.01M Ultrasonic Frequency: 1MHz

% Dioxane	U (m/sec)	ds x 10^3 ($Kg.m^{-3}$)	βs x 10^{-10} (pa^{-1})	Φ_k x 10^{-6} ($m^3mol^{-1}pa^{-1}$)	Φ_v x 10^{-5} (m^3mol^{-1})	R_A	L_f x 10^{-11} (m^{-1})	Z x 10^3 ($kg\ m^{-2}sec^{-1}$)
75	1452.040	0.9947	4.7681	-13.4580	1.0020	1.0011	4.5228	1444.344
80	1450.392	0.9752	4.8745	-11.1955	1.0241	0.9819	4.5730	1414.422
85	1479.992	0.9729	4.6925	-12.8737	1.0268	0.9730	4.4868	1439.884
90	1465.584	0.9700	4.7996	-11.6252	1.0302	0.9733	4.5377	1421.616

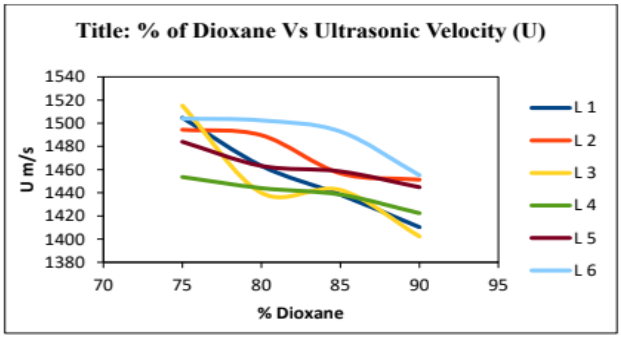
Temp. = 304K Conc.= 0.01M Ultrasonic Frequency: 1MHz

% Dioxane	U (m/sec)	ds x 10^3 ($Kg.m^{-3}$)	βs x 10^{-10} (pa^{-1})	Φ_k x 10^{-6} ($m^3mol^{-1}pa^{-1}$)	Φ_v x 10^{-5} (m^3mol^{-1})	R_A	L_f x 10^{-11} (m^{-1})	Z x 10^3 ($kg\ m^{-2}sec^{-1}$)
75	1540.000	0.9941	4.2415	-19.4982	1.0025	0.9805	4.2812	1530.914
80	1512.000	0.9882	4.4264	-17.2825	1.0091	0.9806	4.3735	1494.158
85	1464.024	0.9882	4.7212	-14.3339	1.0091	0.9912	4.5168	1446.748
90	1460.760	0.9823	4.7708	-13.4704	1.9580	0.9860	4.5405	1434.904

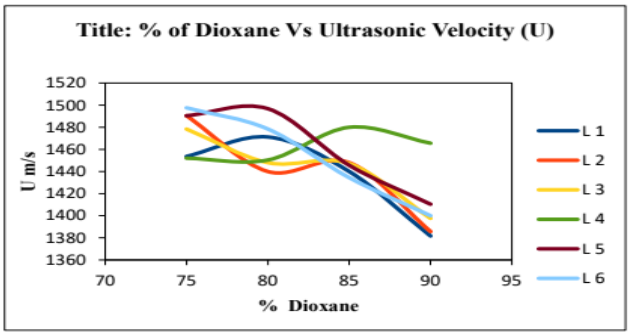
Graph 1: At 298K Conc.: 0.01M



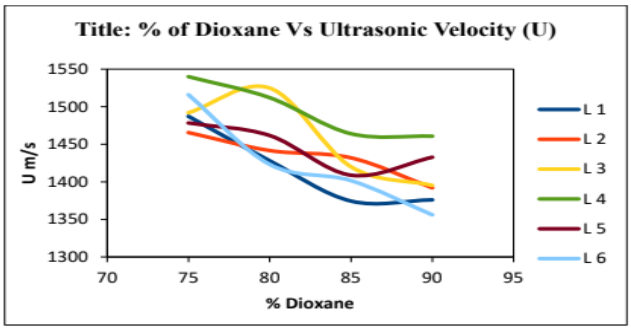
Graph 2: At 300K Conc.: 0.01M



Graph 3: At 302K Conc.: 0.01M



Graph 4: At 304K Conc.: 0.01M



Ultrasonic is the widely considered method to investigate the physical and chemical behaviour of the liquids, liquid mixtures, electrolytic solutions and polymeric solutions. The different acoustical parameters explain the nature and strength of molecular interaction that present in the system.

The ultrasonic velocity of the system either increases or decreases due to changes in the structure and properties of solute. Therefore, the solutes that increase the ultrasonic velocity are structure maker while those decreases the ultrasonic velocities are structure breakers.

Conclusion

From the viscometrical data, it is seen that viscosity of solvent decreases on dilution because, ions freely move in a solution and average speed of molecule is also increases.

The decrease in ultrasonic velocity indicates that the interaction between solute and solvent is becoming less dominant. This is due to the replacement of strong intermolecular attraction between solvent molecules by weaker intermolecular interactions. This indicates that the solvent- solvent interaction is replaced by solute-solvent interaction. The speed of sound velocity in liquids largely depends on the structure, size, shape and molecular association. Thus, the concentration dependencies of ultrasonic velocity and density of 1,4 Dioxane and water binary system have been measured at different temperatures. The nonlinear variation of the related parameters such as ultrasonic velocity, density, adiabatic compressibility, intermolecular free length and acoustic impedance were elaborated to understand the molecular interactions that leads to the process of complex formation between the solute molecules through dipole-induced dipole interactions.

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Antibody-Antigen Interactions with Antibody Loops, Rainbow's Spectrum of Various Imidazole Scaffolds against Various Microbes Using Molecular Docking

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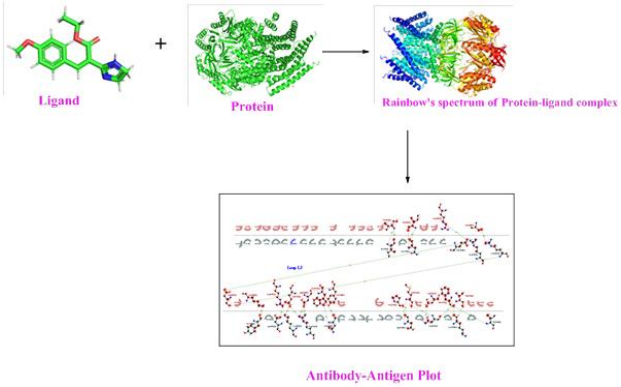
ABSTRACT

In this research article we have systematically presented antibody plot as most common computational structure-based of protein ligand interaction studies. This technique approach can be mainly used in various analysis process for drug design. Application of Antibody plot can be used as effective tool to study terms of visualizing protein ligand interaction, protein- protein interaction and its application to study pharmakinetics as multiple target drug discoveries. The use of this tool can also be used to study with molecular mechanic position. All results provide valuable information for designing and developing antibody drug for different microbes.

Keywords: Imidazole, molecular interaction, Antibody-Antigen interactions, Multiple Target Drug Discovery, Antibody Loops, Rainbow's spectrum.

Graphical Abstract



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INTRODUCTION

Imidazole and its derivatives possess versatility of finding applications in medicines, drugs, synthetic chemistry, and industry [1-3]. It is aromatic heterocyclic compounds containing-Nitrogen atom [4]. In recent years, particularly imidazoles have significant attention in research and biological activities mainly due to their versatile range of pharmaceutical chemistry, industrial chemistry [5-8]. They play important role in the synthesis of biologically active molecules such as antimicrobial, antiviral drugs, antidiabetic and enzyme inhibitors [9-10].

Molecular docking studies have main application of virtual screening and shows interaction between multiple protein-ligand complexes and also used to visualize interaction between enzymes and their substrates [11-15]. Molecular docking and Ligplot+ v.2.2.9 /DIMPLOT /Antibody plot are used for automatic generation of protein-ligand complex diagrams is a graphical front-end to the LIGPLOT and DIMPLOT ,Antibody program for printing or conversion to various image formats[16-20].

Related Ligplot+ v.2.2.9 /DIMPLOTs /Antibody plot to similarities and differences between related proteins binding the same/similar ligand,[21-24] the same/similar ligand binding to different proteins, or the interfaces of related proteins [25-30], **LIGPLOT** + is a schematic diagram of the interactions between protein and ligand, **DIMPLOT** is a plot of the interactions across a selected protein-protein, or domain-domain, interface, **Antibody plot** - this is an extension of DIMPLOT specifically for plotting antibody/antigen interactions, with the antibody loops colour-coded and labelled.[30-35]. Generally, it is a graphical front-end program. In all cases, the interactions plotted are hydrogen bonds and non-bonded contacts [35-40].

We comprehensively and systematically investigated the binding stability of various microbes protein are 4HWA, 5BUN, 4MCT. We identified possible antibody drug from PDB (protein Data Bank). In this paper, we have focused on protein-ligand docking which provides visualized interactions for imidazole scaffolds for different antimicrobial activity such as Escherichia coli (E. coli) (Protein Id: 4HWA), S.typhi (Protein Id: 5BUN) and P.Vulgaris (Protein Id: 4MCT).

Escherichia coli (E. coli) is a bacterium that naturally resides in the intestines of humans and animals. While many strains support digestion and are harmless, certain types can cause severe foodborne diseases. Maintaining good hygiene, ensuring proper food preparation, and using clean water can help prevent infection.

Proteus vulgaris (P. Vulgaris) is a rod-shaped bacterium found in soil, water, and the human intestinal tract. As an opportunistic pathogen, it can cause urinary tract infections, wound infections, and, in severe cases, septicaemia. Its strong motility and urease production contribute to kidney stone formation. Some strains are resistant to antibiotics, making treatment more challenging. Preventive measures include good hygiene, infection control, and careful antibiotic use.

Salmonella Typhi (S. Typhi) is the bacterium responsible for typhoid fever, a serious infection that affects the digestive system. It spreads through contaminated food, water, or close contact with an infected person. Common symptoms include high fever, abdominal pain, weakness, and digestive disturbances. If left untreated, it can cause severe complications and become life-threatening. Preventive measures include vaccination, proper sanitation, and safe food handling practices.

Objective

The objective of the present research work is to perform Antibody plot diagram and rainbow's spectrum helps to study the evaluate interactions through binding affinity with different sites of the target protein of E. coli, P.vulgaris and S.typhi of Imidazole Scaffolds.

Material and Methods

2.1 Softwares and Tools- AutoDock Vina , LigPlot+ v.2.2.9, Protein Data Bank (PDB), PyMOL, and AutoDockTool-1.5.7, Command Prompt ,Chem 3D Ulita8.0, GaussView0.9 software, PubChem, NMR spectroscopy.

2.2 Protein Preparation- The preparation of protein structures of microbes antibody was obtained using Protein Date Bank for Escherichia coli (E. coli) (Protein Id: 4HWA), S.typhi (Protein Id: 5BUN), P.Vulgaris (Protein Id: 4MCT).

2.3 Ligand Preparation- The preparation of ligand used for the due to the NMR structure data for the chosen ligands and tool of Chem 3D Ulita8.0, GaussView0.9 software, PubChem.

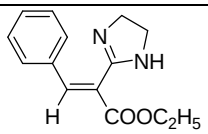
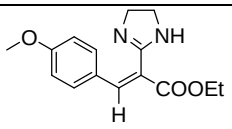
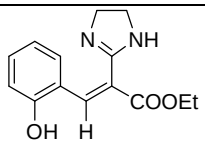
2.4 Docking Studies Using AutoDock Vina-The ligands docked with target proteins using AutoDock Vina 1.5.7. The receptor and ligand files were represented in PDBQT file format, a modified PDB format containing atomic charges, atom type definitions for ligands, For docking, the entire receptor was enclosed inside a grid box , keeping the receptor rigid and the ligand as a flexible molecule. The ligand's backbone and side-chain were flexible and allowed to dock with the receptor to form all possible conformations. After defining the binding site and receptor–ligand preparation, docking runs were launched from the command prompt. The interaction energy between the ligand and the receptor was calculated for the entire binding site and expressed as affinity (kcal/mol).

2.5 Protein–Ligand Interactions Ligplot+ v.2.2.9 software was downloaded from website (https://www.ebi.ac.uk/thornton-srv/software/LigPlus/). Was analysed the molecular interaction with the complex structure of microbes antibody during the analysis the antibody Ligplot+ module was employed to DIMPLOT then explore with Antibody plot this is an extension of DIMPLOT specifically for plotting antibody-antigen interactions. The antibody loops colour-coded and labelled domain-domain and protein-protein interactions and helps to understand the target binding sites for docking. The molecule is Visualization of protein –ligand interaction was carried out using PyMoL software (www.pymol.com). We have determined the bonding free energy for different compounds. Different software is widely available for performing molecular docking.

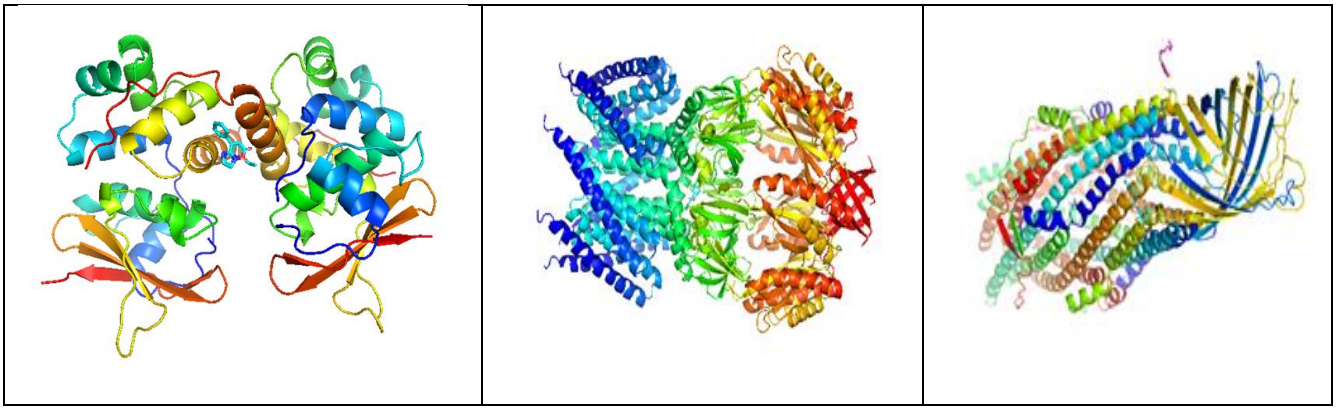
Result and Discussion

Structure and compound name are tabularized in table 1.

Table 1: Structure and Name of Imidazole Scaffolds

Sr. No	Compound	Structure	Compound Name
1)	**6a**		(E)-ethyl 2-(4,5-dihydro-1H-imidazol-2-yl)-3-phenylacrylate
2)	**6b**		(E)-ethyl 2-(4,5-dihydro-1H-imidazol-2-yl)-3(4-methoxyphenyl)acrylate
3)	**6c**		Ethyl 2-(4,5-dihydro-1H-imidazol-2-yl)-3-(2-hydroxyphenyl)acrylate

Different energy minimized proteins (rainbow spectrum) used in docking studies/ Rainbow's spectrum of compound 6a, 6b and 6c are shown below



Antibody plot:

Antigen-antibody interactions for compound 6a is reported in figure 2. Interaction of Imidazole compound with cell division protein of P.Vulgaris for compound **6a** is shown below

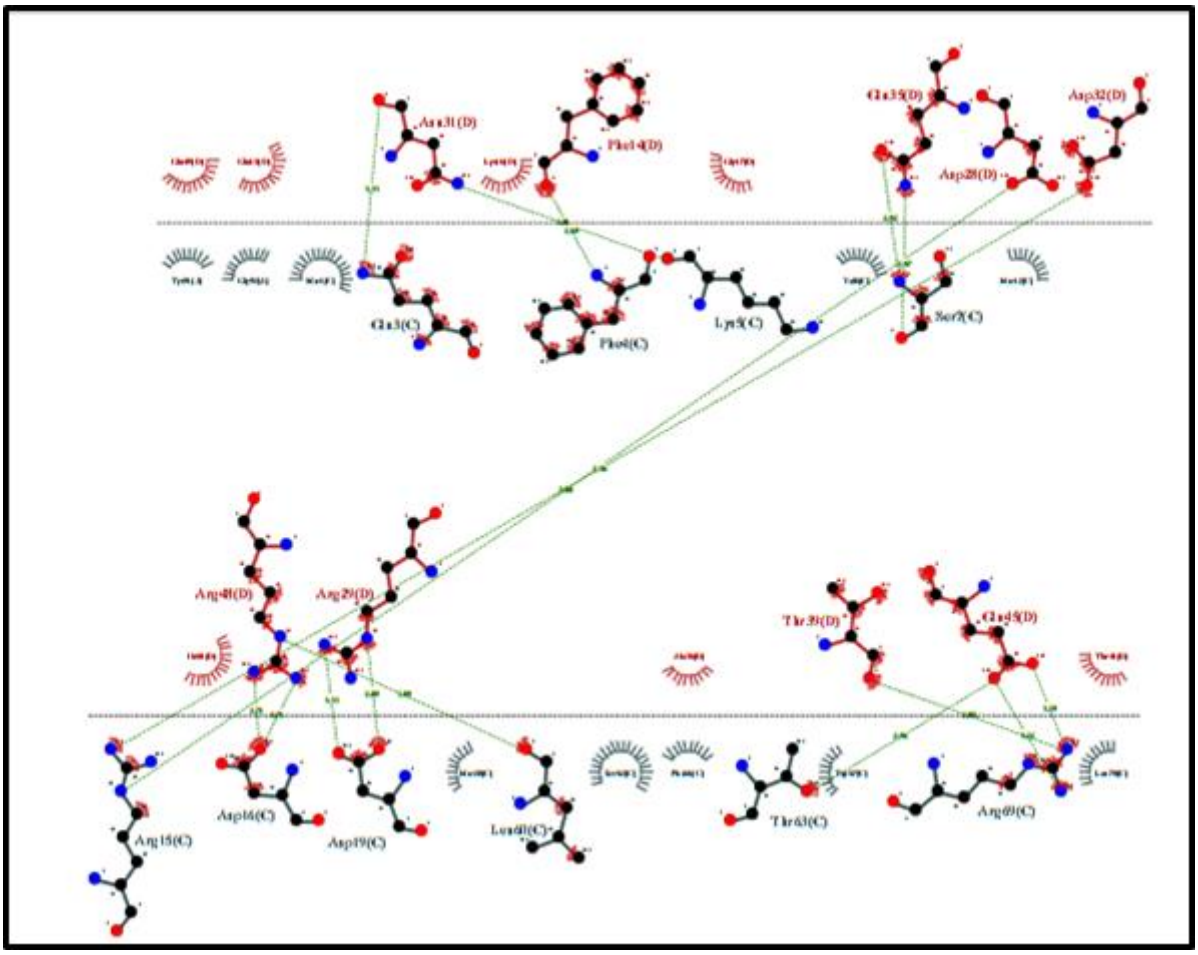


Figure 2 antigen-antibody interactions in lower loop for compound 6a with protein

In the above figure, we have found the interactive residue in terms of hydrophilic interaction between Asp 32(D) and Arg 15(D) with distance 2.56 A^0 while interaction between Asp 28(D) and Arg 15(D) is 3.88 A^0. From the interactions it is clear that there is large favourable binding for antibodies while hydrophobic interaction reveals unfavourable for binding to antibodies.

Antibody plot for antigen-antibody interactions in lower loop for compound **6b** is shown in figure 3

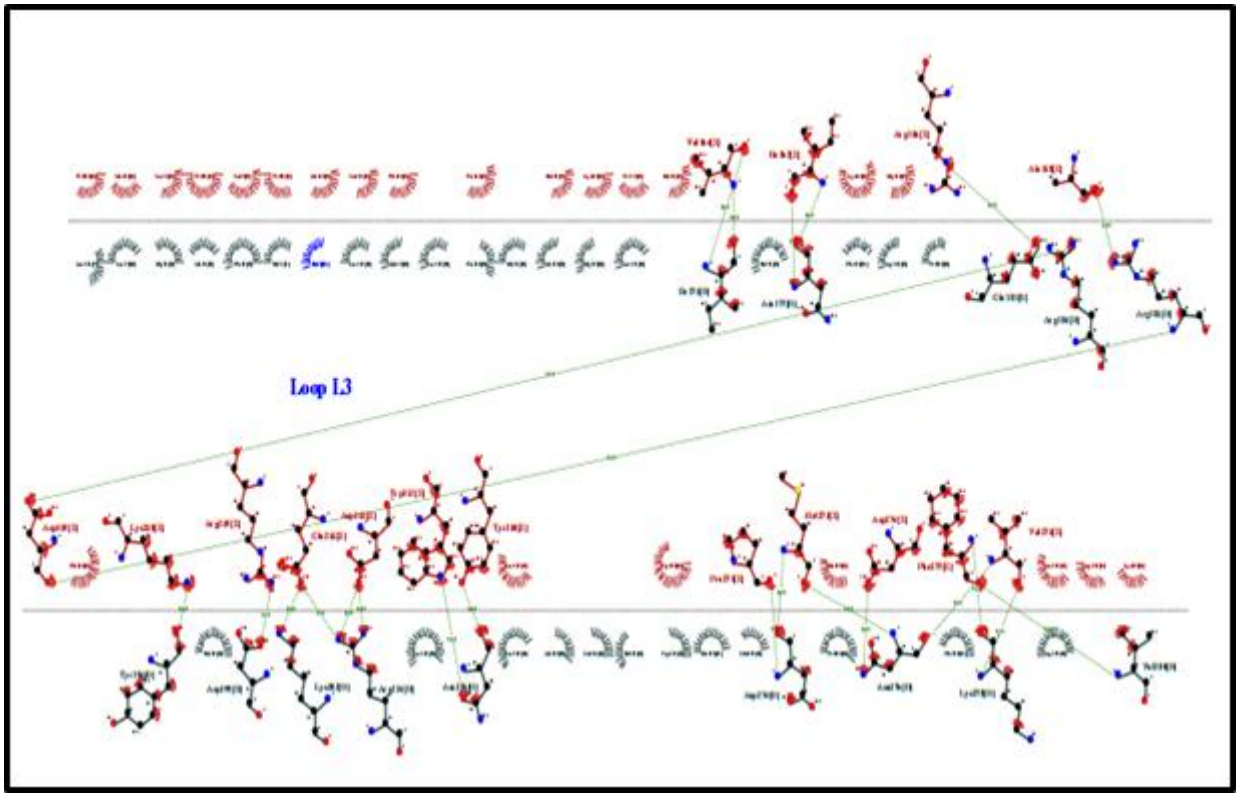


Figure 3 antigen-antibody interactions in lower loop for compound 6b with protein

Interaction of Imidazole compounds with cell division protein of antibacterial Escherichia coli (E. coli) are presented in figure 3. It clearly shows cross hydrophilic interactions between protein and the compound. The hydrophobic interactions are represented by arc with spokes radiating towards the ligand atom to which they are in contact. There are several intermolecular interactions present within the protein molecule. The interaction between Arg185 (D) with Asp159 (E) is 3.02 A^0 while Arg184 (D) interact with Asp159 (E) with 2.78 A for compound **6b**

Antibody-antigen plow showing hydrophilic interaction of compound **6c** is shown in figure 4.

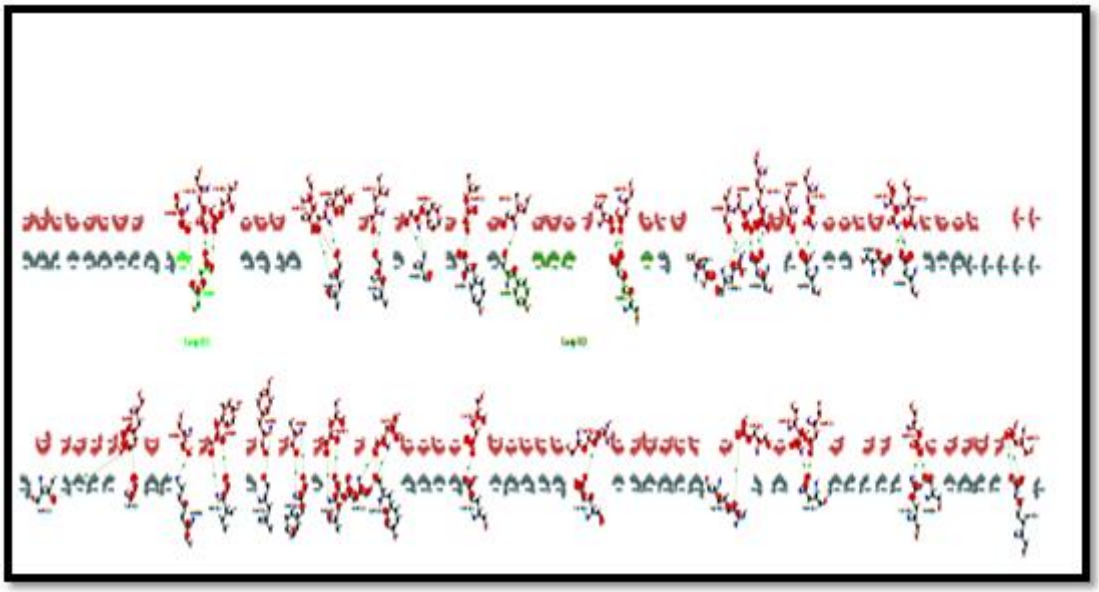


Figure 4 Interaction of Imidazole compound c with cell division protein of S.typhi

For compound **c** hydrophilic interactions is present between protein and compound which disrupts the interactions and act unfavourable antibody effect against S.typhi.

Conclusions

In the study we have adopted antibody plot to study antigen effect of imidazole scaffolds as effective microbial agent against E. Coli, P. Vulgaris and S. Typhi. Our study provide insight into the structural hotspot in terms of higher and lower loop which detects the ability of imidazole scaffolds. The result of our study will definitely assist in the development of new antibacterial agent to protect against different microbes.

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Conflict of Interest

The authors declare no conflict of interest.

Funding Declaration

No Funding

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Photocatalytic, Antimicrobial, Swiss-ADME Studies and Characterization of Hydrothermally Synthesized Pure and Ni-Doped Indium Oxide

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ABSTRACT

In the present study, the pure and Ni-doped indium oxide was successfully synthesized by the hydrothermal method and characterized by several analytical tools for its structural and microstructural properties, such as FTIR, UVDRS, SEM-EDS, and XRD. The UVDRS proves the pure and doped oxides have good bandwidth; hence, they can be used as photocatalysts for the degradation of harmful water pollutants like dyes, insecticides, herbicides, etc. Also, the oxides found are antimicrobial active for E. coli, Pseudomonas aeruginosa, and Candida albicans. Also focused on the challenges in bioavailability using the ADMET study by the Swiss-ADME model.

Keywords—Indium oxide, Ni-doped indium oxide, Antimicrobial, Photocatalyst, Band gap, Swiss-ADME.

INTRODUCTION

The creation of useful materials with a wide range of uses in energy conservation and environmental remediation has been spurred by the growing need for sustainable environmental solutions [1-4]. Metal oxide semiconductors have a lot of interest because of their special antibacterial and photocatalytic abilities. A tried-and-true method for enhancing semiconductors' photocatalytic efficiency and antibacterial activity is to incorporate metal dopants into their structure [5]. Through improved charge carrier dynamics and increased absorption into the visible spectrum, nickel (Ni) doping in indium oxide has demonstrated promise in boosting its photocatalytic activity. Additionally, it has been observed that adding Ni to the In_2O_3 lattice has promising antibacterial effects. Several methods can be adopted for the synthesis of metal oxide at the nano level; among these, the hydrothermal method gives assurance for a comparably low size of oxides with maximum purity. In the present work, pure and doped indium oxide was hydrothermally synthesized and characterized by X-ray

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powder diffraction (XRD) [6-10], UV-visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), and Scanning Electron Microscopy with energy dispersive x-ray analysis (SEM-EDS) [11-18]. The detailed discussion is focused on photocatalytic and antimicrobial studies [19-20]. A variety of dyes and pigments are utilized for textile industries, which creates hazardous pollution. Metal oxide in pure and doped state with amazing particle size and band gap can be effectively used as a photocatalyst for degradation of hazardous pollutants like dyes, pesticides, herbicides, etc. The photocatalytic and antimicrobial activities of nanomaterials are strongly governed by their morphology [21-24]. Malachite green is a synthetic dye that has diverse applications in textile industry, and it is one of the toxic dyes [25-27]. In this present work, synthesized metal oxide is successfully applied as a photocatalyst for continuous degradation of malachite green dye. The activity of oxides is evaluated against gram-positive E. coli, Pseudomonas aeruginosa, Candida albicans, and Staphylococcus aureus [28-31].

EXPERIMENTAL

2.1 Material Synthesis

According to literature review and previous study, we optimized the reaction temperature and time as well as the precursor contents to prepare indium oxide and Ni-doped indium oxide with the required particle size. First, prepare the 30 ml of 5 mM solution by dissolving $In(NO_3)_3.6H_2O$ (99.9%, SRL) in deionized water with continuous vigorous shaking on a magnetic stirrer till a clear solution is obtained, followed by the addition of excess 1 M NaOH solution in deionized water under stirring for 30 minutes. Then, the so-obtained reaction solution was carefully transferred to a Teflon-lined autoclave. The synthesis reaction was conducted at 170°C for 10 hours in an electric oven, which was naturally cooled to room temperature after the reaction completion. The resulting precipitate was collected by centrifugation at 12,000 rpm for 10 min, washed with distilled water and ethanol several times to remove unnecessary compounds, dried at 60°C for 1 h, and, finally, calcined at 500°C for 2 h and 600°C in a muffle furnace with an increasing temperature rate of 1^0C/min till complete conversion of hydroxide into oxide to obtain In_2O_3 NCs. A similar method was adopted for Ni-doped indium oxide using nickel nitrate hexahydrate (99.9 % purity SRL) as a dopant and indium nitrate hexahydrate.

2.2 Material Characterisation

The crystal structure of the synthesized In_2O_3 NCs was investigated by using an X-ray diffractometry (XRD) system (D/Max 2005, Rigaku) with Cu Ka radiation (l ¼ 1.54178 Å). The microstructure of the fabricated In_2O_3 NCs sensor was examined by a field emission scanning electron microscopy (FESEM), and elemental composition was confirmed by an EDS study. The functional groups on the prepared materials were further measured by Fourier transform infrared spectra. Fourier transform infrared spectroscopy (FTIR) spectra of powders were recorded over the range 400–4000 cm^{-1} (PerkinElmer, Spectrum 100 FTIR). Optical properties of In_2O_3 were studied using UV-visible spectroscopy (JASCO V-670).

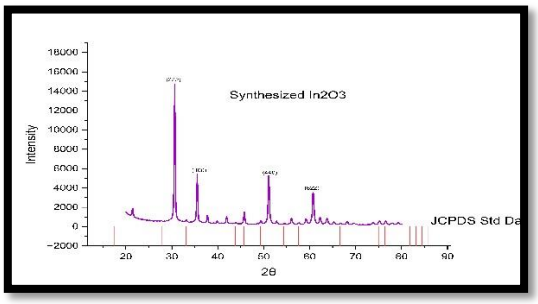
RESULTS AND DISCUSSION

3.1 Structural Analysis

3.1.1 XRD analysis

Figure 1a indicates the XRD pattern of calcinated pure indium oxide, while 1b indicates the XRD of Ni-doped indium oxide. The XRD pattern of indium oxide closely matched with cubic indium oxide (JCPDS card number 76-0152) and cubic bixbyite for Ni-doped indium oxide (JCPDS card number 06-0416). This confirms that the high-purity nanocrystalline indium oxide and doped indium oxide are formed, which is free from impurity with x-ray detection limits. The crystal plane was found to be (222) for pure and (211) for doped indium oxide particles, synthesized using the hydrothermal method. The XRD pattern indicates the formation of crystalline

indium oxide with an average particle size of 29.89 nm for pure indium oxide and 10.73 nm for Ni-doped indium oxide, which is calculated from the Scherrer equation ($D = K\lambda / \beta Cos\theta$).



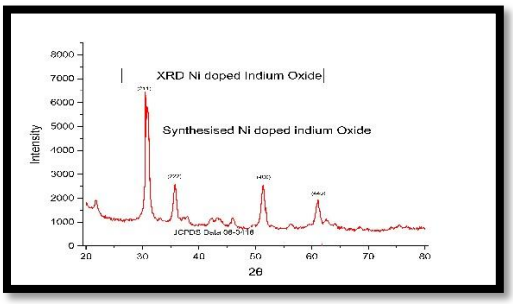
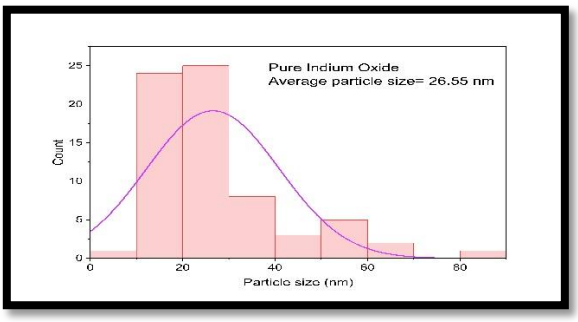


Figure 1a **Figure 1b**

Figure 1a XRD of pure indium oxide and 1b XRD of Ni doped indium oxide.

In the figure 2 histogram, the average particle size for pure (26.55 nm) and Ni-doped (13.07 nm) indium oxide is determined by the ImageJ software, which closely matches the particle size obtained by the Scherrer equation from XRD data.



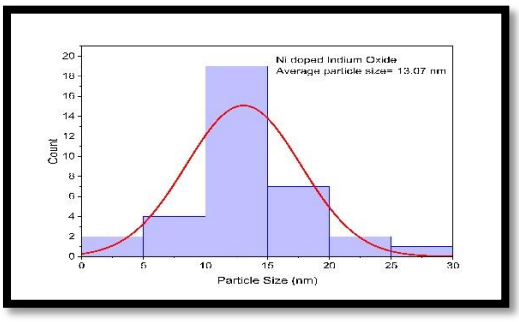
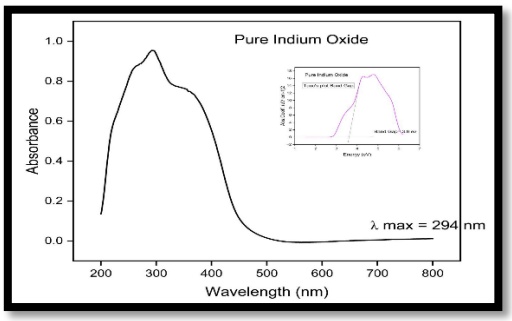


Figure 2a **Figure 2b**

Figure 2a histogram average particle size pure indium oxide and 2b Ni doped indium oxide.

3.1.2 UV Visible spectroscopy

UV-visible absorption spectra of pure and Ni-doped indium oxide show well-defined absorption peaks at 294 nm having a band gap of 3.6 eV and 295 nm having a band gap of 3.21 eV, respectively, as shown in Figures 3a and 3b given below.



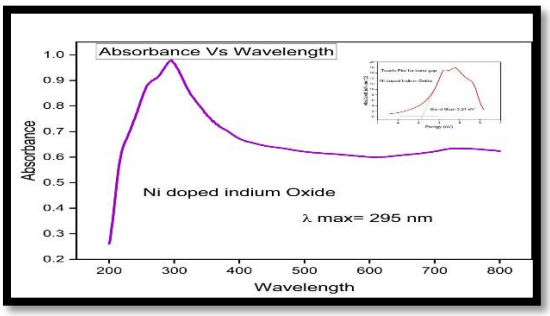


Figure 3a pure indium oxide **Figure 3b Ni doped Indium oxide**

Figure 3 Uv- visible absorption spectra and Tauc plot for pure indium oxide and Ni doped indium oxide.

3.1.3 FT-IR spectra

Figures 4a and 4b reveal the IR spectra of the calcinated powder of pure and doped indium oxide, respectively. The peaks at 400-500 cm^{-1} O-In-O bending vibration, 500-600 cm^{-1} In-O stretching vibration, and 601 cm^{-1}

O-In-O bending vibration for pure indium oxide, while 400-500 cm^{-1} In-O stretching vibration, 537-603 cm^{-1} Ni-O stretching vibration for Ni-doped indium oxide.

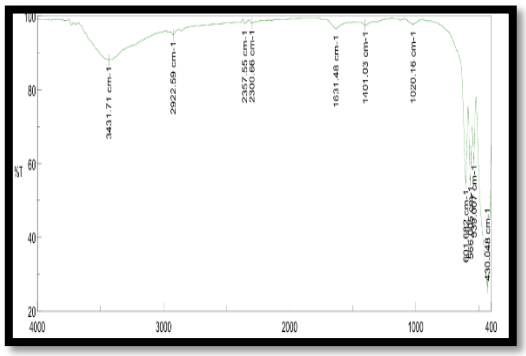


Figure 4a

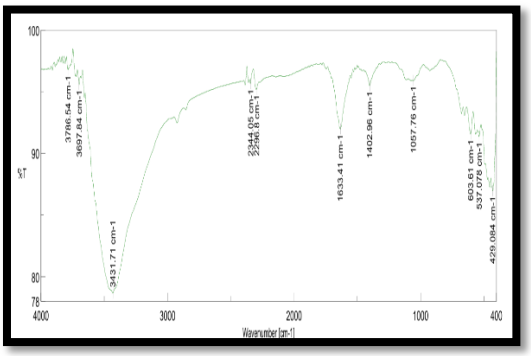


Figure 4b

Figure 4a FTIR spectra for pure indium oxide and figure 4b FTIR spectra of Ni doped indium oxide.

3.1.4 SEM EDS

Figure 5a shows SEM images of the synthesized pure indium oxide sample; it can be clearly observed that indium oxide forms micron-sized cubes, which are the result of the aggregation of multiple indium oxide particles with smaller sizes. Also, the EDS study proves the composition of synthesized indium oxide illustrated in figures 5b and 5c.

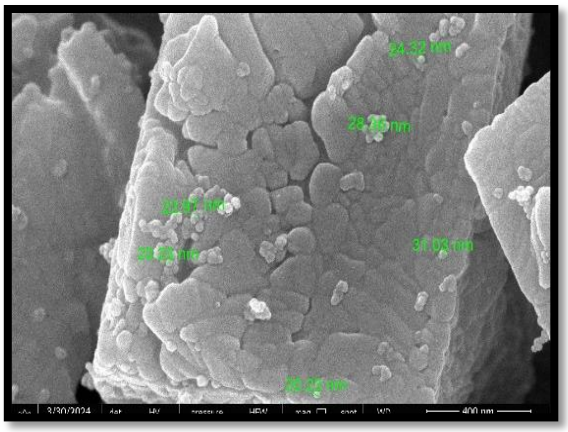


Figure 5a SEM image

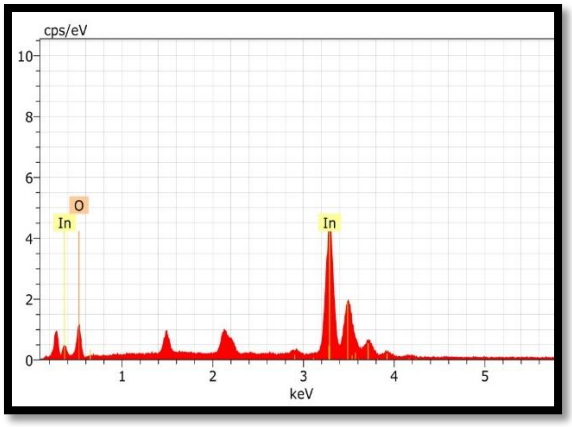


Figure 5b EDS data

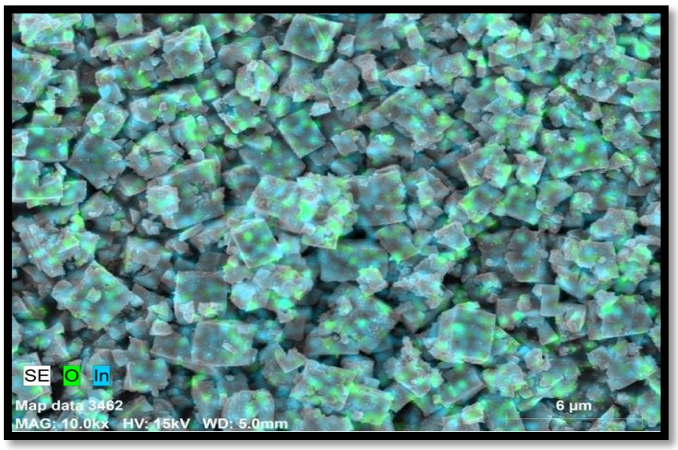


Figure 5c EDS image for pure indium oxide

Similarly, figure 6a gives morphology using SEM, and figures 6b and 6c are for EDS data of Ni-doped indium oxide.

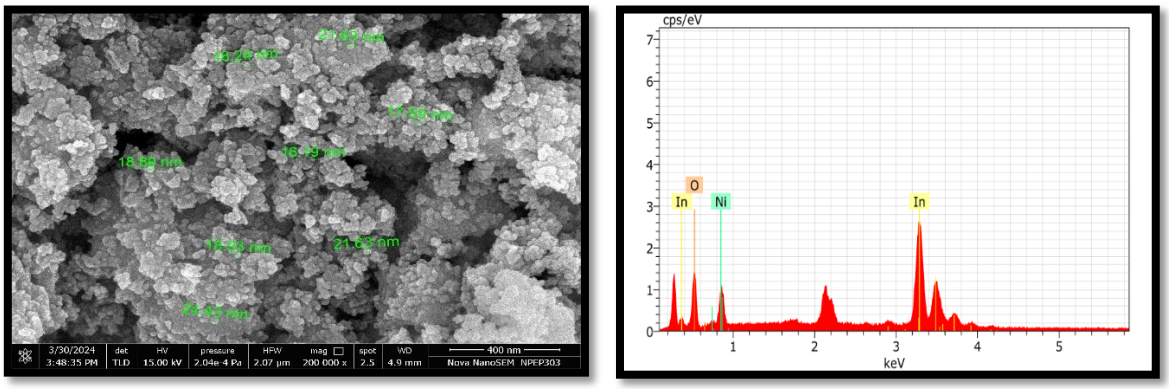


Figure 6a SEM image of Ni doped indium oxide. Figure 6b EDS analysis for Ni doped Indium oxide.

Application of Indium oxide and Ni doped indium oxide for photocatalytic degradation of malachite green dye

Malachite green, a dye used in various industries, poses biohazardous risks to humans, including potential for carcinogenicity, mutagenesis, and teratogenicity, especially through direct contact and exposure. The Swiss-ADME shows the level of toxicity; hence, MG degraded from waste effluent.The process of photocatalysis is taking place on the surface of the photocatalyst. In this study, the aqueous solution of malachite green dye is degraded under UV light in the absence and in the presence of photocatalyst. The continuous degradation of MG dye is studied using indium oxide. The 100 ml of 100 ppm solution of MG dye was kept in the dark along with the photocatalyst overnight. No change in absorbance indicated that in the absence of light, the catalyst was not able to degrade the dye. The photocatalytic degradation of MG dye using indium oxide and Ni-doped indium oxide particles as a photocatalyst was assessed by the degradation of the dye solution with an initial concentration of 20 ppm under the UV reactor, and the sample was taken periodically and centrifuged at 120000 rpm to remove nanoparticles from the test solution. The maximum absorbance λ_{max} of the supernatant dye solution was analyzed by a double beam UV-visible spectrophotometer to measure the concentration of MG dye at 617 nm. The percentage of degradation was calculated from the formula.

Degradation = $(C_0 - C_t / C_0) \times 100 = ((A_0 - A_t) / A_0) \times 100$

C_0 and C_t are the initial and final concentrations of dyes at time t, respectively. A_0 and A_t are the initial and absorbance at time t, respectively.

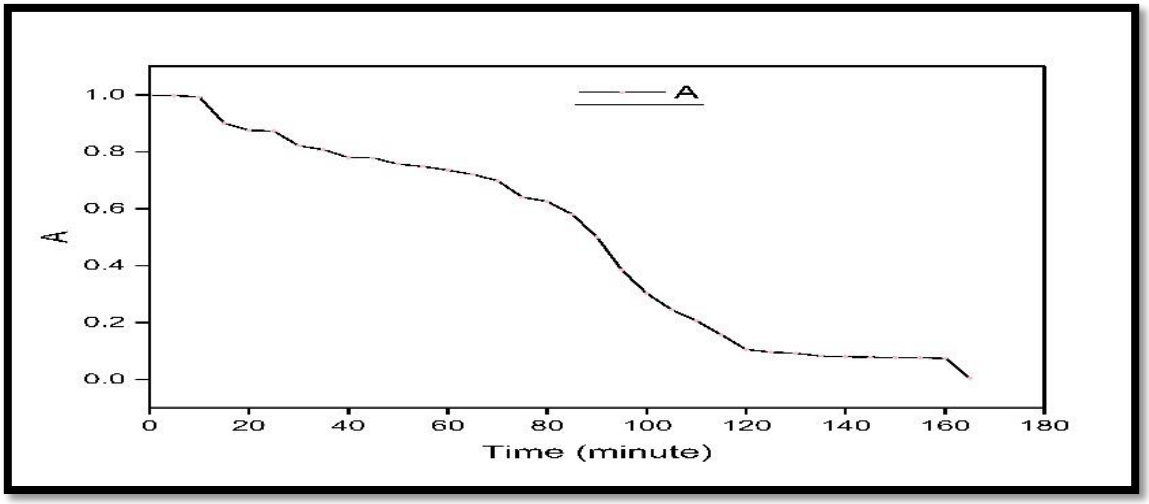


Figure 7a Continuous degradation of MG dye using Indium oxide.

Figure 7b shows the percentage degradation of dye; it is clearly observed that 94% of the dye degraded in 165 minutes.

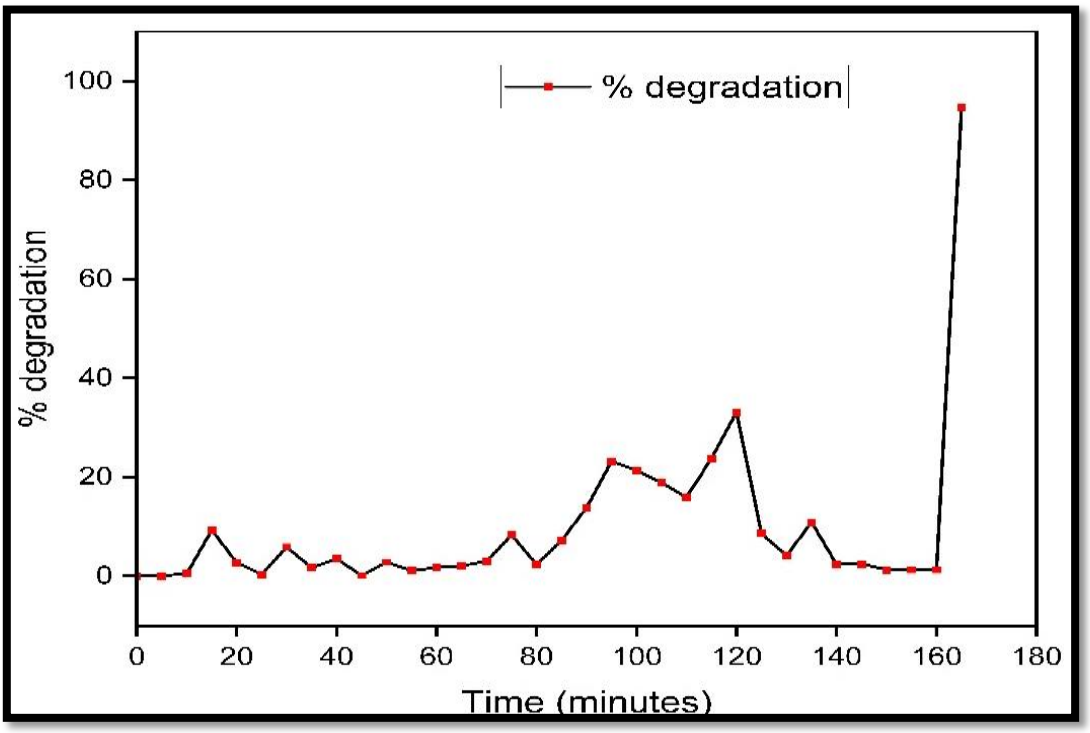


Figure 7b. % degradation of MG dye.

Swiss-ADME study of malachite green dye

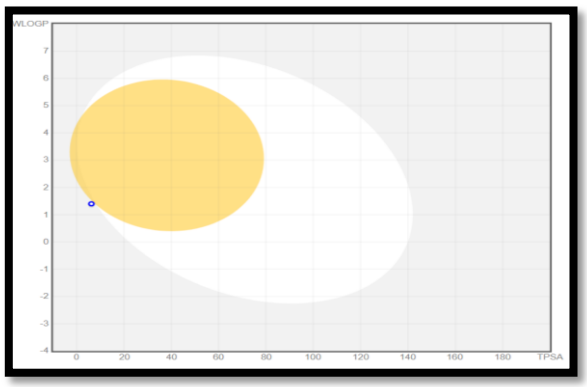


Figure 7c Boiled-Egg model

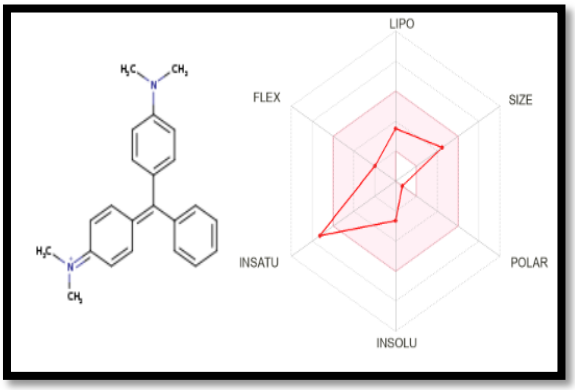


Figure 7d Bioavailability Radar

ANTIMICROBIAL STUDY

The antimicrobial activity of pure and Ni-doped indium oxide was tested against E. coli (ATCC 25922), Pseudomonas aeruginosa (ATCC 27853), Staphylococcus aureus (ATCC 25923), and Candida albicans (ATCC 14053) against gentamicin and nystatin as a standard using the well diffusion method. The development of the zone near the pure and doped oxide was measured and recorded. It was clearly noted that there was no positive activity found due to pure indium oxide.

The antimicrobial activities shown by pure and doped indium oxide with respect to the standard are illustrated as below.

Sr. No.	Name of the compound	Antimicrobial			Antifungal
		E. Coli	Pseudomonas aeruginosa	Staphylococcus aureus	Candida albicans
		ATCC 25922	ATCC 27853	ATCC 25923	ATCC 14053
1.	Pure indium oxide	-	-	-	-
2.	Ni doped indium oxide	7 mm	7mm	-	7 mm
3.	Gentamicin	23 mm	24 mm	26 mm	-
4.	Nystatin	-	-	-	21 mm

Table No. 1 Results of antimicrobial activity.

The graph in figure 9 indicates the antimicrobial activity shown by Ni-doped indium oxide's comparative study.

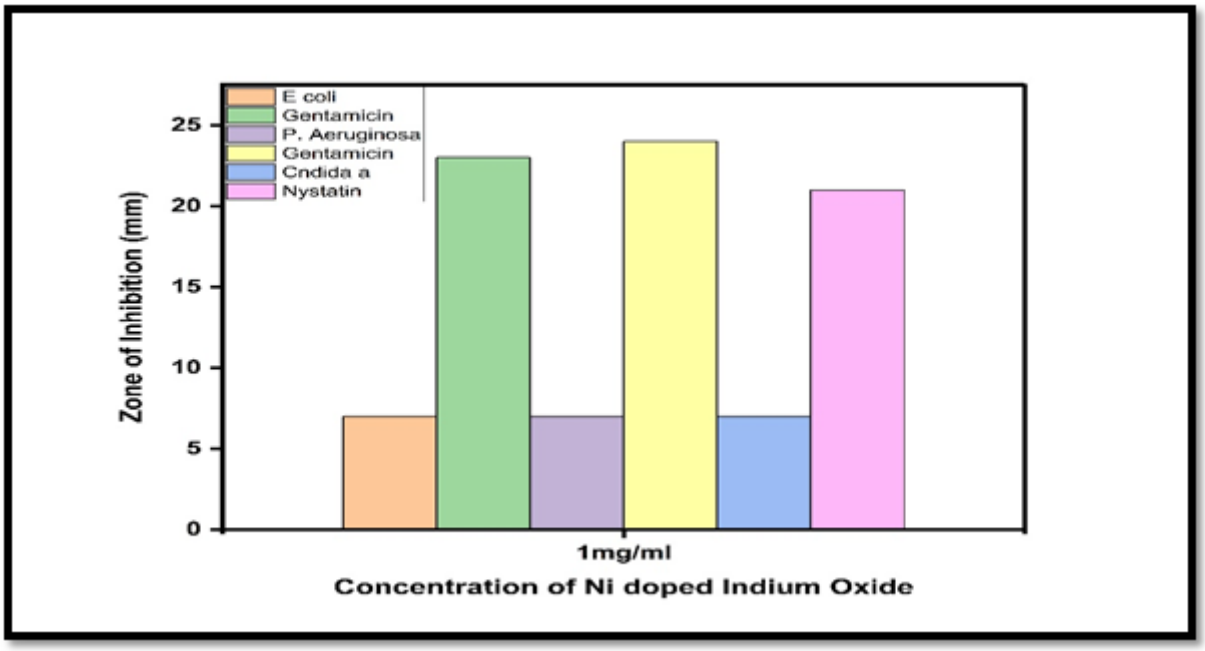


Figure 9 Graph for antimicrobial activity shown by Ni doped Indium Oxide.

SwissADME study of Ni doped indium oxide

The physicochemical properties like lipophilicity, water solubility, molecular weight, TPSA, drug likeness, bioavailability score, and pharmacokinetics, involving gastrointestinal absorption prediction, blood-brain barrier permeation, etc., are studied by the ADMET data guide using SwissADME. The BOILED Egg model was predicted as shown in figures 10a and 10b, while figures 10c and 10d indicate the bioavailability radar for the material. As in figure 10b, the molecule extending beyond the pink region indicates it may face challenges in pharmacokinetics or bioavailability.

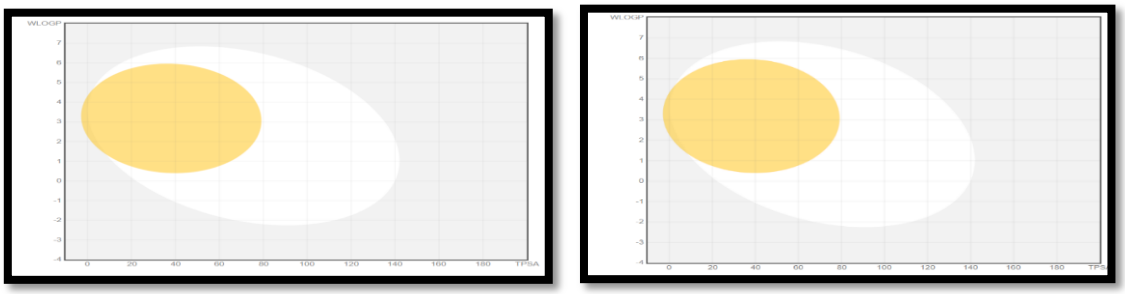


Figure 10a Figure 10 a Boiled-Egg model

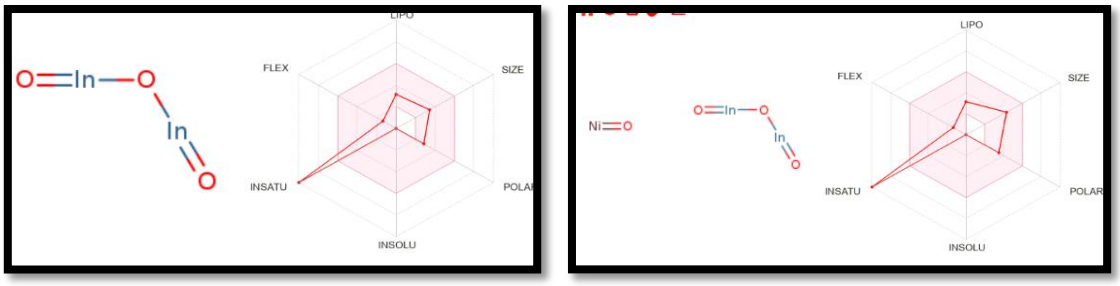


Figure 10b Bioavailability Radar

Conclusion

The pure indium oxide and Ni-doped indium oxide were synthesized by a simple hydrothermal method. The cubic structure of the exhibited significantly improves photocatalytic activity for degradation of malachite green dye. Moreover, doping by nickel enhances its antimicrobial activity towards E. coli, Pseudomonas aeruginosa, and Candida albicans. Also, the ADMET study using SwissADME focused on pharmacokinetics or bioavailability of synthesized metal oxides.

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The Investigation of Thermo-Acoustical Behavior of Binary Liquid Mixtures of Benzene and Tetra Butyl Ammonium Iodide at Different Temperatures

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ABSTRACT

The study of ultrasonic velocity is crucial for understanding molecular interactions in binary liquid mixtures. in the present study the first liquid is taken is nonpolar and the other two components are ionic liquid in nature. The ultrasonic velocity, density, and viscosity for binary liquid mixtures containing benzene with tetra ammonium iodide has been measured at different temperatures T=301.15k,305.15k,309.15k,313. 15k at different composition of liquid mixture. From these experimental values derives the ultrasonic parameter via impedance, intermolecular free length, adiabatic compressibility, molar volume, free volume and relaxation time. Ionic liquids (ILs) are widely used, therefore experimental study on their physio-chemical properties has increased. This study indicates the importance of the speed of sound in ionic liquids and their mixtures. The Reviewing of relevant theoretical frameworks. This investigation is anticipated to yield valuable insights into subsequent research concerning the physicochemical properties within ionic liquid (IL) mixture systems.

Keywords: Benzene, Tetra Butyl Ammonium Iodide, Molecular Interaction, Adiabatic Compressibility

INTRODUCTION

In binary liquid mixtures, the ultrasonic method is one of the most effective methods for examining bulk characteristics and intermolecular forces. The examination of molecular interactions within mixed solvent systems holds considerable importance due to the practical uses of these systems across various technologies, as they offer a diverse range of solutions with suitable properties. The speed of ultrasonic waves, along with measurements of density and viscosity, provides a rich array of insights into the interactions among ions, dipoles, hydrogen bonding, and various forces such as multipolar and dispersive interactions. [1-3]

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Ionic liquids (ILs) are molten salts that melt slowly and are made completely of ions. The melting points are lower than 100 degrees Celsius. The characteristics of ionic liquids differ greatly from those of ordinary conventional liquids. ILs have garnered a lot of attention over the past few decades due to the distinctive characteristics that they possess such as nearly negligible vapor pressure, high chemical, thermal stability, low flammability, a large liquidus range, high ionic conductivity, a large electrochemical window, and an excellent ability to solvate a wide variety of compounds. In recent years, there has been a significant amount of interest in study about the physicochemical studies that involve the volumetric, acoustic, viscometrical properties of room temperature ionic liquids and their mixes with other organic solvents. [4-6]

A quaternary ammonium compound tetrabutylammonium iodide (TBAI) is a powerful electrolyte that dissolves in water and has a variety of physical, chemical, and biological characteristics. Tetra butyl is a viable alternative as a catalyst for the functioning of C–H bonds in recent times because of its inexpensive cost and low toxicity. tetrabutylammonium iodide (TBAI) is used in industry as an active component in paper and textile softeners, conditioners, antistatic agents, and detergent sanitizers. [7]

The nature of molecular interactions between the components is understood by analyzing thermo-acoustical metrics such as adiabatic compressibility, intermolecular free length, acoustic impedance, molar volume, free volume, relaxation time, etc. The thermo-acoustical characteristics at different temperatures, this research attempts to shed light on solute-solvent interactions, ion-dipole interactions, and intermolecular forces. The results will expand our knowledge of ionic liquid-based mixtures, which are useful in advanced solvent systems, green chemistry, and catalysis.

MATERIAL AND METHOD

Chemicals

The tetra butyl ammonium chloride ionic liquid obtained from Loba Pvt Ltd. India (central scientific, Nagpur, Maharashtra).It was used as it is without any purification. The purity was 99% AR grade. The physical state is solid.it was received in off white crystalline powder.

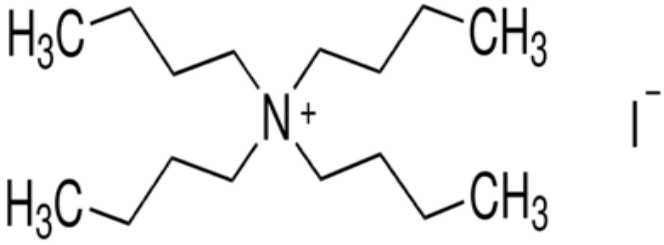

Fig 1. chemical structure of tetra butyl ammonium iodide

The Benzene AR grade 99.5% pure was obtained from sigma Sigma–Aldrich Pvt Ltd India. The supplier is Upper India Scientific, Nagpur, Maharashtra. It was used as it is without any purification.it was not found impurities. One of the most well-known aromatic compounds is benzene, which has the chemical formula C6H6. [8]

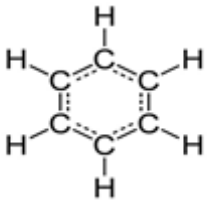

Fig 2. chemical structure of Benzene

METHODS

- Ultrasonic Velocity: The ultrasonic velocities (u) of binary mixture of tetra butyl ammonium iodide with benzene were determined at a constant frequency of 5 MHz in these solutions at various temperatures, namely 301.15k, 305.15k, 309.15k, and 313.15k, using an interferometric technique, specifically Mittal's M-81 model. The water bath is managed entirely through electronic or digital controls for precise temperature regulation of the water. Through unit measuring cells, the water flows. It has two walls and is entirely composed of steel. The temperature was precisely controlled by adjusting the thermostat to within ± 0.05%. The temperature of the water temperature controlling bath ranges from 0°C to 100°C. The obtained ultrasonic velocity (u) for pure liquids benzene and tetra butyl ammonium iodide at 301.15K is in good agreement with the value reported in the literature.
- DENSITY: Pure liquids and their mixtures are weighed using the electronically controlled Dona single monopan balance. The weighing balance has an accuracy of 0.1 mg. The densities of pure liquids and their mixes were measured using an 80 mL tasting tube. This taste tube was submerged in a water temperature-controlled bath after being filled with a 15 ml liquid combination. then taken out of the water bath at a steady temperature after 30 to 60 minutes. then immediately weighing the liquid mixture to determine its density. The obtained density for pure liquids benzene and tetra butyl ammonium iodide at 301.15K is in good agreement with the value reported in the literature.
- VISCOSITY: Ostwald's viscometer was used to test the dynamic viscosity. One thousand $Nm^{-2}s$ is the precision. ±0.1 s is the usual time of uncertainty. To guarantee thermal stability, the viscometer was submerged in the water bath for 30 to 60 minutes. We recorded the flow's duration using a digital stopwatch. For every mix, a flow time measurement was taken five times. The viscometer is calibrated using acetone, distilled water, and benzene that have known densities and viscosities. The obtained viscosity for pure liquids benzene and tetra butyl ammonium iodide at 301.15K is in good agreement with the value reported in the literature. The obtained viscosity for pure liquids benzene and tetra butyl ammonium iodide at 301.15K is in good agreement with the value reported in the literature.

RESULT AND DISCUSSION

This research examines the binary mixture of tetra-butyl ammonium iodide (TBAI) and benzene across various temperatures (301.15K, 305.15K, 309.15K, and 313.15K) to analyze the influence of ionic solutes on the structural and acoustical properties of a nonpolar medium. The findings of this research enhance our comprehension of solute-solvent interactions within ionic-organic systems, which may have significant implications for ultrasonic fluid technologies, solvation chemistry, and the study of molecular interactions.

The acoustical parameters: adiabatic compressibility, intermolecular free length, acoustic impedance, molar volume, free volume, and relaxation time has been calculated using experimentally measured values for binary mixtures of benzene with tetra-butyl ammonium iodide at various temperatures viz.301.15K, 303.15K, 309.15K, and 313.15K

- **Adiabatic Compressibility**

The ultrasonic velocity is experimentally obtained all over the composition of range of binary mixtures as a function of tetra butyl ammonium iodide mole fraction(x)at different temperatures adiabatic compressibility is calculated though experimental value such as ultrasonic velocity and density. The following formula was used to determine the adiabatic compressibility

$$\beta = \frac{1}{u^2 \times \rho}$$

Where ρ-density of liquids-ultrasonic velocity, β-adiabatic compressibility

The obtained values of adiabatic compressibility (βa) for the binary mixture of TBAI and benzene are plotted against the mole fraction in Fig. 1. The trend shows an initial increase in βa with increasing TBAI concentration, suggesting a decrease in intermolecular interactions and an increase in free space between molecules. This rise in compressibility indicates that the structural arrangement of molecules becomes less rigid, reducing the cohesive forces within the mixture

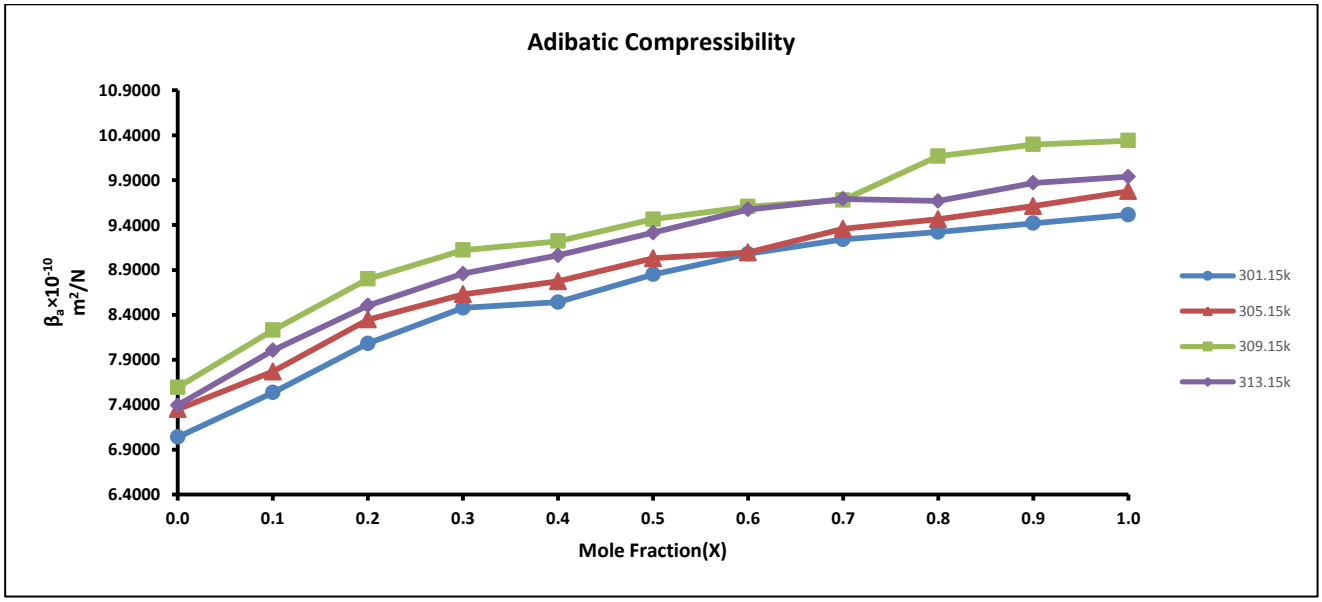

Figure 1: Graph depicting the adiabatic compressibility(β) for binary liquid mixture of benzene and tetrabutylammonium iodide at a temperature 301.15k,3035.15k,309.15k,313.15k

The increase in molecular motion weakens intermolecular forces, leading to greater free space between molecules and higher compressibility

❖ **Intermolecular free length**

The distance between the two molecules' surfaces is known as the intermolecular free length (L_f), which is another acoustical parameter that describes the type and intensity of intermolecular interactions that exist in a liquid mixture. It also depends on molecular size, shape, and mixture composition. When isentropic compressibility increases, free length also increases The intermolecular free length is calculated by using the ultrasonic velocity and density. The following formula was used to determine the acoustic free length

$$L_F = K\sqrt{\beta}$$

Here K-Jacobsen constant, T- Absolute Température $=(93.875+0.375\times T)\times 10^{-8}$

Figure 2. shows the intermolecular free length plotted against the mole fraction. the mole fraction of Tetra butyl ammonium iodide is added to benzene then it shows a non-linearly increased with increased in temperature is shown in fig.2. The observation revealed that the intermolecular free length (L_f) rises as the mole fraction of TBAI increases. Ultrasonic velocity (u) in the TBAI-benzene mixture systematically decreases as intermolecular free length rises with increasing TBAI concentration. This inverse relationship indicates that the system is more compressible due to a weakening of intermolecular interactions. Higher temperatures intensify the trend because of more thermal agitation.

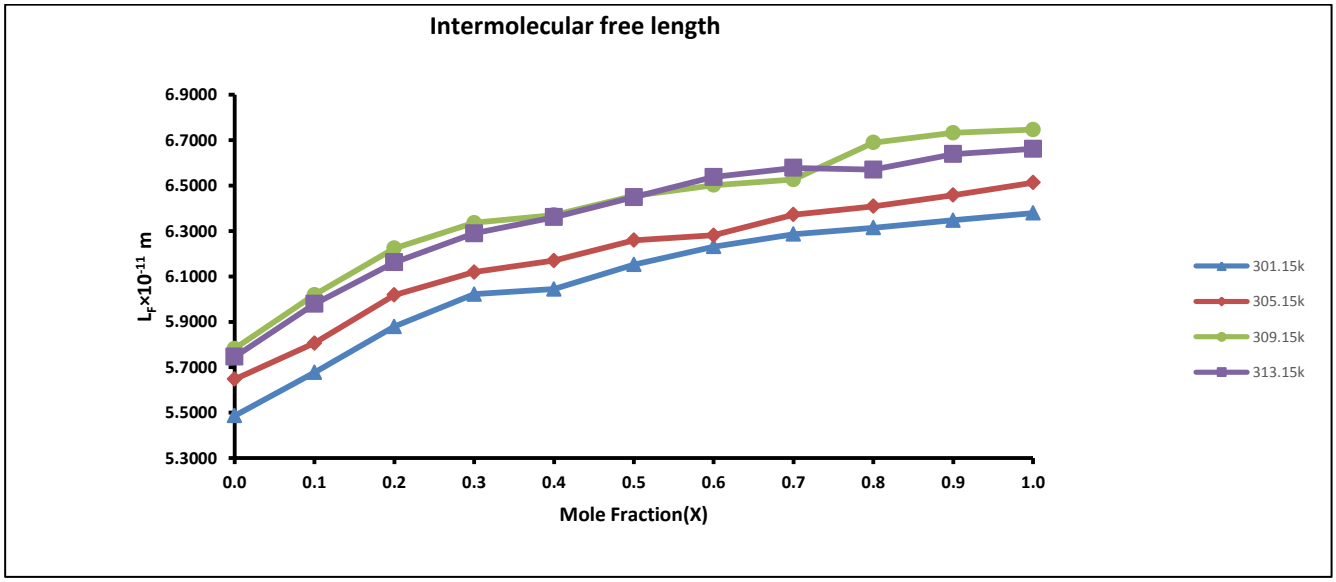

Figure 2: Graph depicting the intermolecular free length (L_f) for for binary liquid mixture of benzene and tetrabutylammonium iodide at a temperature 301.15k,3035.15k,309.15k,313.15k

❖ **Acoustic impedance**

The acoustic impedance (Z) of the TBAI-benzene mixture exhibits a systematic decrease as the mole fraction of TBAI increases is shown in figure3. The observed decline can be explained by the concurrent decrease in both density (ρ) and ultrasonic velocity (u), as evidenced by the experimental data. The observed lower impedance values indicate that the incorporation of TBAI modifies the structural configuration of the mixture, leading to a decrease in its resistance to the propagation of sound waves. Furthermore, at increased temperatures, this pattern becomes more pronounced as a result of alterations in molecular interactions and the overall compressibility of the substance. The acoustic impedance is calculated by using the ultrasonic velocity and density. The following formula was used to determine the acoustic impedance

$$Z = u \times \rho$$

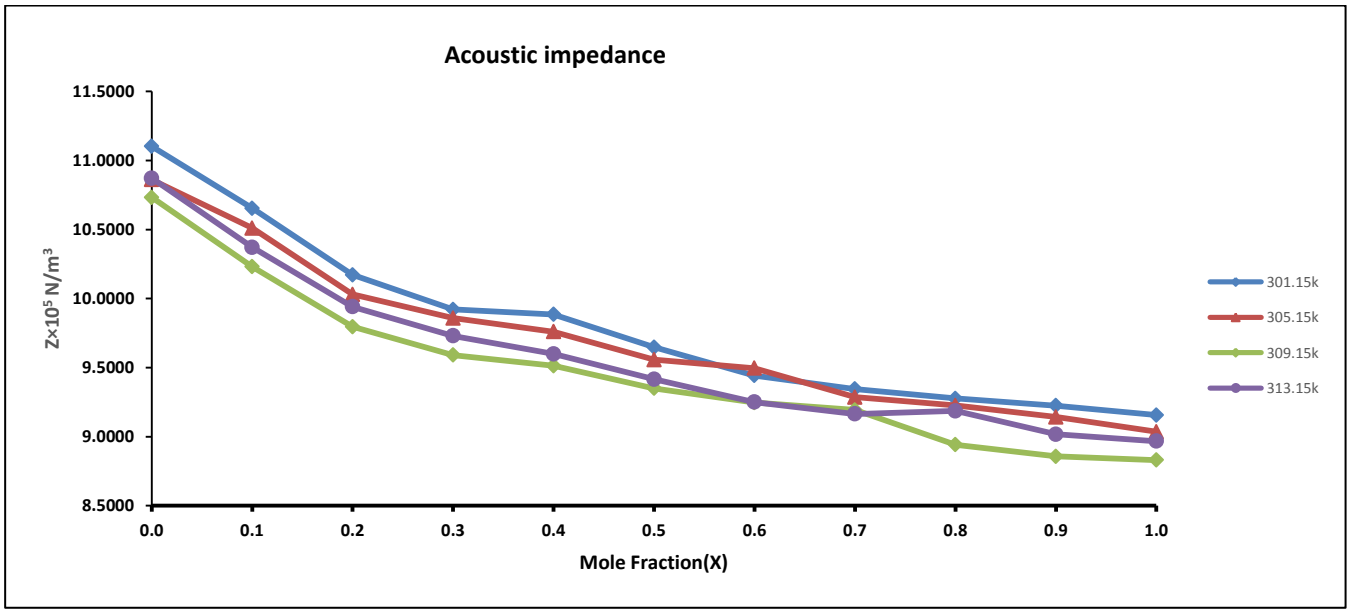

Figure 3: Graph depicting the acoustic impedance(Z) for for binary liquid mixture of benzene and tetrabutylammonium iodide at a temperature 301.15k,3035.15k,309.15k,313.15k

The interaction between TBAI with benzene is mainly influenced by weak ion–π interactions involving the ammonium ion (N +) and the π-electron cloud of benzene. Furthermore, the presence of weak van der Waals forces plays a significant role in the process of molecular association. The observed increase in intermolecular free length (Lf) alongside a decrease in ultrasonic velocity (u) indicates that the interactions present are comparatively weak, resulting in a mixture that is more loosely bound and exhibits reduced structural rigidity.

❖ **Molar Volume**

The calculated data of molar volume represented against the mole fraction in fig.4.The molar volume curves show a sharply increase as mole fraction of tetra butyl ammonium iodide is added into benzene at different temperature viz 301.15k,3035.15k,309.15k,313.15k .

The molar volume is calculated by using the density and molecular weight of liquid. The following formula was used to determine the molar volume,

$$V_m = \frac{XM_1 + (1 - X)M_2}{\rho}$$

Where X- mole fraction of tetra butyl ammonium iodide, M_1 and M_2- molecular weight of pure liquids tetra butyl ammonium iodide and benzene, ρ-density of pure liquid and liquid mixture

The molar volume (Vm) of the TBAI-benzene mixture shows a notable increase as the concentration of TBAI rises, suggesting structural expansion attributed to diminished molecular packing and the occurrence of ion–π interactions. The noted positive deviation from ideal mixing indicates a limited presence of attractive forces among the components. Furthermore, a minor reduction in (Vm) at increased temperatures indicates that temperature-dependent compressibility effects are impacting the volumetric characteristics of the system. This examination offers significant understanding of the molecular structure and interaction mechanisms within the TBAI-benzene binary system, which is crucial for comprehending the physicochemical characteristics of ionic liquid-based mixtures.

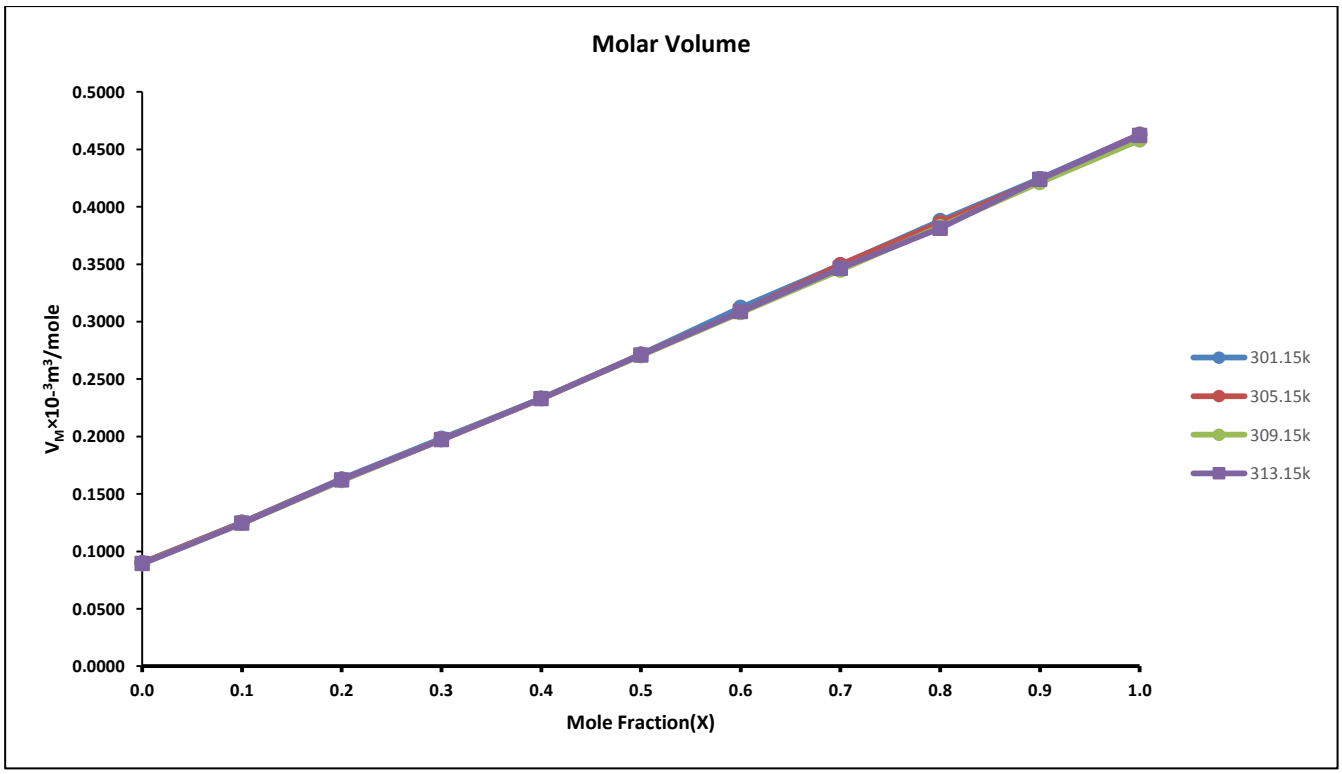

Figure 4: Graph depicting the molar volume (V_m) for binary liquid mixture of benzene and tetrabutylammonium iodide at a temperature 301.15k,3035.15k,309.15k,313.15k

❖ **Free Volume**

The calculated data of free volume represented against the mole fraction in fig.5.The free volume curves show a sharp increase as mole fraction of tetra butyl ammonium iodide is added into benzene at different temperature viz 301.15k,3035.15k,309.15k,313.15k .The free volume is calculated by using the ultrasonic velocity, independent temperature constant, viscosity and molecular weight of liquid. The following formula was used to determine the free volume

$$V_f = \left(\frac{M_{Eff} \times U}{K_T \times \eta}\right)^{\frac{3}{2}}$$

Where M_{Eff}- Effective molecular weight of pure liquids of tetra butyl ammonium iodide and benzene, u-ultrasonic velocity, K_T-temeprature independent constant=4.28×10^9 value for all liquids, η-viscosity of liquid. The free volume (V_f)of the TBAI-benzene mixture exhibits a notable increase with higher TBAI concentrations, suggesting a disturbance in the molecular arrangement attributed to the presence of large TBAI molecules and ion–π interactions. This positive deviation indicates a reduction in cohesive forces within the mixture. The documented temperature-dependent rise in (V_f) further substantiates that thermal agitation promotes molecular spacing, thereby facilitating the expansion of the liquid system. This examination offers critical insights into the microstructural behavior of the TBAI-benzene binary system, pertinent for comprehending solvation dynamics and ionic liquid interactions in nonpolar solvents.

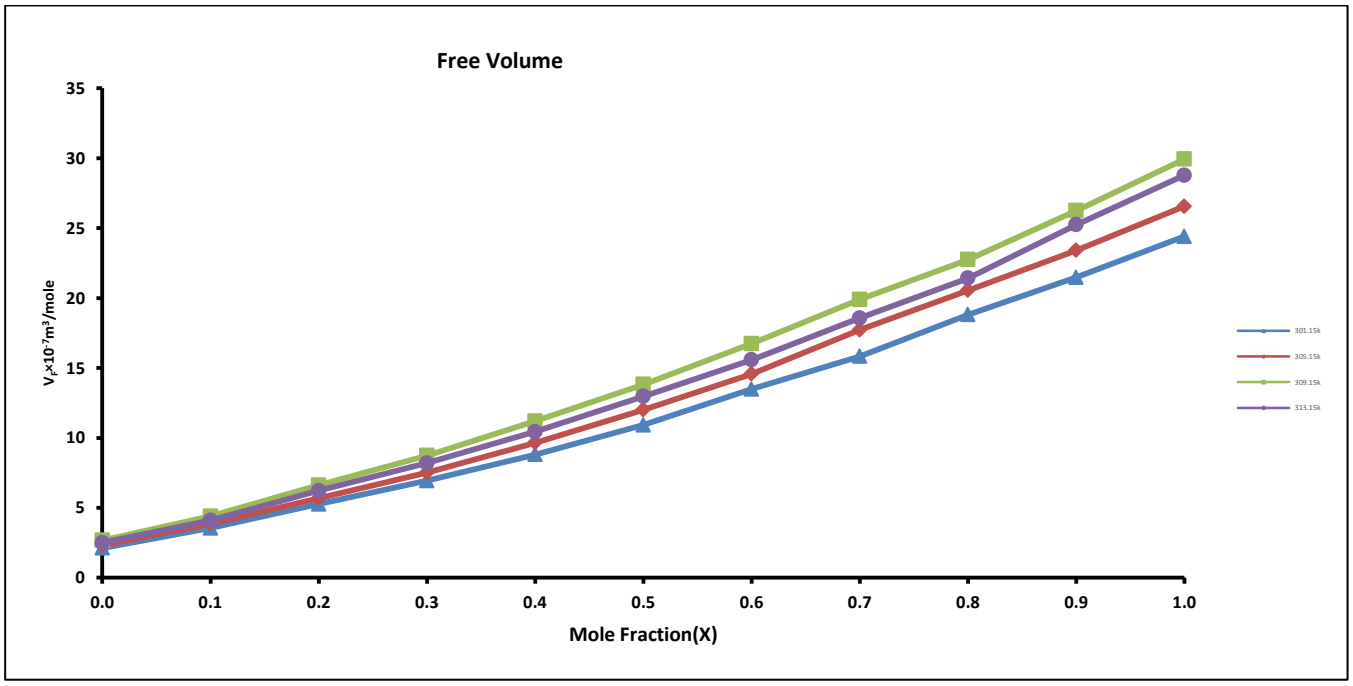

Figure 5: Graph depicting the free volume (V_f) for binary liquid mixture of benzene and tetrabutylammonium iodide at a temperature 301.15k,3035.15k,309.15k,313.15k

❖ **Relaxation Time**

The calculated data of relaxation time represented against the mole fraction in fig.6.The relaxation time curves shows a non-linearly increased as mole fraction of tetra butyl ammonium iodide is added into benzene at different temperature viz 301.15k,3035.15k,309.15k,313.15k . Relaxation time is calculated by using the adiabatic compressibility and viscosity of liquid. The following formula was used to determine the Relaxation time

$$\tau = \tfrac{4}{3}\beta \times \eta$$

Where β-adiabatic compressibility-viscosity of pure liquid and mixture of liquid

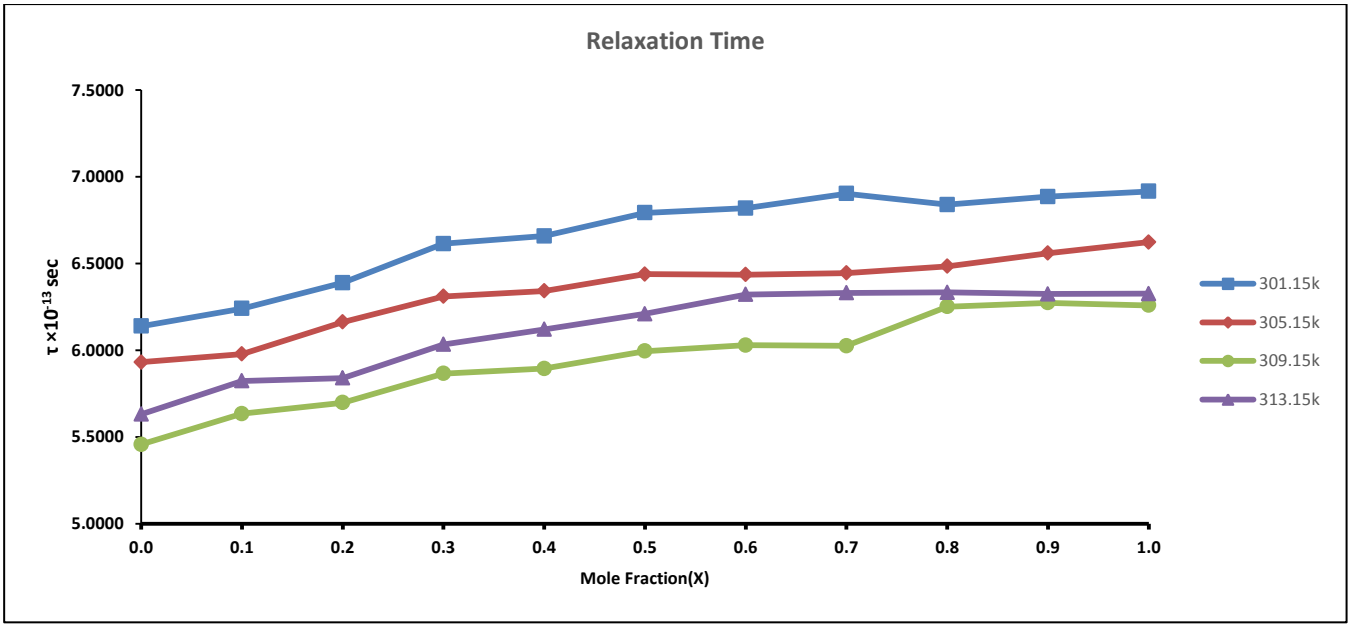

Figure 6: Graph depicting the relaxation time for binary liquid mixture of benzene and tetra butyl ammonium iodide at a temperature 301.15k,3035.15k,309.15k,313.15k

In the TBAI-benzene mixture, the relaxation time (τ) rises with mole fraction, suggesting improved viscosity and molecular interactions. Because heat agitation weakens intermolecular interactions, this rise stabilizes at higher temperatures. This behavior illustrates how ion–π interactions fundamentally affect the system's molecular energy dissipation and acoustic absorption. This finding is important for comprehending acoustic relaxation and solute–solvent interactions in ionic-organic liquid systems.

CONCLUSION

The present investigation demonstrated that incorporating tetrabutylammonium iodide (TBAI) into benzene resulted in an elevation of adiabatic compressibility, intermolecular free length, and free volume, suggesting diminished molecular interactions and a decrease in structural compactness. The reduction in acoustic impedance and ultrasonic velocity indicated that the mixture exhibited diminished resistance to sound propagation, consistent with the loosening of molecular packing. The observed increase in relaxation time suggests a deceleration in the energy dissipation mechanism, potentially attributable to alterations in the interactions between solute and solvent molecules. Temperature fluctuations additionally affected these characteristics, improving molecular mobility and the dynamics of interactions. The results yielded significant understanding of the acoustical properties and solvation influences within ionic–nonpolar binary systems.

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A Comparative Study on Decomposition Rates and Environmental Impacts of Sal Leaves vs. Common Leaf Litter and Challenges to convert it into Compost

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ABSTRACT

This study investigates the decomposition rates of Sal tree (Shorea robusta) leaves compared to other common leaf litter, such as oak (Quercus spp.), pine (Pinus spp.), and maple (Acer spp.) leaves and other leaves. Leaf litter decomposition is a crucial process in nutrient cycling and soil health, influencing forest ecosystem productivity and carbon sequestration. The research involved studies consisting of field and laboratory experiments to measure the mass loss and nutrient release over time under controlled conditions. The results indicated that sal leaves decompose at a significantly slower rate compared to the other leaf types, attributed to their higher lignin content and tougher physical structure. The study also highlighted the role of microbial communities and environmental factors such as temperature and moisture in the decomposition process. Understanding these differences provides insights into forest management practices, especially in tropical regions where Sal trees are prevalent, and underscores the importance of species-specific strategies for enhancing soil fertility and carbon management. The study also examines key challenges such as prolonged decomposition time, nutrient imbalance, and possible Allelopathic effects on plant growth. By addressing these issues, optimized composting techniques can improve the efficiency of Sal leaf decomposition, promoting sustainable waste management and organic farming practices. The findings contribute to developing an eco-friendly approach to converting Sal leaves into a valuable bio-fertilizer, supporting agricultural sustainability and environmental conservation.

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Keywords: - Sal leaves, decomposition, nutrient cycle, soil fertility, bio-fertilizer.

INTRODUCTION

Leaf litter decomposition is a fundamental ecological process that contributes to nutrient cycling and soil fertility. Understanding the decomposition rates of different types of leaf litter is essential for managing ecosystems and enhancing soil health. This study focuses on the comparative decomposition rates of Sal (Shorea robusta) leaves and other common leaf litters. Sal is a predominant tree species in tropical and subtropical regions, known for its economic and ecological significance.

TABLE-1: TAXONOMICAL CLASSIFICATION OF SHOREA ROBUSTA

TAXONOMICAL CLASSIFICATION		
1	Kingdom	Plantae
2	Sub Kingdom	Viridiplantae
3	Division	Tracheophyta
4	Class	Magnoliopsida
5	Order	Malvales
6	Family	Dipterocarpacae
7	Genus	Shorea
8	Species	Shorea Robusta

Note: - Table1 is adapted from [1].

The leaves of Sal trees, due to their tough and leathery texture, are often considered resistant to decomposition. In contrast, other common leaf litters, such as those from deciduous and evergreen trees, vary significantly in their decomposition rates depending on their chemical composition and environmental conditions.

Sal (Shorea robusta) is the one of major forestry species of the Chhattisgarh forests and other forest laden states of India. This tree has numerous religious, traditional, ayurvedic medicinal, environmental as well as commercial benefits and uses. Considering the innumerous importance of Sal tree in Chhattisgarh, the Shorea Robusta had been declared as the State tree of Chhattisgarh. Shorea Robusta is the vernacular species of the Indian Sub-continental ranging from following states i.e Assam, West Bengal, Odisha, Jharkhand, mountain ranges like Shivalik hills to the Vindhya & Satpura range of Central India [2].

The only Biosphere Reserve (BR) located in Chhattisgarh dominated by Sal (Shorea Robusta) trees is the 14th National Biosphere Reserve of India established on 30th March 2005 that is Achanakmar-Amarkantak Biosphere Reserve (AABR)[3]. It lies between 220°15’ to 200° 58’ North latitude and 810° 25’ to 820 °05’ East longitude. Its total geographical area is 3,83,551 km^2 [3]. This forest genetic resource of AABR is a projected as the biodiversity hub of the central India. The AABR occupied mostly Sal Forest, mixed forest, degraded forest and agro-forestry ecosystems[4].

India's National Forest Policy aims for at least 33% of the country's geographical area to be forested, but currently, only around 24% is covered, according to the Forest Survey of India. To reach the target, more trees

plantation is needed in unoccupied areas. Native to the Indian subcontinent, Shorea Robusta (Sal) forests stretch from the sub-Himalayan region to Assam, with a dense canopy that shapes the diversity of understory plants. Common species found in Sal forests include Mallotus Philip Pensis, Moghaniachappar, and Terminalia tomentosa, among others [5].

As Sal tree is deciduous it sheds its leaves during autumn and covered the whole area below the tree thus protecting the sunlight to reach the surface which makes the surroundings infertile and results in barren land. Preparing a decomposer for degradation of Sal leaves can prove beneficial in terms of making the soil more fertile and utilizing the vast Sal Forest area into agricultural field or for planting other forest crops. This paper mainly consists of ways to decompose the Sal leaves and solve the problem of infertility of Sal Forest area and utilize the decomposed Sal leaves into valuable compost.

For this purpose, the paper consists of discussions about comparative decomposition rate of different leaf litters along with Sal leaves, role of microbial community in the decomposition of Sal leaves, Environmental influences in the decomposition of Sal litter, nutrient release dynamics of Sal leaves, implications of forest ecosystem, Carbon Sequestration in the decomposition process, management practices in the conversion of Sal leaves into compost and limitations and further research. This work discusses the comparative decomposition rate of different leaf litter along with Sal leaves, and the role of microbial community in the decomposition of Sal.

COMPARATIVE DECOMPOSITION RATES

Leaf-litter decomposition in terrestrial ecosystems plays a crucial role in nutrient recycling within the soil. Nutrient dynamics refers to the process by which nutrients cycle through an ecosystem. A study was carried out in tropical lowland (about 450 m altitude) of Makawanpur district, central Nepal to examine the decomposition rates and nutrient mineralization patterns of leaf litter from five tropical tree species—Shorea Robusta, Ficus Hookeri, Mallotus Philippensis, Artocarpus Lakoocha, and Dillenia Pentagyna species over one year using the litter-bag method. Results showed that M. Philippensis had the highest decomposition rate and weight loss (73.49% weight loss; k = 0.33), while S. robusta had the lowest (54.01% weight loss; k = -0.18). Generally, the remaining weight of the litter negatively correlated strongly with nitrogen (N) and phosphorus (P) concentrations and weakly with potassium (K). However, there was a strong positive correlation between the remaining weight of the litter and the carbon to nitrogen/carbon ratio, indicating it as a good predictor of mass loss and nutrient mineralization [6].

A study in Bangladesh's Madhupur Sal Forest (MSF), a vital area for both national economy and environment, investigated the role of litter formation and decomposition in maintaining nutrient dynamics and a balanced forest ecosystem. This pioneering research focused on the nutrient dynamics associated with leaf litter production and decomposition. The results showed that Shorea robusta, the dominant tree species, produced the most leaf litter followed by Dipterocarpus Indicus, Terminalia Bellirica, Tectona Grandis, and Grewia Microcosm. However, the decomposition rate of these species was found to be in the reverse order [7].

Bangladesh's Madhupur Sal Forest is a vital asset, providing significant natural resources and playing a crucial role in the country's economy and environment. Research revealed that Shorea robusta, the dominant tree species, produced the most leaf litter, followed by Dipterocarpus indicus, Terminalia bellirica, Tectona grandis, and Grewia microcos. Interestingly, the decomposition rate of these species was in the opposite order. Nutrient analysis showed that leaf litter primarily released Calcium and Potassium, along with essential micronutrients like Manganese, Iron, Cobalt, and Zinc [8].

ROLE OF MICROBIAL COMMUNITIES

The decomposition of Shorea robusta branch wood was studied in a subtropical Sal forest. Researchers measured termite population, respiration, and density at the site. After two years, the average dry weight of the branch wood had decreased by 89%. During winter and rainy seasons, the soil showed a lower carbon-to-nitrogen (C/N) ratio, indicating positive microbial activity. In contrast, the higher C/N ratio in the summer suggested more significant faunal activity, particularly from termites. The rainy season showed a faster decay rate due to the increased availability of organic matter and nitrogen in the soil, which supported microbial colonization and decomposition [9].

Collembola (Cyphoderusjavanus Borner) is a predominant group of detritivores micro-arthropod fauna in soil, and density and diversity of this detritivores depend on the quality and quantity of decomposing plant litter which act as a source of nutrition. The macronutrient composition was comparable across different types of litter, but the levels of non-nutrients such as polyphenols, tannins, and lignin were significantly higher in the litter from Acacia auriculiformis and Shorea robusta trees compared to that from Cassia siamea and Dalbergia sissoo trees. This experiment revealed that Collembola consistently preferred to inhabit litter from Cassia and Dalbergia trees, showing a significantly higher presence compared to Acacia and Shorea trees, which had noticeably fewer Collembola. The quality of leaf litter, which affects the growth of decomposer organisms, varies in its chemical makeup. The study discovered that Acacia litter initially contained high levels of polyphenols and ash, while Shorea robusta litter had high levels of tannins and lignin. Interestingly, Collembola (C. javanus) fed on Cassia and Dalbergia litter had higher levels of carbohydrates and proteins in their bodies, whereas those fed on Acacia and Shorea robusta litter had higher levels of lipids [10].

Another study focuses on the isolation and identification of fungi associated with litter decomposition in the Sal (Shorea Robusta) forests of central India. Seasonal successional changes in litter mycoflora were analyzed within four main seasons. The decomposition of litter was studied across four periods: March-May, June-August, September-November, and December-February. Certain fungi like Aspergillus flavus and Rhizopus stolonifera were present throughout the year, while others like Aspergillus fumigatus and Curvularia indica appeared in three seasons. Some fungi, including ecto-mycorrhizal species, were only found during the rainy season (June-August). The rainy season also saw an increase in litter decomposition. Initially, imperfect fungi like Alternaria and Cladosporium colonized fresh litter, while basidiomycetes, including ecto-mycorrhizal fungi, emerged in August and September, facilitating further decomposition. Finally, dematiaceous fungi appeared in later stages of decomposition [11].

ENVIRONMENTAL INFLUENCES

In one of the studies conducted at monthly interval at five different sites by using litter bag technique and observed annually in dry tropical deciduous forest of Vindhyan highland, India. It was found that, due to strong environmental control drastically influences the litter decay rates. Litter decomposition rate of eight dry tropical woody species of trees are observed, viz. Shorea robusta, Buchanania lanzan, Diospyros melanoxylon, Lagerstroemia parviflora, Lannea coromandelica, Terminalia tomentosa, Holarrhena antidysenterica and Lantana camara. The percentage of weight loss varied significantly among the trees and over time, with the lowest loss of 15.38% observed in L. camara at the Kotwa site in January, and the highest loss of 30.72% seen in T. tomentosa at the Hathi Nala site in August. On average, the greatest weight loss across all species and sites occurred in August, with a mean loss of 46.2%. This study found that S. robusta had distinctive thick leaves with noticeable midribs and veins, and notably lower levels of essential nutrients like Nitrogen and Phosphorous compared to the other species examined [12].

NUTRIENT RELEASE DYNAMICS

A study on deciduous trees (Dalbergia sissoo, Azadirachta indica, Pongamia pinnata, and Shorea robusta) planted on a mine spoil habitat found varying rates of litter fall, leaf decomposition, and nutrient release. Litter fall ranged from 1220 kg/ha/year (S. robusta) to 3620 kg/ha/year (A. indica), with fast-growing species (A. indica and D. sissoo) producing more litter than slow-growing ones (P. pinnata and S. robusta). The amount of nitrogen returned to the soil through litter fall varied from 8.6 kgs/ha/year (S. robusta) to 36.5 kgs/ha/year (D. sissoo). Leaf litter decomposition rates also differed, with A. indica (73%) and D. sissoo (69%) showing faster decomposition than P. pinnata (59%) and S. robusta (47%) [17].

A controlled leaf litter decomposition study was conducted in Rampur, Chitwan, Nepal, with a split-plot design experiment. The study examined the effects of C/N ratio, moisture, and tree species (Shorea robusta, Quercus semicarpifolia, and Pinus wallichiana) on decomposition. The results showed that these factors significantly impacted decomposition ($p<0.05$), with optimal decomposition occurring at a C/N ratio of 20:1 and 75% moisture content. This led to the release of minerals, including nitrogen, with varying amounts from each species. The study highlights the importance of moisture content in leaf litter decomposition and suggests that temperature can be managed using plastic houses or covers in cooler areas or during winter [18].

A study at Ramna Reserve Forest in West Bengal, India, examined how litter decomposition affects nutrient return to the soil. The results showed that Shorea robusta (Sal) had higher nutrient use efficiency and accumulation than Tectona grandis (Teak). As leaves aged, phosphorus, nitrogen, and potassium were reabsorbed in that order. The amount of nitrogen, phosphorus, and potassium added to the soil through litter fall differed significantly between the two species, with Shorea robusta returning more potassium and phosphorus, and Tectona grandis returning more nitrogen, ultimately benefiting soil fertility[19].

In Bangladesh's Madhupur Sal forest, researchers studied the nutrient content of Sal leaves litter by measuring leaf litter production and standing crop. They also conducted a laboratory experiment to observe mass loss and nutrient release through leaching over 192 hours. The results showed that Sal leaves litter contains significant amounts of N, K, and P, with mean leaf litter production and standing crop estimated at 12.94 g/m^2/day and 89.20 g/m^2, respectively. Leaching caused a 10% mass loss after 48 hours, with marginal reductions in N and P concentrations after 24 hours and a significant reduction in K concentration after 12 hours. The study found that leaching can extract approximately 25% of N, 45% of P, and 92% of K from the initial content [20].

IMPLICATIONS FOR FOREST ECOSYSTEMS

A study was conducted in various forest regions of Chhattisgarh to investigate the ability of native tree species to absorb high levels of toxic chemicals and heavy metals. The research aimed to explore the species-area relationship, focusing on red-wood tree species, which not only indicate iron and aluminum reserves but also play a crucial role in mitigating the release of heavy metals, fluorides, and nitrates from soil and groundwater. The study revealed that large biomass tree species, such as Shorea robusta (Sal), Pterocarpus marsupium, and Terminalia spp., absorb significant amounts of water, produce more energy, and accumulate higher levels of toxic substances, resulting in their distinctive reddish coloration. This adaptation enables them to thrive in metal-rich environments [21].

In one of the studies in eastern Nepal was conducted to understand the effect of variation in altitude in the soil characteristics in Tarai (low land) Sal Forest (TSF) and Hill (high land) Sal Forest (HSF). Soil samples are collected from both the forest which has sandy and loamy soil. Moisture content, bulk density and water holding capacity are higher in TSF than HSF. While, pH, soil organic carbon and total nitrogen are higher in HSF. Total Phosphorous is almost the same in both the forest types [22].

CARBON SEQUESTRATION

Biochar Production: Sal leaves can be converted into biochar through pyrolysis (heating in the absence of oxygen). Biochar can be used as a soil amendment, improving soil fertility and water retention while sequestering carbon.

A dynamic growth model (CO_2FIX) was used to estimate how much carbon can be stored by different forests in India, including Sal (Shorea Robusta), Eucalyptus, Poplar, and Teak (Tectona Grandis). The CO_2FIX model is a simulation tool used to estimate carbon storage and exchange in forests, including biomass, soil, and wood products.

It uses a simple accounting approach to convert biomass growth into carbon sequestration and storage, with annual time-steps. The model requires input data on stem volume growth and allocation patterns to other tree parts (leaves, branches, roots). Results from the model indicate that carbon storage in these forests ranges from 101 to 156 megagrams carbon sequestration per hectare, with Sal (Shorea Robusta) forests having the highest carbon storage in living biomass (82 megagrams per hectare). Fast-growing Poplar tree and Eucalyptus plantations have the highest annual carbon sequestration rates at 8 Mg Cha^{-1} per year and 6 Mg Cha^{-1} per year, respectively. Teak forests sequester 2 Mg Cha^{-1} per year annually, while slow-growing Sal forests sequester 1 Mg Cha^{-1} per year. Due to their fast growth and ability to thrive in various environments, short rotation plantations not only store carbon quickly but also produce biomass for energy, helping reduce greenhouse gas emissions [14].

The model was also used to study the effects of changing the rotation length and thinning practices on carbon stocks in Sal and Teak forests of India. It was found that extending the rotation length from 120 to 150 years increased the forest ecosystem's carbon stock of trees and soil by 12%. The net primary productivity was highest (3.7 Mg ha^{-1} per year) with a 60-year rotation but decreased with longer rotations (1.7 Mg ha^{-1} per year at 150 years). To achieve maximum carbon storage and produce more valuable saw logs, longer rotation lengths are beneficial. However, while "no thinning" results in the largest biomass, it means no wood from thinning operations would be available for use, which has economic implications [23].

A relatable study at the Madhupur Sal Forest (MSF) in Bangladesh aimed to measure the amount of carbon stored and the potential for carbon capture by tree species including Shorea Robusta. Researchers focused on two areas, Dokhola Sadar and Chandpur, within the Dokhola range of the MSF. They randomly selected 20 plots (10 from each area) for sampling. In each plot, they recorded the number, names, heights, and trunk diameters of all the trees. They then used these measurements to calculate the carbon stored in the tree biomass of selected tree species. They found 10 different tree species and 154 individual trees in total. Sal trees (Shorea robusta) were the most common, with 137 individuals, and they had the highest potential for carbon capture, storing 239.15 kgs (about 527.23 lb) of carbon per tree. The study estimated that the trees in the Dokhola range store 1.39 million tons of carbon, which equals 5.10 million tons of CO_2. Overall, the MSF stores 3.56 million tons of carbon, equivalent to 13.07 million tons of CO_2. The findings show that MSF significantly helps mitigate global climate change. However, to further increase the forest's carbon capture potential, it is important to manage and maintain the Sal Forest and carry out reforestation and afforestation projects in deforested areas [24].

MANAGEMENT PRACTICES TO CONVERT SAL LEAVES INTO BIO-FERTILIZER

Decomposition of Sal leaves (Shore robusta) though a long process involves several management practices to ensure effective and environmentally friendly processing. Here are some common practices:

1. Collection and Sorting: Collect fallen Sal leaves from forests or plantation areas. Sorting helps in removing any non-leaf materials.
2. Shredding: Shredding the leaves into smaller pieces increases the surface area, promoting faster decomposition.
3. Composting:
    i. Windrow Composting: Leaves are piled in long rows and periodically turned to aerate the pile and facilitate decomposition.
    ii. Pit Composting: Leaves are placed in pits along with layers of soil, cow dung, and other organic materials to enhance decomposition.
    iii. Vermicomposting: Involves the use of earthworms (such as Eiseniafetida) to break down the leaves into high-quality compost.
    iv. Bokashi Composting: this is a fermentation process that involves adding a Bokashi mix (a combination of beneficial microorganism) to the Sal leaves. The leaves are then kept in an airtight container to ferment, the process is relatively fast and produces a nutrient rich compost.
4. Moisture Management: Maintaining optimal moisture levels (around 50-60%) is crucial for microbial activity. This might involve periodic watering of the compost piles.
5. Aeration: Regular turning of compost piles ensures proper aeration, which is necessary for aerobic decomposition.
6. Addition of Microbial Inoculants: Adding microbial inoculants or compost activators can speed up the decomposition process.
7. Monitoring and Control: Regular monitoring of temperature, moisture, and pH levels helps in managing the composting process effectively. Ideal temperatures for composting range between 55-65°C.
8. Curing: After the active composting phase, the material is left to cure for several weeks to months, allowing it to stabilize and mature into high-quality compost. These practices help in converting Sal leaves into valuable compost, which can be used as a soil amendment, improving soil health and fertility.

LIMITATIONS AND FURTHER RESEARCH

Converting Shorea Robusta (Sal) leaves into bio-fertilizer has several limitations, including:

1. High Lignin Content: Shorea Robusta leaves contain high levels of lignin, which makes them resistant to decomposition. This slows down the composting process and requires longer time to break down into usable bio-fertilizer.
2. Low Nitrogen Content: These leaves typically have low nitrogen content, which is essential for microbial activity during composting. This can lead to an imbalance in the carbon to nitrogen (C) ratio, further slowing down the decomposition process. Applying compost made from municipal solid waste is expected to enhance soil fertility by increasing nutrient availability, particularly nitrogen. As a result, the compost treatment was found to boost the total nitrogen content in the top 15 cm of the soil and that's why compost is also known as Black Gold [15].
3. Tannins and Polyphenols: The leaves contain tannins and other polyphenolic compounds that can inhibit microbial activity. This can reduce the efficiency of composting and affect the quality of the final bio-fertilizer.
4. Need for Pre-treatment: To overcome the high lignin content and other inhibitors, the leaves often require pre-treatment methods such as shredding, soaking, or chemical treatments, which add to the complexity and cost of the process.

5. Environmental Factors: Successful composting of Shorea Robusta leaves depends on various environmental factors such as temperature, moisture, and aeration. Managing these factors can be challenging, especially in large-scale operations.
6. Potential Allelopathic Effects: The presence of certain chemicals in Shorea Robusta leaves may have allelopathic effects, inhibiting the growth of certain plants if not properly composted.
7. Labor and Time Intensive: The process of converting these leaves into bio-fertilizer is labor and time-intensive, requiring careful monitoring and management to ensure optimal conditions for decomposition.

Addressing these limitations involves optimizing composting techniques, possibly integrating these leaves with other organic materials to balance nutrient content and improve decomposition rates. As there are many different approaches of making compost out of waste for example the method of utilizing fly ash for different purposes in Agriculture sector in supporting the bio-fertilizer industry is highly commendable and can solve the rising menace of fly ash disposal in an economical as well as ecological way [16]. In the same way utilization of Sal leaves as compost can prove beneficial for ecosystem of Sal tree forests all over the world.

CONCLUSION

The comparative study on the decomposition rates and environmental impacts of Shorea robusta leaves versus common leaf litters has provided valuable insights into their potential for composting and the challenges associated with their conversion into compost. Shorea robusta leaves exhibit slower decomposition rates compared to other common leaf litters, primarily due to their higher lignin content and tougher structure. This characteristic poses a significant challenge for efficient composting and necessitates the development of specialized composting techniques to enhance the breakdown process. Despite these challenges, the environmental benefits of composting Shorea robusta leaves are notable. The process of composting reduces the volume of organic waste, mitigates the release of greenhouse gases, and produces nutrient-rich compost that can improve soil fertility and structure. However, the slower decomposition rate of Shorea robusta leaves necessitates longer composting periods and more intensive management practices. To overcome these challenges, several strategies can be employed. Pre-treatment methods such as shredding, soaking, and the addition of microbial inoculants can accelerate the decomposition process. Furthermore, optimizing composting conditions, such as maintaining proper moisture levels, aeration, and temperature control, is crucial for achieving efficient composting of Shorea robusta leaves. In conclusion, while Shorea robusta leaves present certain challenges for composting due to their slow decomposition rates, the environmental benefits and potential for producing high-quality compost make it a worthwhile endeavor. Further research and development of innovative composting techniques are necessary to enhance the efficiency of composting Shorea robusta leaves and maximize their environmental benefits. This study underscores the importance of adapting composting practices to accommodate different types of leaf litter, ultimately contributing to more sustainable waste management and soil health improvement.

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Natural Synthesis of Superhydrophobic Stainless Steel Mesh for Oil-Water separation

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ABSTRACT

The objective of this review is to highlight recent advances in the application of SiO2-based polymer nanocomposite surfaces for oily wastewater treatment. There is a need to develop methods and materials that show excellent ability to separate the oil and organic contaminants from water. The superhydrophobic coated sponges and metal meshes are used to separate oil from the oil-water mixture. The various surface-modified organic metal oxide nanoparticles are used to develop superhydrophobic surfaces on porous substrates. Metal-oxide-based nanomaterials, including SiO2, TiO2, ZnO, etc. have gained tremendous attention due to their unique mechanical and chemical properties such as micro-hierarchical, hydrophobic, stability, and wettability. Among them, SiO2 nanoparticles are mostly useful for the preparation of superhydrophobic surfaces. The current challenges for the successful development of SiO2-based nanocomposite surfaces and opportunities for future research are also discussed. This review focused on silica-modified porous sponge and metal meshes for scalable oil-water separation applications.

Keywords: Metal Mesh, Oil-Water Separation, Porous Sponge, and Superhydrophobic.

INTRODUCTION

They are high surface energy substrates that attract water and allow wetting of the surface. They typically have a droplet contact angle measurement of less than 90 degrees. Lots of surfaces tend to be more water-friendly including, glass, steel, or stainless steel, and many coatings and paints [1-3]. A hydrophobic surface is a surface that can repel water. The hydrophobic surfaces can be defined as materials that tend to repel with water. Generally, the hydrophobicity of a surface can be measured by the contact angle between the droplets of water with the surface itself. The water droplets on the hydrophobic surface will flow very easily and retain their

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spherical shape with a contact angle of more than 90 degrees. Superhydrophilicity refers to the phenomenon of excess hydrophilicity, or water attraction; in superhydrophilic materials, the contact angle of water is equal to zero degrees. Superhydrophilic material has various advantages [4-5]. For example, it can defog glass, and it can also enable oil spots to be swept away easily with water. Such materials are already commercialized as door mirrors for cars, coatings for buildings, self-cleaning glass, etc. A superhydrophobic surface could efficiently reduce the contact time of bouncing drops because its contact angle is greater than 150° while the sliding angle is lower than 5° [6-7]. However, the contact time of a bouncing water droplet of a certain volume on a superhydrophobic coating is constant.

Wettability of a material refers to its hydrophilic or hydrophobic nature. The wettability of a material has a direct relationship with oxygen incorporation, which in turn affect cell adhesion. Hydrophobic surfaces show more platelet adhesion than hydrophilic surfaces. Platelets strongly attach to hydrophobic surfaces, possess spherical conformation, and therefore experience more shear stress. Even though hydrophilic substances attract platelets, those platelets get detached in a few minutes with the provision of arterial flow conditions [8-10].

A contact angle (also referred to as a wetting angle) is formed when a drop of liquid is placed on a material surface. The surface tension of the liquid and the attraction of the liquid to the surface causes the drop to form a dome shape. If the drop is small and the surface tension of the liquid is high, it will form a perfect hemisphere [11]. The point where the perimeter of a liquid drop, the liquid-solid interface, and the solid all meet is called the three-phase contact point. The contact angle is defined as the angle between a tangent to the liquid surface and the solid surface at this point. Theta (Θ) is the contact angle in the illustration above. If the drop of liquid spreads across a surface, the contact angle becomes smaller. If the drop of liquid beads up on the surface (as you might see with a drop of water on a water-resistant article of clothing or a waxed car), the perimeter of the drop retracts, and the contact angle becomes larger [12].

EXPERIMENTAL WORK:

Material:

Stainless steel mesh, SiO_2 beads and candles were purchased from a local supermarket. Polydimethyl siloxane (PDMS), Polystyrene (PS), H_2SO_4, NaOH, and HCl were purchased from Shri Samarth commercialism Company, Pvt. Ltd., India. Organic solvents including toluene, hexane and chloroform were purchased from Shri Samarth commercialism Company, Pvt. Ltd., India. All the chemicals used for the experiments were standard commercial grade, which were used as received without any further purification.

Method:

1. **Preparation of hydrophobic SiO_2 nanoparticles:**

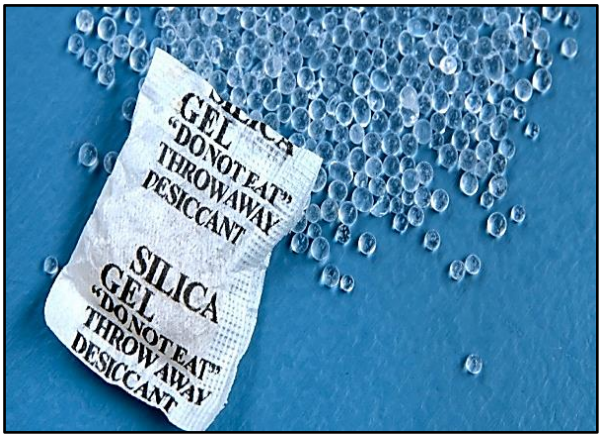


Fig. 1. Photograph of Silica Beads

1.1 Synthesis of sodium silicate from silica beads:

- Dissolve 16 g of NaOH of 20 ml of distilled water with continuous stirring.
- After the dissociation of NaOH, start adding 12 g silica gel (SiO_2). [SiO_2 must be dried]
- The temperature should be about 80°C. Use a hot plate to support the reaction. The temperature rises to 105°C.
- Keep it boiling until all SiO_2 dissolved.
- Water glass is formed. i.e., sodium silicate

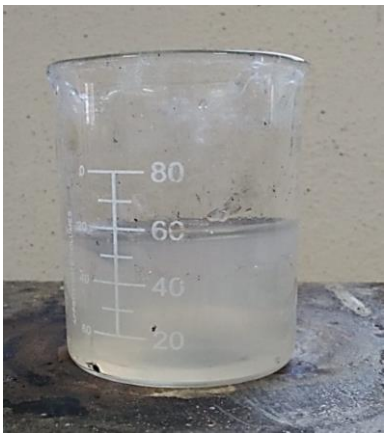


Fig. 2. Formation of sodium silicate

1.2 Synthesis of silica nanoparticles from sodium silicate:

- Take 12 g of sodium silicate.
- Dissolve this in 24 ml of water [1:2 ratio] using a magnetic stirrer.
- Prepare 1 M HCl solution.
- Use 1 M HCl solution to neutralize sodium silicate drop by drop.
- It takes up to one and a half hours to fully neutralize the solution.
- Test with pH paper.
- Silica gel was produced.
- Get obtained was aged for 24 hours at room temperature.
- After that separate the silica gel via filtration.
- Absorb the moisture using filter paper.
- Dry this gel using a hot plate.
- After the drying process, use a mortar pestle to crush the large particles.
- Nanoparticles of SiO_2 is formed.

Fig. 3. Formation of silica nanoparticles

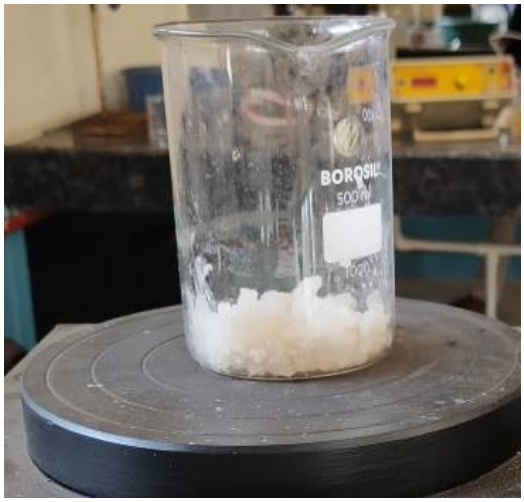


Fig. 4. Drying the product on a hot plate

Fig. 5. Prepared silica nanoparticles

2. Preparation of Polydimethyl siloxane, SiO_2 and Chloroform solution:

We took 20 ml of solution is sufficient for dipping the mesh. So, we have taken 0.2 ml of PDMS and curing agent in 20 ml Chloroform. After adding both, solution stirred for 30 min. without heating at 150-180 rpm. Then, solution is prepared after 30 min. After that add 800 mg of SiO_2 in it and stirring for 1 h without heating at 200-220 rpm. Then, solution is prepared after 1 h.

3. Preparation of Polystyrene and Chloroform solution:

We took concentration as 10 mg/ml 20 ml of solution is sufficient for dipping the mesh. So, we have taken 200 mg of Polystyrene and 20 ml of Chloroform. After adding both, solution stirred for 30 min. without heating at 160-180 rpm. Then, solution is prepared after 30 min. After that add 100 mg of Candle soot in it and stirring for 1 h without heating at 210-220 rpm. Then, solution is prepared after 1 h.

4. Preparation of superhydrophobic/superoleophobic mesh:

The superhydrophobic mesh was prepared by a facile dip coating method. The meshes of 3×2 cm^3 were dipped in deionized water, acetone, and ethanol, respectively by ultrasonic wave washing at room temperature. Subsequently, the pre-cleaned sponge was immersed in a dispersion of SiO_2 and CS in Chloroform and after magnetic stirring for 1 h was dried in the oven at 60°C for 2 h. The relationship between the mass ratio of

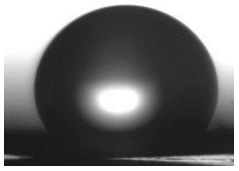
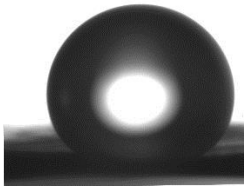
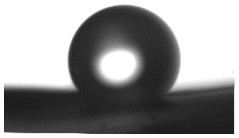
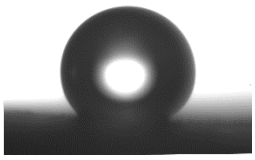
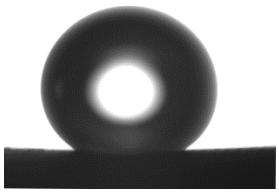
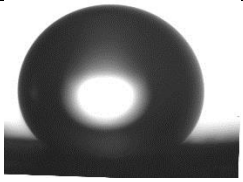
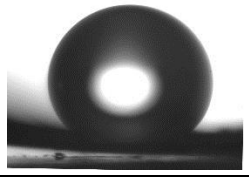
SiO_2/CS NPs and the water CAs on the as-prepared mesh was measured. We can gain the different SiO_2/CS NPs loading by changing the dispersion amount.

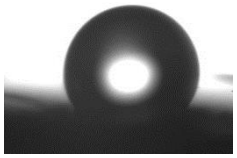
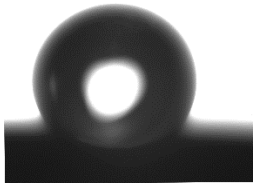
RESULT AND DISCUSSION:

1. Water Contact Angle:

The relationship between the candle soot deposition time, dipping time, and the water CAs on the as-prepared mesh were measured which is shown in the table below:

Table 1: The relationship between candle soot deposition time, dipping time, and the CAs of water on the superhydrophobic mesh.

CS Deposition Time (min.)	Dipping Time (min.)	Water contact angle (°)	Water contact angle image
5	5	151	
	10	153	
	15	154.5	
10	5	162	
	10	**165.5**	
	15	150.5	
15	5	148.2	

	10	146.6	
	15	139.5	

2. SEM:

The surface morphology of the SS mesh and the as-prepared sponges is investigated by SEM at different magnifications, as shown in Fig. It is observed that the SS mesh has a three-dimensional hierarchical porous structure with pore sizes ranging from 100 to 400 μm and the high magnification of the image in the inset of exhibits a smooth surface of sponge skeletons, shows the SEM images of the CS-SiO_2-SS mesh at low and high magnifications [13]. Numerous microscale aggregates are covered on the skeletons of the sponge, indicating that CS and SiO_2 NPs have been coated on the mesh successfully. The higher magnification reveals that lots of CS and SiO_2 NPs aggregate and form micro-nano-rough structures on the skeletons of the mesh. The 3D micro-porous structure of the mesh and the nanoscale CS and SiO_2 NPs form a binary rough structure, which is extremely similar to the structure of lotus leaves.

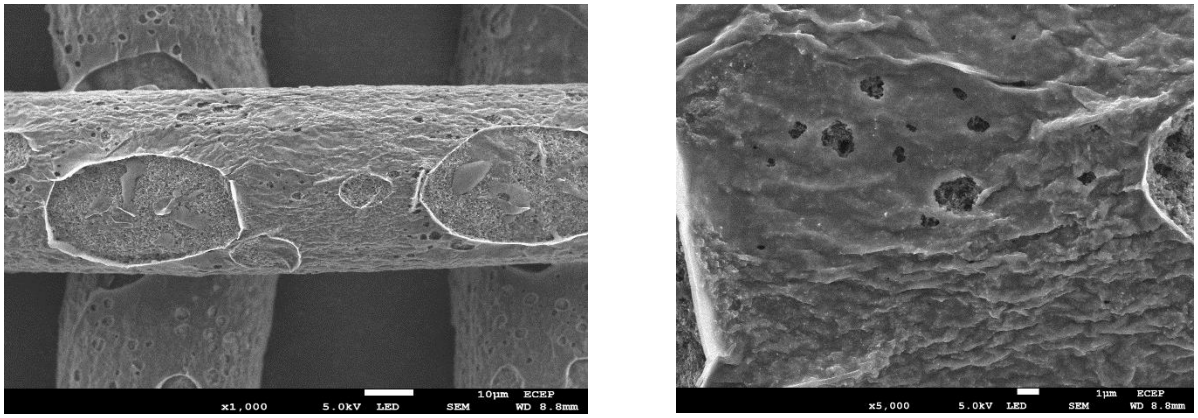


Fig. 6. SEM images of the superhydrophobic mesh surface morphologies at low and high magnifications, respectively.

CONCLUSION:

In conclusion, we successfully prepared stable superhydrophobic mesh by a facile solution dip coating method for clean-up of oil contamination. The superhydrophobic mesh possesses stable superhydrophobicity and excellent ability of selective absorption to oil even at various harsh conditions, including acid, alkali, and salt aqueous solutions at mechanical agitation conditions, hot water, and ice/water mixtures. Finally, the superhydrophobic mesh combination with a vacuum system could continuously absorb and remove oil from the water surface. The superhydrophobic mesh possessed remarkable performance, including a facile fabrication method, high separation efficiency, good recyclability, anti-corrosion, and excellent superhydrophobicity for hot water, which demonstrated that superhydrophobic mesh as an absorptive material has significant value in water remediation for practical applications.

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Recent Developments in Synthesis of Nanomaterials and Composites of Vanadium and Cobalt Sulfides for Supercapacitors - A Review

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ABSTRACT

The growing demand for advanced energy storage solutions has spurred significant research into supercapacitors, known for their exceptional power density, rapid charge-discharge capabilities, and long-term stability. Among the promising materials for supercapacitors, vanadium disulfides (VS_2), cobalt disulfides (CoS_2), and their composites have attracted considerable attention due to their unique electrochemical properties and tunable structural characteristics. This review focuses on recent advancements in the synthesis strategies of nanomaterials and composites based on vanadium and cobalt disulfides. Various methodologies, including hydrothermal, solvothermal, and chemical vapor deposition techniques, are critically analysed for their effectiveness in controlling morphology, particle size, and compositional uniformity. The synergistic effects of combining these disulfides with other materials to enhance conductivity, stability, and energy storage performance are thoroughly discussed. Furthermore, challenges such as material degradation, scalability, and the optimization of composite properties are explored. This review provides a comprehensive perspective on the synthesis and application of vanadium and cobalt disulfides and their composites, contributing to the development of next-generation high-performance supercapacitors.

Keywords: Supercapacitors, Nanomaterials, Vanadium disulfides (VS_2), Cobalt disulfides (CoS_2)

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INTRODUCTION

In the rapidly evolving tech era, optimizing energy storage is crucial. Presently, batteries, supercapacitors, and fuel cells are the most reliable options. Addressing the growing energy needs of advancing technology remains a significant challenge [1]. The global energy crisis can be addressed by supercapacitors, which offer rapid charging and avoid toxic, scarce materials like lead and lithium. Compared to batteries, electrochemical supercapacitors provide greater power density, longer lifespan, and enhanced safety. Consequently, their advancement has drawn significant interest from researchers and industries worldwide [2]. Supercapacitors, based on their energy storage mechanism, are categorized into three types: electric double-layer capacitors (EDLCs), pseudocapacitors, and hybrid supercapacitors, which combine both [3]. Despite extensive research on novel electrode materials, EDLCs face an inherent limit in specific energy due to their reliance on double-layer capacitance for energy storage [4, 5]. It is clear that supercapacitors using pure carbon or carbon-based organic materials have reached their performance limits [6]. Pseudocapacitance arises from rapid, reversible electron exchange at or near the electrode surface, leading to greater capacitance and energy density. However, pseudocapacitors typically have a shorter cycle life than EDLCs [5, 7]. A wide range of pseudocapacitive materials has been extensively investigated for their potential in energy storage applications. These materials include transition metal oxides (such as titanium dioxide, TiO_2), perovskite oxides, two-dimensional transition metal carbides, nitrides, and carbonitrides (MXenes), transition metal dichalcogenides, carbon-based materials, metal-organic frameworks (MOFs), transition metal sulfides, and electronically conducting polymers. Each of these materials exhibits unique electrochemical properties that contribute to improved energy storage capabilities. However, despite their advantages, many of these materials suffer from a key drawback—limited cycling stability, which ultimately leads to a decline in electrochemical performance over time. This instability restricts their widespread use in long-term applications [8]. To overcome these limitations, researchers have developed hybrid supercapacitors, which integrate two different types of electrode materials within the same device to optimize both energy storage and power output. In a typical hybrid supercapacitor, a pseudocapacitive electrode functions as the primary energy storage component, providing high energy density similar to a battery, while an electric double-layer capacitor (EDLC) electrode acts as the power source, delivering high power capabilities and rapid charge/discharge rates. This combination allows hybrid supercapacitors to achieve a balance between high energy density and fast power delivery, making them a promising alternative for advanced energy storage applications. Based on the type of electrode materials used, hybrid supercapacitors are further categorized into symmetric and asymmetric configurations. Symmetric hybrid capacitors use identical electrode materials on both sides, while asymmetric hybrid capacitors combine different materials to optimize performance. Among these, asymmetric hybrid supercapacitors incorporating conducting polymer electrodes have gained significant commercial success due to their superior energy storage capabilities and cost-effectiveness. These advancements continue to drive research and industrial interest in developing next-generation energy storage solutions [9]. Hybrid supercapacitors exhibit superior capacitance and higher energy density compared to EDLCs. However, their performance is hindered by the limited cycling stability of faradaic electrodes, which degrades over repeated charge-discharge cycles. To address this issue, extensive research has explored various combinations of positive and negative electrodes in both aqueous and organic electrolytes, aiming to optimize their electrochemical performance. Achieving an ideal balance between high-power, high-energy density, and long cycle life in hybrid capacitors requires innovative electrode material systems. This involves the strategic design of electrode materials, considering their composition, morphology, and nanoscale structure, to enhance conductivity, stability, and electrochemical efficiency. Additionally, the selection of electrolytes plays a crucial role in determining device performance. Electrolytes with high ionic conductivity,

broad electrochemical stability, and the ability to sustain high operating voltages are essential for improving the overall efficiency and lifespan of hybrid supercapacitors. By integrating rational material design, optimized electrode pairing, and advanced electrolytes, researchers aim to develop next-generation hybrid supercapacitors capable of delivering both long-lasting durability and superior energy storage performance for advanced technological applications [9, 10]. In recent years, the use of 2D layered inorganic materials, specifically transition metal dichalcogenides (TMDs), has grown in supercapacitor technology. TMDs consist of a transition metal atom (M) and two chalcogen atoms (X)—such as sulfur (S), selenium (Se), or tellurium (Te)—arranged in an X–M–X structure, with the general chemical formula MX_2. Several TMDs have been extensively studied for their potential as supercapacitor electrodes, including molybdenum disulfide (MoS_2), molybdenum diselenide ($MoSe_2$), tungsten disulfide (WS_2), tungsten diselenide (WSe_2), tungsten ditelluride (WTe_2), tantalum disulfide (TaS_2), tantalum diselenide ($TaSe_2$), titanium disulfide (TiS_2), niobium disulfide (NbS_2), zirconium disulfide (ZrS_2), vanadium disulfide (VS_2), and vanadium diselenide (VSe_2), among others. While these materials exhibit great potential, their semiconducting nature makes them less than ideal for supercapacitor electrodes, as they tend to have limited electrical conductivity. To address this limitation, researchers have enhanced the conductivity of TMDs by blending them with carbon-based materials and conducting polymers, resulting in nanocomposites. These hybrid materials improve the overall electrochemical performance of supercapacitors by offering better conductivity and stability, making them more suitable for high-performance energy storage applications [11, 12]. Despite the progress made with TMD-based nanocomposites, several challenges remain in optimizing their performance for supercapacitor applications. One key issue is interfacial adhesion between the TMD materials and other components (such as carbon-based materials or conducting polymers), which can affect the stability and efficiency of the electrodes. Another challenge is the electronic mobility within the materials. Although nanocomposites improve conductivity to some extent, the overall electron transport can still be hindered due to the complex interactions between the different components. This limits the efficiency of charge storage and transfer, particularly at higher current densities, where rapid electron movement is crucial. Moreover, the use of binders in the electrode materials, which are essential for holding the materials together and ensuring structural integrity, can sometimes negatively affect the overall electrochemical performance. Binders, typically used to enhance mechanical strength, can introduce resistance and reduce conductivity, further complicating the system. Lastly, selecting the appropriate electrolyte is critical for the hybrid system's performance. The electrolyte must match the specific materials used in the electrodes, ensuring high ionic conductivity, stability, and the ability to operate at high voltages. The choice of electrolyte can influence the charge storage mechanism and cycle stability, and incompatible electrolytes may result in poor performance or degradation of the materials. Addressing these challenges through improved material design, better interfacial engineering, optimized binders, and careful electrolyte selection remains a key focus for researchers aiming to maximize the efficiency and longevity of hybrid supercapacitors [13].

To the best of our knowledge, no review has yet been conducted on the combined use of vanadium sulfide (VS_2) and cobalt sulfide (CoS_2) in supercapacitor applications. Therefore, we are undertaking a comprehensive review that focuses on both VS_2 and CoS_2 for their potential in supercapacitive applications. This review aims to provide an in-depth analysis of recent research related to the electrochemical properties of both materials, highlighting their performance, advantages, and challenges in the context of energy storage. By examining these two materials together, the review seeks to offer new insights into their combined potential and their role in advancing the development of high-performance supercapacitors.

CRYSTAL STRUCTURES AND FUNDAMENTAL ELECTROCHEMICAL PROPERTIES

2.1 Vanadium sulfides

Vanadium sulfides primarily include VS2 and VS4, as well as many phases such as V2S5, V2S3, VS, V3S and VS6. Of those sulfides, VS2 and VS4 are two typical ones that have drawn intense attention in the past few years. The VS2 crystal exhibits layered structures with an interlayer spacing of 5.76 Å and consists of a hexagonally packed metal V layer sandwiched between two layers of S atoms. The VS_4 crystal is a quasi-one-dimensional, chain-like compound consisting of V(IV) ions coordinated with S_2^{2-} dimers. These linear structural units are held together by weak van der Waals interactions, with an interchain distance of 5.83 Å [14]. The oxidation states of vanadium in VS_2 and VS_4 are identical, but the oxidation states of the sulfides differ. In VS_2, there is an S^{2-} monomer, whereas in VS_4, there is an S_2^{2-} dimer. Electrical conductivity is indeed a crucial parameter for determining electrochemical activity. In recent years, researchers have computed the density of states (DOS) for both VS_2 and VS_4. This analysis helps in understanding the electronic properties and potential applications of these materials in various electrochemical devices. The VS_2 layer exhibits metallicity with significant electronic states at the Fermi level, which is advantageous for enhancing electronic and electrochemical activities. It was found that potential dimerization through metal-metal bonding existed in VS_4 [15]. This characteristic contributes to the unique properties and potential applications of VS_4 in various electrochemical devices. This phenomenon was linked to a Peierls distortion. Researchers also noted variations in the V-V distances, measuring 2.8 and 3.2 Å. Using density functional theory (DFT) computations, they discovered that the band gap of diamagnetic VS_4 is approximately 1 eV [16]. The 1T VS_2 monolayer, where vanadium is in octahedral coordination, has also been studied as an anode material for Li-, Na-, Mg-, Ca-, and Al-ion storages through first principal simulations. This research highlights the potential of VS_2 in various ion storage applications, contributing to the development of advanced energy storage solutions [17]. The 1T VS_2 monolayer was found to be unsuitable for Mg or Al ion storage due to ultralow or positive absorption. However, the surface of the 1T VS_2 monolayer can strongly interact with single Li, Na, or Ca adatoms, efficiently accepting electron charge density. The open circuit voltage profiles were predicted to range from approximately 1.56 V to 0.46 V for Li-ion storage and from 1.5 V to 0.37 V for Na-ion storage. Similarly, through first-principles calculations, Chen et al. investigated VS_2 monolayers as electrode materials for Li-, K-, Mg-, and Al-ion batteries [18].

2.2 Cobalt sulfides

According to the phase diagram of CoS, cobalt sulfides can exist in various stoichiometric compositions, including Co_4S_3, Co_9S_8, CoS, Co_3S_4, Co_2S_3, and CoS_2. These compositions exhibit diverse structural chemistry and unique properties, making them suitable for a range of applications. Since the performance of advanced functional materials is closely linked to their accessible surface area, significant research efforts have been dedicated to the precise synthesis and morphological control of cobalt sulfide nanostructures [49].

FABRICATION METHODS

3.1 Vanadium sulfides

While pure phase vanadium sulfides exhibit considerable theoretical capacity, they may not provide desirable performance in energy storage applications due to volume expansion during the ion intercalation process. This expansion results in low capacity and poor rate performance. Additionally, when applied as catalysts in energy conversion, nanoscale vanadium sulfides offer more active sites compared to their bulk counterparts. However,

the catalytic activity of pure nanoscale vanadium sulfides for energy conversion does not meet the practical usage requirements.

To address these issues, several synthetic strategies have been developed:

Constructing heterogeneous structures: By combining vanadium sulfides with other oxides or sulfides, the electronic properties of vanadium sulfides can be adjusted, thereby enhancing their activity.

Hybridizing with carbon materials: To improve conductivity and mitigate volume expansion during the ion intercalation process, vanadium sulfides are hybridized with carbon materials. Graphene or carbon nanotubes (CNTs) are often used as substrates for vanadium sulfides. For example, VS_4/rGO hybrids were synthesized by introducing graphene oxides (GO) into the reaction system.

These strategies aim to optimize the performance of vanadium sulfides in energy storage and conversion applications, making them more suitable for practical use. The best synthetic strategy depends on the intrinsic characteristics of the target products. In the following sections, several strategies and examples will be reviewed in detail.

Hydrothermal/Solvothermal Methods

Hydrothermal and solvothermal synthesis methods, which are based on liquid-phase reactions, have proven to be highly effective techniques for the controlled fabrication of materials with uniform size, morphology, and crystallinity. The key distinction between these two methods lies in the choice of solvent: hydrothermal synthesis employs water as the reaction medium, while solvothermal synthesis utilizes an organic liquid as the solvent. The reaction conditions, including solvent type, temperature, duration, and pH, play a crucial role in determining the phase composition, crystal structure, and morphological characteristics of the final products.

Unlike conventional synthetic approaches, hydrothermal and solvothermal processes allow researchers to achieve reaction conditions that would otherwise be difficult or impossible under standard laboratory settings. These conditions enable precise tuning of particle size, morphology, and crystallinity, making these methods particularly suitable for the synthesis of nanostructured materials. Furthermore, hydrothermal and solvothermal methods offer significant advantages, such as ease of operation, cost-effectiveness, and low energy consumption, making them attractive for large-scale material fabrication [19].

A notable example of hydrothermal synthesis was reported by Xie et al. in 2001, where they successfully prepared $VS_2{\cdot}3NH_3$ (vanadium disulfide-ammonia complex) materials. The synthesized $VS_2{\cdot}3NH_3$ was then exfoliated to obtain ultrathin vanadium disulfide nanosheets (VS_2 NSs). The presence of ammonia molecules, which exhibit both physical activity and chemical reactivity, facilitated the intercalation into the layered VS_2 structure. As a result, $VS_2{\cdot}3NH_3$ flakes with a thickness of approximately 110 nm were obtained. Further exfoliation of these flakes through sonication led to the formation of ultrathin VS_2 nanosheets with a reduced thickness of approximately 2.5 nm [20].

By carefully adjusting the reaction parameters, such as temperature and solvent composition, researchers have successfully synthesized a variety of VS_2 nanostructures. For instance, the incorporation of ethylene glycol (EG) into the solvent system has been shown to enhance crystallinity, leading to the formation of highly crystalline VS_2 nanosheets. Conversely, the addition of cetyltrimethylammonium bromide (CTAB) as a growth modifier resulted in reduced crystallinity of the synthesized VS_2 nanosheets. Moreover, poly(vinyl pyrrolidone) (PVP)-assisted hydrothermal synthesis has been employed to fabricate layered VS_2 nanosheets with a stacked architecture. The versatility of the hydrothermal process is further demonstrated by its ability to facilitate the direct growth of VS_2 nanostructures onto various substrates by introducing them prior to the reaction. [21, 22]

In addition to the synthesis of pristine VS_2, the hydrothermal method has been extensively utilized for fabricating VS_2-based hybrid materials. Huang et al. successfully prepared vanadium oxyhydroxide (VOOH)-

coated VS_2 microflowers through a one-step hydrothermal reaction. By modulating the reaction temperature, the crystallinity of the VOOH coating could be precisely controlled. Notably, when the reaction temperature was increased to 180°C, the diffraction peaks corresponding to VOOH disappeared in the X-ray diffraction (XRD) pattern, indicating a significant change in phase composition. Furthermore, Yu et al. developed a two-step hydrothermal method to synthesize MoS_2-VS_2 heterostructures, wherein molybdenum disulfide (MoS_2) nanosheets were hybridized with 1T-phase VS_2 nanoflowers. This approach enabled the formation of heterostructures with enhanced electrochemical properties, making them promising candidates for applications in energy storage and catalysis. Beyond VS_2 synthesis, the hydrothermal technique has also been widely applied in the preparation of vanadium sulfide (VS_4)-based materials. Shin et al. successfully grew VS_4 nanostructures using this method, further demonstrating the versatility and adaptability of hydrothermal synthesis for tailoring the structural and compositional characteristics of transition metal sulfides. [23, 26]

Solvothermal synthesis has also been extensively utilized for the fabrication of VS_4-based nanostructures, offering precise control over their morphology and crystallinity. These methods leverage organic solvents to create reaction conditions that enable the growth of highly uniform vanadium sulfide nanostructures with desirable electrochemical properties. A notable example of solvothermal synthesis involves the growth of VS_4 nanoparticles (NPs) directly onto carbon nanofibers (CNFs). This process was achieved through a solvothermal reaction between sodium orthovanadate (Na_3VO_4) and thioacetamide (C_2H_5NS, TAA) in an ethylene glycol (EG) solution. The presence of carbon nanofibers, which contain abundant surface defects, played a crucial role in facilitating the nucleation and growth of VS_4 nanoparticles. These structural defects acted as active sites for the deposition of VS_4, thereby enhancing the interaction between the vanadium sulfide and the carbon matrix. The resulting VS_4@CNF composite exhibited improved electrical conductivity and structural stability, making it a promising candidate for energy storage applications.

In another study, Ma et al. successfully synthesized VS_4 nanospheres using a solvothermal method in an ethylene glycol-based solvent system. These VS_4 nanospheres served as versatile precursors for the fabrication of other vanadium sulfide-based materials. Specifically, the synthesized VS_4 nanospheres were encapsulated within polyacrylonitrile (PAN) fibers to form a composite material. This composite was subsequently subjected to an annealing process under an argon/hydrogen (Ar/H_2) atmosphere at a temperature of 600°C. During this thermal treatment, a controlled transformation occurred, leading to the formation of V_3S_4 microspheres encapsulated within nitrogen-doped carbon nanofibers (N-doped CNFs). The incorporation of nitrogen-doped carbon not only enhanced the electrical conductivity of the material but also provided structural stability, making it highly suitable for applications in energy storage and catalysis. [27]

The ability to tailor the structural and compositional characteristics of VS_4-based materials through solvothermal synthesis highlights the versatility of this approach. By optimizing reaction parameters such as solvent composition, precursor concentration, and temperature, researchers can fine-tune the properties of VS_4 nanostructures, thereby expanding their potential applications in supercapacitors, lithium-ion batteries, and electrocatalysis.

Exfoliation Method

The exfoliation method is a "top-down" approach used to break down bulk layered crystals into thin nanosheets (NSs). This process works by overcoming weak van der Waals forces that hold layers together. There are different types of exfoliation methods:

Mechanical Exfoliation: Uses adhesive tape (Scotch-tape method) to peel off thin layers, producing high-quality single-layer sheets.

Mechanical Force-Assisted Liquid Exfoliation: Uses solvents and mechanical force to separate layers.

Ion Intercalation-Assisted Liquid Exfoliation: Inserts small ions between layers, pushing them apart.
Ion Exchange-Assisted Liquid Exfoliation: Replaces large ions with smaller ones to weaken layer interactions.
Oxidation-Assisted Liquid Exfoliation: Uses oxidizing agents to add oxygen-containing groups, reducing layer bonding (used for graphite).
Researchers have used these techniques to synthesize vanadium sulfide (VS) nanosheets. Xie et al. used solvent-assisted liquid exfoliation to obtain VS_2 nanosheets thinner than 2 nm while modifying their electronic properties. High-resolution microscopy confirmed their 1T crystal structure. Similarly, VS_4 nanorods were obtained from bulk VS_4 using mechanical force-assisted liquid exfoliation in isopropanol. [28, 29, 30]

CVD Method

The Chemical Vapor Deposition (CVD) method is widely used for synthesizing high-quality, impurity-free 2D materials on a large scale. In 2005, Lou et al. successfully synthesized VS_2 nanosheets (NSs) using CVD. Since then, many VS_2-based materials have been produced using this method. By using vanadium chloride (VCl_3) and sulfur as precursors under an argon/hydrogen (Ar/H_2) atmosphere, researchers have grown ultrathin VS_2 nanosheets (less than 10 nm thick) on substrates. Key factors influencing growth include the evaporation temperature of VCl_3 and the placement of SiO_2/Si substrates. CVD is also useful for creating vanadium sulfide hybrid materials. Kortatkar et al. used CVD to deposit highly crystalline VS_2 flakes onto carbon nanotube (CNT) substrates. Additionally, a thin TiS_2 layer (~2.5 nm thick) was coated onto VS_2 flakes using atomic layer deposition, forming VS_2-TiS_2 hybrid structures, which show potential as cathode materials in lithium-ion batteries (LIBs). [15, 27, 31, 32]

3.2 Cobalt sulfides

Different synthetic strategies have been employed to fabricate cobalt sulfide nanoparticles with varying morphologies, including:

Hydrothermal and Solvothermal Synthesis: Dong et al. synthesized hierarchical CoS nanostructures via a simple one-pot hydrothermal method. $Co(NO_3)_2{\cdot}6H_2O$ and thiourea were dissolved in deionized water/ethanol and heated in a Teflon-lined autoclave. Thiourea acted as both an S^{2-} source and a structural directing agent. Morphologies were tailored by adjusting reactant ratios, solvents, time, temperature, and ligands. The flower-like CoS nanostructure formation involved three stages: (i) nanoflake formation, (ii) skeleton sphere development via Ostwald ripening, and (iii) hierarchical structure growth through dissolution-recrystallization. [33]. Similarly, Xing et al.$^+$ synthesized hierarchical CoS_2 nanostructures using $CoCl_2{\cdot}6H_2O$, citric acid monohydrate, ethanolamine, and CS_2 as the sulfur source [34]. Wang et al. studied temperature effects on CoS hierarchitectures, achieving diverse flower-like structures using $CoCl_2{\cdot}6H_2O$ and thioacetamide (TAA) as precursors, with temperature as the sole variable [35].

Sulfidation: Yin et al.[325] synthesized hollow Co_9S_8 and Co_3S_4 via thermal decomposition of $Co_2(CO)_8$ to CoO nanocrystals, followed by sulfidation in anhydrous o-dichlorobenzene. CoS and Co_9S_8 were also obtained through anion exchange and MOF-derived polyhedral nanocages. [36].

SUPERCAPACITOR PERFORMANCE

4.1 Vanadium Sulfide

With the growing demand for eco-friendly energy storage solutions, supercapacitors (SCs) have gained significant attention due to their long operational lifetimes, high power densities, and ultrafast charge-discharge rates. For instance, a supercapacitor demonstrated an impressive specific capacitance of 4760 μF/cm² and excellent stability after 1000 cycles. Dong et al. synthesized VS_2 nanoplates with abundant in-plane and out-

plane defects, significantly enhancing their energy storage capacity. At 1 A g^{-1}, these rich-defect VS_2 nanoplates exhibited a capacitance of 2200 F g^{-1}. An asymmetric SC using these nanoplates as the anode and commercial activated carbon as the cathode achieved a specific capacitance of 225 F g^{-1} at 0.5 A g^{-1}, delivering a power density of 6.62 kW kg^{-1} at 31.25 Wh kg^{-1} energy density, with good stability over 5000 cycles [37]. VS_4, another vanadium sulfide, has a higher sulfur content and theoretical capacity than VS_2. A VS_4/SWCNT/rGO hybrid exhibited a specific capacitance of 558.7 F g^{-1} at 1 A g^{-1}. Additionally, a VS_4/rGO/CoS_2@Co nanocomposite was developed as a cathode material, enhancing voltage window, conductivity, and stability. This cathode delivered a specific capacitance of 1353 F g^{-1} at 0.625 A g^{-1}, retaining 89.6% capacity after 20,000 cycles. An asymmetric SC using rGO/Co_9S_8@GO as the anode achieved an energy density of 106 Wh kg^{-1} at 2.67 kW kg^{-1} power density, maintaining 96.2% retention after 3000 cycles [38, 39].

4.2 Cobalt Sulfide

In SC applications, energy storage and release occur through the faradaic reaction of CoS_x with OH^-, facilitating electron transition between the Co^{2+}/Co^{3+} redox couple. The simplified reaction expressions are: $CoS_x + OH^- \leftrightarrow CoS_xOH + e^-$ and $CoS_xOH + OH^- \leftrightarrow CoS_xO + H_2O + e^-$ [40, 41, 42]. To enhance capacitive performance, extensive research has focused on tailoring the morphology of cobalt sulfide nanostructures, resulting in various forms such as hierarchical structures, nanosheets, nanowires, nanotubes, ellipsoids, and hollow structures [43, 44, 45, 46].

Peng et al. successfully synthesized hollow CoS_2 spheres via a hydrothermal method, demonstrating that different concentrations of carbon disulfide (CS_2) and ethylenediamine (EN) produce diverse morphologies, including solid, yolkshell, doubleshell, and hollow structures. These CoS_2 hollow nanostructures exhibit a wall thickness of ~150 nm, with nanosheet subunits (~5 nm), contributing to enhanced electrochemical properties. The specific capacitances of CoS_2 hollow nanostructures at current densities of 1, 2.5, 5, 10, and 20 A g^{-1} were 1301, 1073, 883, 650, and 450 F g^{-1}, respectively, surpassing other CoS_2 forms. Furthermore, their cycling stability was superior, retaining performance over 2000 cycles [46].

To improve SC power density, a binder-free approach was adopted to reduce equivalent series resistance (ESR). Pu et al. synthesized nickel foam-supported Co_9S_8 nanotube arrays using a two-step hydrothermal method, leveraging the nanoscale Kirkendall effect for tubule formation. These nanotube arrays delivered specific capacitances of 1775, 1635, 1600, 1563, 1520, and 1483 F g^{-1} at current densities of 4, 8, 12, 16, 20, and 24 A g^{-1}, respectively, with 83.5% capacitance retention after 2000 cycles at 16 A g^{-1} [47].

Similarly, Xia et al. employed anion conversion to prepare freestanding CoS nanoarrays on carbon fiber and nickel foam substrates. The Co_3O_4 or $Co(OH)_2$ nanoarrays underwent sulfidation using Na_2S, preserving their 1D morphology with diameters of ~80 nm and lengths of ~5 μm. These CoS nanoarrays exhibited excellent rate performance with capacities of 129 and 102 mAh g^{-1} at 2 and 40 A g^{-1}, respectively, maintaining 91% retention over 3000 cycles [48].

Comparative studies between self-supported CoS nanowire arrays and their powder counterparts revealed that freestanding CoS nanoarrays reduce electrode polarization, improving electrochemical performance. Xu et al. achieved direct growth of Co_9S_8 arrays on carbon cloth, with optimized samples exhibiting a specific capacitance of 2.35 F cm^{-2} (783.3 F g^{-1} for active material, 113.5 F g^{-1} for the entire electrode) at 5 mV s^{-1}, retaining 0.56 F cm^{-2} at 200 mV s^{-1}. The vertically aligned Co_9S_8 structure enabled superior performance at high current densities, achieving areal capacitances of 0.86 and 0.84 F cm^{-2} at 10 and 50 mA cm^{-2}, respectively. The binder-free Co_9S_8 arrays reduced internal resistance and charge transfer resistance at electrode/electrolyte interfaces, further enhancing their electrochemical capabilities [42].

CHALLENGES AND FUTURE PERSPECTIVES

Despite their promising properties, vanadium sulfide and cobalt sulfide-based supercapacitors face challenges such as:

- Poor Cycling Stability: Caused by structural degradation and volume expansion during cycling.
- Low-Rate Capability: A result of insufficient conductivity in certain morphologies.
- Environmental and Cost Concerns: Related to the synthesis and disposal of transition metal sulfides.

Future research should focus on optimizing synthesis routes, exploring hybrid materials, and developing scalable fabrication techniques to enhance the commercial viability of

CONCLUSION

Vanadium sulfide and cobalt sulfide nanoparticles have emerged as promising materials for supercapacitor applications due to their diverse morphologies, high surface area, and excellent electrochemical properties. Their unique structural features enable efficient charge storage through fast redox reactions, high electrical conductivity, and enhanced ion diffusion, leading to superior energy and power densities. Various synthesis techniques, such as hydrothermal, solvothermal, and template-assisted methods, have been developed to control their morphology and optimize their electrochemical behavior. Additionally, advancements in structural engineering, including doping, compositional tuning, and hybridization with carbon-based materials, further enhance their stability and capacitance retention over multiple charge-discharge cycles. These innovations make vanadium and cobalt sulfide nanoparticles viable candidates for next-generation energy storage devices, addressing the increasing demand for high-performance, environmentally friendly, and cost-effective supercapacitors. As research continues, the development of scalable and sustainable synthesis methods will be key to their widespread adoption in real-world applications.

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Advances in Medicinal Chemistry: Multidisciplinary Approaches to Drug Design, Synthesis, and Evaluation

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ABSTRACT

Novel therapeutic compounds that target a variety of illnesses, including as cancer, infectious illnesses, metabolic conditions, and drug-resistant infections, have been developed as a result of recent developments in medicinal chemistry. To improve therapeutic efficacy and safety, researchers have concentrated on investigating new bioactive chemicals, refining their molecular makeup, and determining their mechanisms of action. The design and synthesis of nitrogen-based derivatives and heterocyclic molecules, as well as the use of ecologically friendly synthetic techniques, are important innovations. By combining synthetic chemistry, computational modeling, and biological evaluation, efforts to prevent antimicrobial resistance, create dual-action drugs for complicated diseases, and improve drug delivery systems highlight the field's multidisciplinary nature. This all-encompassing strategy has the potential to improve therapeutic results and solve important issues in contemporary drug research.

Keywords: Medicinal chemistry, therapeutic compounds, drug design, bioactive molecules, antimicrobial resistance, drug delivery, green synthesis.

INTRODUCTION

Due to the need for novel therapeutic molecules to treat a variety of illnesses, including as cancer, infectious illnesses, metabolic conditions, and drug-resistant infections, medicinal chemistry has advanced significantly in recent years. To create more potent and specialized medications, researchers from all over the world have been aggressively investigating new bioactive chemicals, refining their structures, and clarifying their modes of action.

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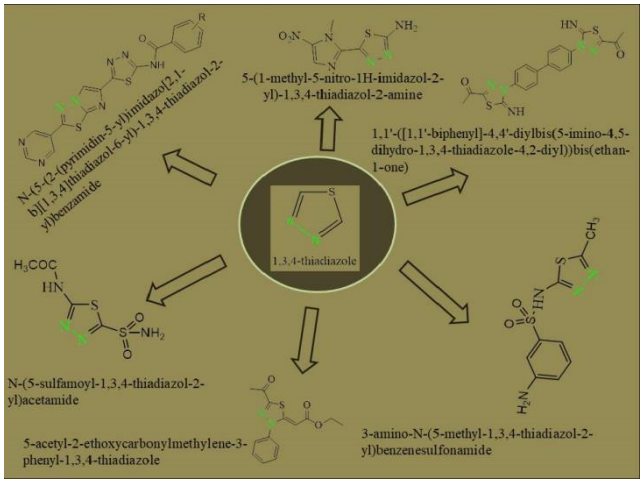
The design, synthesis, and assessment of heterocyclic molecules, nitrogen-based derivatives in particular and other structural scaffolds with encouraging pharmacological profiles have advanced as a result of this work. In order to address urgent issues in drug discovery, the corpus of work covered here takes a multidisciplinary strategy that blends synthetic chemistry, computer modeling, and biological evaluation.

Together, these investigations seek to increase medication efficacy, bioavailability, and safety, from developing environmentally friendly synthesis processes [14, 15] to designing anticancer medicines with improved specificity [1, 8, 9]. Antimicrobial resistance [20], dual-action compounds for complicated disorders [16], and improving the delivery of drugs for targeted therapy [22, 23] have all been the focus of research efforts.

The importance of pharmaceutical chemistry in overcoming the gap between fundamental science and use in medicine is highlighted by this corpus of research. These studies open the door to the development of next-generation therapeutics that tackle both new and enduring health issues by constructing novel compounds and comprehending their molecular interactions.

Recent developments in the field of medicine have brought to light a variety of methods for creating and examining bioactive substances that may have therapeutic uses. Gowramma et al. (2016) [2] examined innovative drug design techniques in anti-infective research, while Kalirajan et al. (2019) [1] studied anticancer drugs, emphasizing structural optimization for increased activity. Furthermore, focusing on their molecular processes, Gowramma and colleagues (2018) [3] developed bioactive compounds that target metabolic diseases. Similarly, the synthesis of organic molecules with possible antioxidative characteristics was described in detail by Kaviarasan et al. (2020) [4]. Synthetic approaches for creating heterocyclic compounds—which are essential scaffolding in drug discovery—were advanced by Sridhar et al. (2020) [5].

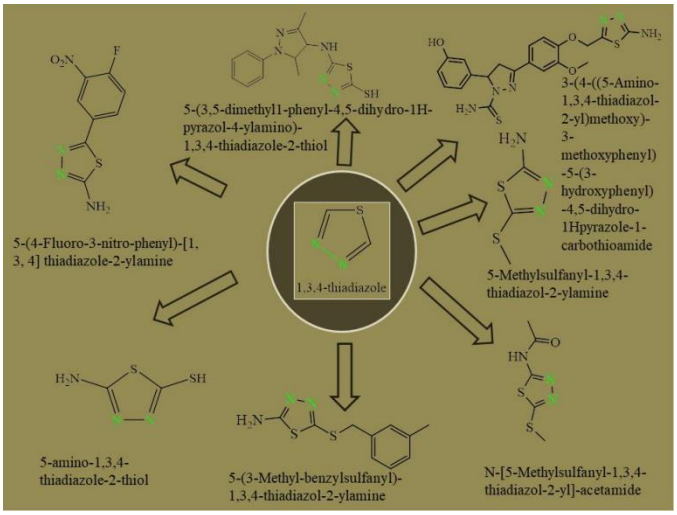


Graphical extract 1

Different techniques to the synthesis and analysis of bioactive molecules with potential therapeutic uses have been highlighted by recent developments in medicinal chemistry. While Gowramma et al. (2016) [2] investigated novel drug design methodologies in anti-infective research, Kalirajan et al. (2019) [1] studied anticancer drugs, concentrating on the optimization of the structure for increased activity. Additionally, Gowramma et al. (2018) [3] developed bioactive compounds that target metabolic diseases, focusing on their molecular pathways. Similar to this, Kaviarasan et al. (2020) [4] described in detail how organic molecules with possible antioxidative qualities were synthesized. Sridhar et al. (2020) [5] made contributions to synthetic approaches for creating heterocyclic molecules, which are essential building blocks for drug development.

In support of sustainable pharmaceutical practices, Upadhyay and Mishra (2017) [14] and Tahtaci et al. (2018) [15] created more environmentally friendly synthesis processes for physiologically active substances. Multitarget drugs were introduced by El-Naggar et al. (2019) [16] and have dual uses in neuroprotection and

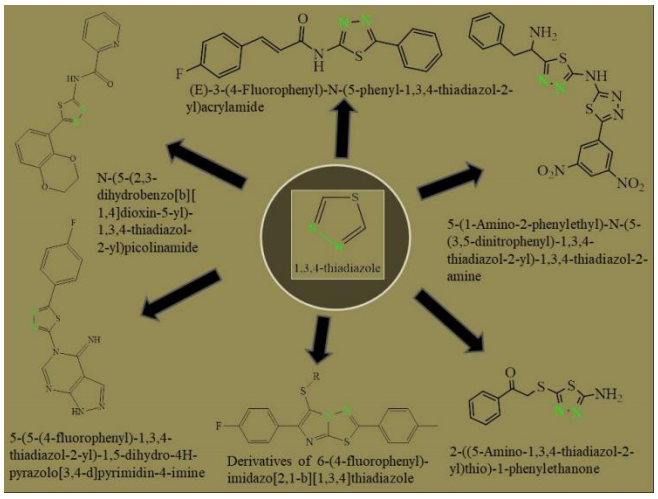
cancer. Simultaneously, Hemachander and Sugumaran (2012) [17] described methods for improving the bioavailability and solubility of lipophilic medications.



Graphical abstract 2

Derivatives with improved receptor-specific interactions were created by Farghaly et al. (2012) [18] and Luo et al. (2013) [19], offering information on the mechanisms underlying drug resistance. Cui et al. (2017) [21] introduced sophisticated computational methods for forecasting medication efficacy, while Taflan et al. (2019) [20] emphasized bioactive chemicals for antimicrobial resistance. Two notable studies that looked into hydrophilic moieties for better drug delivery systems were Noolvi et al. (2016) [22] and Polkam et al. (2015) [23]. Camoutsis et al. (2010) [25] and Vudhgiri et al. (2017) [24] emphasized the significance of aromatic replacements in augmenting pharmacological effectiveness. In order to meet unmet clinical needs, studies by Chandrakantha et al. (2014) [26] and Dubey et al. (2012) [27] broadened the range of antimalarial and antifungal medicines.

Synthetic pathways for chiral molecules with potential uses in asymmetric catalysis were created by Yazdanian et al. (2020) [28]. As noted by Qu et al. (2018) [29] and Clerici et al. (2001) [30], steric and electronic effects are crucial for regulating drug-target interactions.



Graphical abstract 3

This thorough analysis demonstrates the link among synthetic ingenuity and therapeutic applications, highlighting the dynamic breakthroughs in medicinal chemistry. Together, the contributions push the limits of molecular design and drug discovery.

CONCLUSION

To sum up, the examined literature emphasizes how important medicinal chemistry is to the advancement of therapeutic development and discovery. Researchers have made great strides in discovering bioactive chemicals with great promise in tackling serious health issues including infectious illnesses, cancer, and medication resistance through creative synthesis, optimization of structure, and in-depth biological evaluation. These studies demonstrate how contemporary methods, such as structure-activity relationship analysis, green chemistry, and computer modeling, can be integrated to improve the sustainability, safety, and effectiveness of drug development procedures. The development of dual-action drugs, nitrogen-based derivatives, and heterocyclic molecules demonstrates the adaptability and diversity of medicinal chemistry in treating complicated illnesses.

Furthermore, the field's dedication to converting lab results into clinically feasible solutions is seen in the focus on enhancing pharmacokinetic characteristics, bioavailability, and tailored drug delivery systems.

The discoveries and breakthroughs from these investigations will surely provide a basis for further research and development as the field of global health continues to change. Medicinal chemistry continues to be at the forefront of developing revolutionary treatments to meet unmet medical needs by encouraging interdisciplinary collaboration and utilizing state-of-the-art techniques.

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Review on Green Synthesis of Nanoparticles: Sustainable Approaches and Applications

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ABSTRACT

Now a day, nanoparticles being important in a variety of applications that is environmental science, medicine, material engineering, use in battery and supercapacitor applications. Nanotechnology has become a very important focus area of study. In day-to-day research, conventional synthesis methods frequently use hazardous chemicals and lot of electricity also use, which create lots of problems about sustainability and environmental safety like water pollution, air pollution, soil pollution. By using biological approach including plant extracts, bacteria, fungi and algae, green synthesis of nanoparticles provides a sustainable ecofriendly and environmentally friendly alternative. This review paper focus on the promise of green synthesis as a comparative alternative to traditional chemical and physical methods by study all concepts, methodologies, benefits and different uses.

Keywords: Nanoparticles, engineering Nanotechnology, Green Methods, Supercapacitor, plant fungi etc.

INTRODUCTION

Nanomaterial exhibits distinctive and unique physiochemical properties, nanoparticles (NPs) are essential part in a wide range of scientific and industrial areas [1]. There are many problems regarding toxicity and environmental contamination because of common traditional synthesis methods, such as physical and chemical approaches, usually required lots of electricity inputs and harmful chemicals [2]. Green synthesis, which utilize biological materials like plant extract, biomolecules and microbes has become a vital substitute because of its environmental friendly nature, non-toxic and sustainable processes. Green approach of nanotechnology reduces waste and uses renewable resources, which differentiate the great ideas of green chemistry.

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A fascinating field in nanoscience and technology is the synthesis of nanomaterial, including Carbon nanotubes, metal nanoparticles, graphene and their composites [3]. Green synthesis of nanoparticles, which are design through process of regular growth of size, all processes in control manner, after completion of reaction cleanup not needed, will essentially immediately contribute to their increased environmental friendliness. The number best factors of green synthesis of nanomaterials are minimum waste side products, minimum pollution and generally use the nontoxic solvents. In green synthesis methods use of plant extract is simple approach and synthesizing metal oxide nanomaterial on large scale also compared to other methods like fungi, algae. In green synthesis method, reaction is carried out with some parameters are mainly consider, the pH of reaction (neutral, acidic and basic), temperature, pressure, solvent, reaction time. In many medicinal base plants and algae contain some phytochemicals functional groups such as aldehyde, ketone terpenoids, carboxylic acids, phenols, ester [4]. These functional groups reduce the metal oxide in to nanomaterials. The main applications these green methods are biomedical diagnostics, antimicrobials drug synthesis, sensor development, talcum powder, supercapacitor and developed catalyst for many reactions. Overall objective of this review paper is to provide a helpful guidance for readers with a general interest in this green chemistry methods.

SIZE OF NANOPARTICLES

According to nanotechnology, a particle is a tiny thing that behaves as a whole unit in terms of its transport and properties. Particles are further categorized base on their size in terms of diameter; Course particles range in size from 10000 to 2500 nanometers. Size of fine particles ranges from 2500 to 100 nanometers. Nanoparticles is also known as ultrafine particles, range in size from 100 to 01 nanometer. The size related characteristics may or may not be substantially different from those of tiny particles or bulk materials. Individual molecules are typically not referred as nanoparticles, even though majority of molecules size would fall inside the above outline.

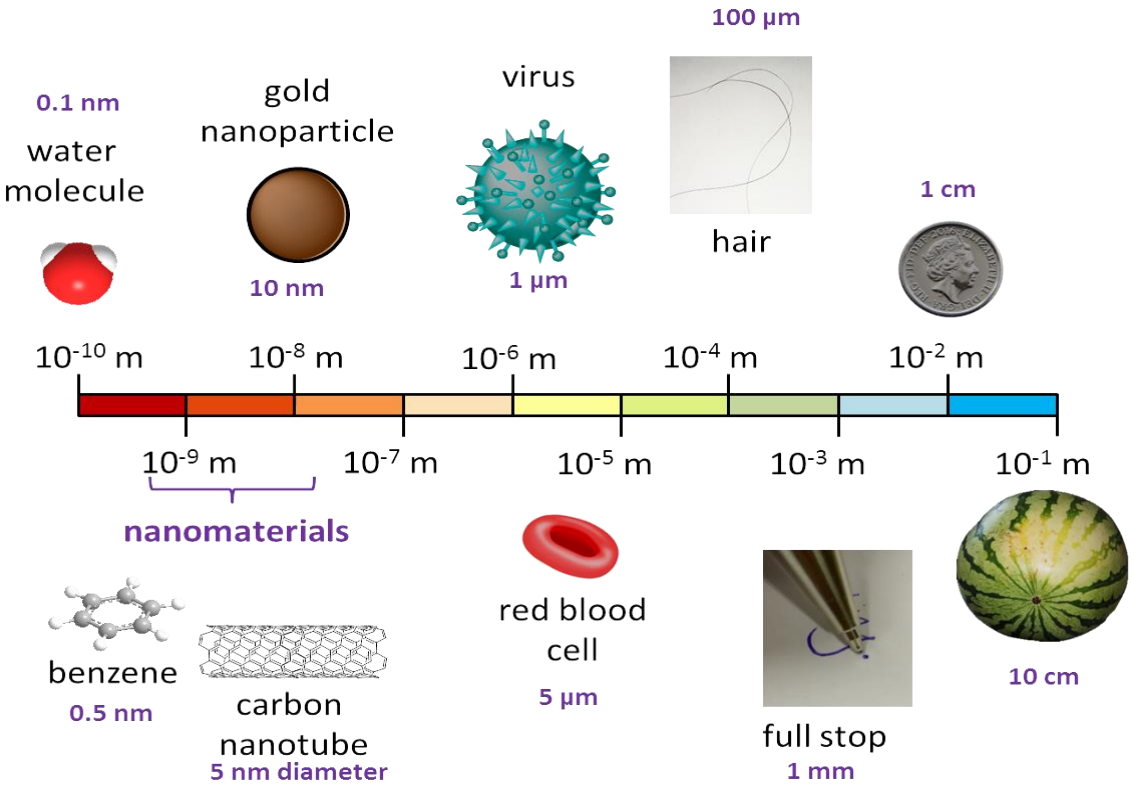

Diagram: Size of different particles

CHARACTERISTICS/PROPERTIES OF NANOPARTICLES:

Small size and large surface area, nanoparticles have special physical, chemical and biological properties. Among the important properties are:

a. Physical properties of nanoparticles:

- Their Small size: Generally ranging from 01 to 100 nm gives extraordinary thermal, mechanical and optical properties.
- High surface area: nanoparticles have a large surface area therefore reactivity and interactions with other materials are improved [5].
- High mechanical properties: Nanoparticles like carbon nanotubes are very strong and long-lasting properties [6].

b. Chemical properties of nanoparticles:

- Nanoparticles with a greater number of surface area atoms are more reactive. Due to high surface area nanoparticles used in catalyst development process [7]. Compare to other bulk material several nanoparticles increase stability and reactivity.

c. Biological properties of nanoparticles:

- Antibacterial: Utilize in coating and medications, silver nanoparticles contain antimicrobial properties [8].
- Drug delivery: In critical patients delivering medications straight to targeted cells therefore increase the effectiveness of treatment [9].

METHODS USED IN NANOPARTICLES SYNTHESIS:

There are different ways to synthesize nanoparticles, but they can be broadly divided in to two types: top down and bottom up

4.1 Top down:

By using this approach physical and mechanical methods to reduce bulk materials in to nanoparticles.

a. Ball milling
b. Laser ablation
c. Lithography
d. Arc discharge methods

4.2 Bottom up:

By using this approach creating nanoparticles either molecule by molecule or atom by atom

a. Sol gel method
b. Chemical vapor deposition
c. Coprecipitation method
d. Microemulsion method
e. Green synthesis method

The cost, scalability, application and desired nanoparticle qualities all influence the synthesis technique selection. For accurate control, bottom-up approaches are favored. Whereas top-down approaches are employed for large scale manufacturing [41].

SYNTHESIS OF NANOPARTICLES BY GREEN METHOD MECHANISM

There are **three steps** are usually involved in the synthesis of nanoparticle by green method are as follows:

Metal ion reduction by plant extract or any other biological species, Stabilization of metal ion and capping of nanoparticles.

a. Metal ion reduction:

Bioactive substances decrease the given metal salt utilized in the production of nanoparticles, such as $CuSO_4$, $NiCl_2$ $CoCl_2$ precursors. Aldehyde, ketone, carboxylic acid, ester, polyphenols, alkaloids, flavonoids, proteins and sugars derived from biological sources are the examples of these reducing agents [10].

b. Growth and stabilization of nanoparticles:

Biomolecules like aldehydes, ketones, flavonoids, proteins, sugar molecules regulate the size of the nanoparticles and stop them from aggregating after they have formed.

c. Capping of nanoparticles:

Capping of nanoparticles is the most important step in the synthesis of nanoparticles. In which for industrial or biomedical applications, the organic compounds derived from biological extracts serve as capping agents, offering stability and shape control of nanoparticles [11].

BIOLOGICAL INGREDIENTS FOR GREEN SYNTHESIS OF NANOPARTICLES:

Number of Biological substances, each with unique characteristics, have been investigated for the synthesis of nanoparticles.

6.1 Extract from Plants:

Because of its ease of use, speed and capacity to synthesize nanoparticles with precise size and shape, plant extract extensively employed. Aldehydes, ketones terpenoids alkaloids, flavonoids, proteins and carboxylic acids are examples of phytochemicals that have reducing and stabilizing characteristics. Here are a few examples are as follows;

a. Extract from Neem tree:

Botanical name of neem tree is Azadirachta indica, which is rich in bioactive chemicals, efficiently synthesizes gold and silver nanoparticles [12][42].

b. Aloe vera extract:

The botanical name of aloe vera is Aloe barbadensis miller. The proteins and polysaccharides in aloe vera help to stabilize nanoparticles [13].

c. Tulsi extract:

The botanical name of tulsi is Ocimum sanctum. Tulsi plant contains lots of antioxidants that stabilize nanoparticles and reduce metal ion in to nanosized [14].

d. Apple Juice:

The botanical name apple is pyrus malus. For the synthesis of nanoparticles, apple juice can be utilized as a green stabilizing and reducing agent. Apple juice contain following phytochemicals, flavonoids, organic acids and polyphenols aid in stabilizing and reducing metal ions to nanoparticles [15].

e. Tea plant extract:

The botanical name of tea is Camellia sinensis. Tea plant extract contain polyphenols are strong reducing components that promote the synthesis of nanoparticles [16].

6.2 The bacteria:

Metal ions can be reduced to nanoparticles by some bacterial species through the use of secreted proteins and enzymatic process. We see some examples;

a. Escherichia coli:

Helps to reduce metal ions, especially those that are silver and iron nanoparticles [17].

b. Pseudomonas aeruginosa:

Used to synthesize gold and silver nanoparticles [18][43].

c. Bacillus subtilis:

Uses biomineralization mechanisms to produce extracellular nanoparticles [19].

6.3 Fungi

Benefits of fungi include increased biomass production, effective enzyme Secretion and the formation of extracellular nanoparticles. We see following Examples:

a. Fusarium oxysporum:

Generates stable nanoparticles of silver and gold [20].

b. Penicillium sp:

Produces more stable, biocompatible nanoparticles [21].

c. Aspergillus niger:

Used to synthesize titanium dioxide and silver nanoparticles [22].

6.4 Algae

Algae contain more amount of bioactive ingredients, freshwater and marine algae can be used to produce environmentally friendly nanoparticles.

a. Spirulina platensis:

It is one of the best reducing agent in the production of gold and silver Nanoparticles [23][44].

b. Chlorella vulgaris:

For the manufacture of gold and zinc oxide nanoparticles this algae is used Preferentially [24].

Table 1: Nanoparticles synthesis by using green methods via plant source

Nanoparticle made by	Size in nm	Green method source	Reference
Zinc oxide	1.56 to 19.57	Neem	12
Silver	Below 50	Neem	35
Silver	5-35	Neem	36
Silver	10-20	Tulsi	14
Gold	30	Tulsi	14
Silver	42	Tulsi	37
Silver	-	Aloe vera	38
Silver	-	Aloe vera	13
Aluminum	8.04 to 24.81	Apple	15
Silver	5.26 to 30.25	Apple	39
Silver	-	Tea	16
Siver	20- 90	Tea	40

Table 2: Nanoparticles synthesis by using green methods via Bacteria source

Nanoparticle made by	Size in nm	Green method source	Reference
Silver	10-90	Escherichia coli	17
Gold	40	Pseudomonas aeruginosa	18
TiO_2	66-77	Basillus subtils	19

Table 3: Nanoparticles synthesis by using green methods via Fungi source

Nanoparticle made by	Size in nm	Green method source	Reference
Silver	5-50	Fusarium oxysporum	20
Silver	75	Penicillium sps.	21
Silver	20	Aspergillus niger	22

Table 4: Nanoparticles synthesis by using green methods via Algae source

Nanoparticle made by	Size in nm	Green method source	Reference
Silver	20-90	Spirulina platensis	23
Palladium		Chlorella vulgaris	24

DIFFERENT TYPES OF NANOPARTICLES SYNTHESIZED BY USING GREEN TECHNIQUES APPROACH

Green techniques have been applied in the synthesis of several metal and metal oxide nanoparticles [45].

a. Gold Nanoparticles:

Gold nanoparticles possess biocompatibility and some specific properties so this nanoparticle used in cancer therapy, biosensing and drug delivery.

b. Silver Nanoparticles:

Extensively used for medical coating and wound dressing because of their well known antibacterial and antiviral properties.

c. Zinc oxide NPs:

Zinc oxide nanoparticles are actively utilized in antibacterial coating, as a catalyst and as a UV blocker agent.

d. Copper oxide Nps:

Copper nanoparticles used in conducting materials as well as in antibacterial coating also.

e. Iron oxide Nps:

Fe2O3 nanoparticles always used in water filtration technique, targeted medication drug delivery and magnetic resonance imaging.

USEFUL APPLICATION OF NANOPARTICLES SYNTHESIZED VIA GREEN METHOD.

a. Solve the environmental related problems:

1) Waste water contains heavy metals, that metals are remove via suitable nanoparticles [25].
2) By the use nanoparticles degradation of pollutants and air cleansing also done [26].

b. Application in Biomedicine:

1. Now a day nanoparticle used in targeted medication drug delivery for cancer treatment [27].
2. Nanoparticles tremendously useful in antibacterial coating of medical equipment's [28].
3. The main use of nanoparticles is identifying illness via biosensors [29].

c. Agriculture applications:

1. Use of nano-fertilizers to improve the growth of plants [30][46].
2. Minimum use of pesticides via nanoparticles based pesticides [31].

d. Application in catalysis:

1. Due to large surface area nanoparticles use in catalysis [32].
2. The main used of nanoparticles in catalysis is the carbon capture and hydrogen production.

e. Talcum powder enhancement:

1. In each an every home talcum powder is used for beautification that powder antibacterial qualities enhance by the use of Ag, ZnO and TiO2 nanoparticles [33].
2. Some other qualities also improve like moisture absorption, smooth texture, scent retention, UV protection and skin calming effects are all improved by the nanoparticles.

f. Supercapacitors applications:

Nanoparticles enhance the power of supercapacitors like increasing energy density, improving conductivity, boosting cycle life and enabling flexible designs [34].

OBSTACLES AND PROSPECTS FOR THE FUTURE

Difficulties:

- Reproducibility: Inconsistencies arise due to biological extract variability.
- Scalability: Production on a large scale is still difficult.
- Stability of storage: Overtime, certain nanoparticles may agglomerate.
- Approvals from regulatory: Guaranteeing uniformity and safety for business uses.

Prospectus for the future:

- Synthesis techniques are optimized for better control.
- Investigating new biological sources to increase effectiveness.
- Widespread applicability through integration with commercial businesses.

CONCLUSION:

Synthesis of nanoparticles by green method is an inventive and sustainable method that complies with both economic viability and environmental safety. This approach saves energy use, decreases chemical waste and encourages safer uses across a range of industries by utilizing biological resources. Green nanotechnology has the power to transform a number of industries and contribute to a healthier and more environmentally friendly future with continued breakthroughs.

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Assessment of Genotoxic Potential of Carbendazim on Channa Punctatus Using Micronucleus Assay

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ABSTRACT

Pesticides are commonly employed in agricultural innovation to boost crop yields. They also have the potential to contaminate water and soil, causing long-term environmental harm. Pesticides can enter adjacent rivers, lakes, and groundwater through runoff from treated fields, disrupting ecosystems and perhaps endangering aquatic life. This may cause local ecosystems to be disrupted and biodiversity to decline. However by damaging earthworms, fungus, and beneficial microbes that is essential to the upkeep of healthy soil ecosystems, pesticides can lower soil fertility. Somehow, its excessive exposure does not end with target creatures; it also impacts a number of non-target organisms like beneficial insects like bees, butterflies, and natural pest predators. But the most prominent species to get affected is fish. Since biodiversity-rich freshwater ecosystems are currently losing biodiversity more quickly than marine or terrestrial ecosystems, making them the most vulnerable habitats on Earth and facing threats from anthropocentrism, fish micronucleus testing has great potential for continuous and effective pollution assessment. In the present study micronucleus assay was used to evaluate the genotoxic potential of the fungicide carbendazim in Channa punctatus. Two distinct approaches were used: three dosages of carbendazim (1.5, 3, and 4.5 mg/kg body weight) were administered intraperitoneally, and the skin was exposed to varied concentrations of the drug (15, 25, and 35 ppm) in lab aquariums. Giemsa solution (pH 7.0) at concentrations of 15 to 20% was used to stain peripheral blood smears. Blood smear slides were prepared after 24, 48 and 72 hours of exposure. The chemical produced several nuclear and cytoplasmic abnormalities in addition to micronuclei. The biological

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specimens of Channa punctatus were shown to be significantly impacted by high amounts of carbendazim. The study highlights the potential detrimental effects of improper use of carbendazim containing pesticides in agriculture on Channa punctatus and emphasizes the need for careful management of such chemicals to protect aquatic ecosystems. Further research employing different test systems necessary to reconcile the contradictory results observed in various test systems.
Keywords: Channa punctatus, carbendazim, micro nucleus assay, genotoxic potential, peripheral blood smear

INTRODUCTION

Regardless of one's social or economic standing, everyone has the fundamental right to receive healthy food (FAO, 2009). It is anticipated that the agriculture industry will face numerous obstacles in the upcoming years as it works to ensure food production for the exponentially growing increasing human population; according to United Nations projections, it will reach 9.7 billion in 2050 and 10.9 billion in 2100. The demand for food and other essential resources will unavoidably rise sharply as a result of such development (Viola and Marinelli, 2016). To fulfill the nutritional needs of the growing population, the food industry should specifically boost production by 15% over the next ten years (OECD-FAO, 2019), with a 50% rise predicted by 2050 (FAO, 2017). For many years, agrochemicals have been used extensively to try to protect crops from insect pests. Nevertheless, a wide range of novel chemicals are released into the market each year due to the growing resistance, which results in unfavorable side effects and higher food production costs. Pesticides are, more precisely, chemicals that are purposefully released into the environment to control pests. These poisons then remain in the soil, water, and food, causing toxicity to both humans and animals (Schulz, 2004; Carvalho, 2006; Moraes *et al*., 2009). Despite this, pesticide use is still widespread, particularly in tropical areas (Carvalho, 2006). Monitoring a number of indicators, such as the measurement of pesticide residues, is necessary for environmental quality control. The study of bioindicators is essential for identifying the harmful consequences that these cause. Fish have been the primary subject of research on the bioconcentration and transformation processes of pesticides. This is because these animals live close to places where pesticides are frequently applied, putting them in direct touch with aquatic sediments. When compared to the water column overall, a large number of weakly water-soluble chemicals eventually settle in these pools of water, increasing the level of local pollution (Grisolia, 2005; Umbuziero *et al.,* 2006). These days, a number of well-developed and standardized tests are available to evaluate the genotoxic profile of a broad range of drugs. Counting the micronuclei in erythrocytes is made easier by the micronucleus test's simplicity when compared to other techniques. As a result, the test has been widely used to assess novel chemicals' and medications' potential to cause mutations. It is also recommended for routine screening and environmental monitoring (Al-Sabti *et al.,* 1994; Bücker *et al.,* 2006). When the nuclear membrane is rebuilt around the daughter cells' chromosomes during the telophase of mitosis or meiosis, micronuclei are created (Udroiu, 2006). Chromosome acentric fragments (clastogenic effect) or entire chromosomes that have been excluded from the main core due to inadequate migration (aneugenic effect) are the causes of micronuclei. Micronuclei are hence a loss of chromatin due to either chromosome structure (fragmentation) or the mitotic apparatus being damaged. An early shift in cellular metabolism may

also be indicated by the development of bilobed nuclei (Fenech, 2000; Grisolia and Cordeiro, 2000; Bombail *et al.,* 2001; Grisolia and Starling, 2001). Within this context, the aim was to survey the genotxic effect of carbendazim on *Channa punctatus* through micronucleus testing, determine the risk and toxicological impact of carbendazim.

MATERIALS AND METHODS

2.1 Test Chemical: The study used premium carbendazim, a 50% pure fungicide sold under the trade name "bavistin," which was obtained from Biostadt (India) Ltd. The solvent used in the experiment was glass double-distilled (g.d.d.) water.

2.2 Dose: Three different doses of 1.5, 3, and 4.5 mg/kg body weight were given to *Channa punctatus* intraperitoneally (i.p.). In a further set of investigations, the specimen was exposed to carbendazim at concentrations of 15, 25, and 35 parts per million in lab aquariums to investigate the chemical's effects on fish through cutaneous exposure.

2.3 Experimental animal: Local vendors in the Cuttack district provided live *Channa punctatus* measuring 100–150 grams. These fish were acclimated to laboratory settings before any chemical treatments were started. They spent 15 to 20 days in glass aquariums filled with 40 liters of de-chlorinated tap water throughout this phase. To maintain the appropriate physio-chemical parameters, the aquarium water was aerated and replaced every day, and the fish were fed commercial fish food twice a day. A temperature range of 28°C, a pH level between 6.8 and 7.05, and dissolved oxygen levels between 6.5 and 7.3 mg/L were among these criteria. To mitigate stress and prevent contamination, regular maintenance of the aquaria ensured the removal of leftover food, trash, and any dead organisms.

2.4 TIME: Blood smear slides for analysis were prepared at intervals of 24, 48, and 72 hours following exposure to the chemicals.

2.5 Experimental Protocol: Four fish were assigned to each treatment group for both intraperitoneal and cutaneous exposure. At 24, 48, and 72-hour intervals, blood was taken via caudal incision, and the resulting blood was utilized to create peripheral blood smear slides. Thin smears of peripheral blood were made on sanitized, grease-free slides, examined in an oil immersion, preserved in pure methanol, and stained using Giemsa solution. From 4000 erythrocytes per specimen, micronuclei—smaller, non-refractile particles that resemble nuclei—were scored.

RESULTS

3.1 General Toxicity: There were noticeable signs of external toxicity following intraperitoneal injection (mg/kg) or whole body exposure (dermal exposure) at varying dosages (ppm) of the toxin. On the ventral surface of the *Channa punctatus*, crimson spots emerged.

3.2 Qualitative: The erythrocytes of the fish are fairly large with centrally located nucleus. The nucleo-cytoplasmic ratio is 1:6 in the specimen, which facilitates easy scoring of micronucleus (MN). The location and size of micronuclei varied from cell to cell. In general, one micronucleus per cell was recorded. However more than one micro nuclei were also noticed in some cell. Micronuclei were mostly dot shaped and range from 1/5 to 1/28th (*Channa punctatus*) of the principal nucleus. Throughout the entire course of investigation both small and large size MN were observed in the treated individuals. Besides the induction of micronuclei, several other types of nuclear anomalies such as sickle shaped, thinning in mid region of nuclei and enucleated cells were also recorded. The chemical also induced other anomalies like enucleated cell, and constrictions.

3.3 Quantitative: The incidence of micronuclei induced by different doses of the chemical administered both dermal and intraperitoneal route are summarized in tables 1-2 respectively. The frequency of MN induced by all the doses after different exposure timings differed significantly from respective controls in *Channa punctatus* exposed to 15, 25 and 35ppm of the chemicals. Significant variation of micronuclei number was observed in all treated groups as compared to control (Table1) [*P<0.05,**P<0.01 (Student's t-test)]. Further, significant variations from control were also observed for different dose response analysis (F=13.72; degree of freedom (d.f.) = 35.3;**P<0.01). Moreover, a linear increase in the frequency of micronuclei with doses was marked (Y- intercept (b) =0.068; Coefficient of correlation (r) =0.858;**P<0.05). However, no significant variation was observed in time response analysis [F=1.68;d.f.=36.2;P>0.05](ANOVA).

Frequency of micronuclei also differed from control when the fish *Channa punctatus* injected with 1.5, 3 and 4.5 mg/kg body [*P<0.05; ** P<0.01; (Student's t-test)]. Further significant variations among different doses were also observed (F=12.13; d.f.= 36.3;**P<0.01). However, no significant variation was observed in time response analysis (F=1.72; d.f. =36.2; **P<0.05) (ANOVA). Moreover, a linear increase in the frequency of micronuclei with dose was observed (Y- intercept (b) =0.052; Coefficient of correlation (r) =0.832;*P<0.05)

Table 1: The occurrence of micro nucleated peripheral blood cells in *Channa punctatus* fish exposed to water contaminated with Carbendazim

Dose(ppm)	Time(hrs)	No. of MN	‰ aberration±S.E.	No. of NA	‰ aberration±S.E
	24	1	0.06±0.06	2	0.12±0.07
	48	2	0.12±0.07	2	0.12±0.07
Control	72	2	0.12±0.08	3	0.18±0.06
	24	4	0.37±0.07*	3	0.18±0.06
	48	5	0.50±0.10*	4	0.25±0.00
15	72	5	0.62±0.06*	5	0.25±0.07
	24	5	0.43±0.11**	4	0.25±0.10
	48	5	0.56±0.06**	5	0.31±0.06
25	72	6	0.62±0.07*	5	0.31±0.06
	24	5	0.50±0.06**	4	0.25±0.00
	48	6	0.56±0.07**	5	0.32±0.07
35	72	7	0.68±0.06**	5	0.32±0.07

Results are mean‰ ± S.E of four fish.

Result is significantly different from the control at *P<0.05,**P<0.01(Student's t-test)16000 cells were scored for each point (4000/fish)

Table2: The occurrence of micro nucleated peripheral blood cells in *Channa puntatus* fish injected intraperitoneally with carbendazim

Dose(mg/kg)	Time(hrs)	No. of MN	‰aberration±S.E.	No. of NA	‰ aberration±S.E
	24	1	0.12±0.07	2	0.18±0.06
	48	2	0.12±0.07	2	0.12±0.06
Control	72	2	0.18±0.06	3	0.12±0.07
	24	4	0.50±0.10*	3	0.18±0.06
	48	5	0.56±0.06*	4	0.25±0.00

Dose(mg/kg)	Time(hrs)	No. of MN	‰aberration±S.E.	No. of NA	‰ aberration±S.E
1.5	72	6	0.68±0.07*	4	0.31±0.06
	24	5	0.50±0.10**	4	0.25±0.10
	48	6	0.62±0.07**	5	0.31±0.06
3	72	7	0.75±0.10*	5	0.31±0.06
	24	6	0.62±0.07**	4	0.37±0.10
	48	6	0.68±0.06**	5	0.43±0.06
4.5	72	7	0.87±0.07**	5	0.50±0.10

Results are mean‰ ± S.E of four fish.

Result is significantly different from the control at *P<0.05,**P<0.01(Student's t-test)16000 cells were scored for each point (4000/fish)

DISCUSSION

We evaluate the genotoxicity of carbendazim on *Channa punctatus* using micronucleus assay. Here fishes have exposed to two different routes i.e. dermal route and intraperitoneal route. In general terms, our results allowed us to establish, based upon statistical analysis, and for the doses response, carbendazim has toxic effect on fish specimen. In dermal exposure it has been seen that the number of micronucleus was low in control medium. With increase in concentration of chemical exposure the number of micronuclei increased. Along with the micronuclei, several nuclear abnormalities have also been identified. With increase in concentration of chemical and with increase in time of exposure the number of micronucleus and nuclear abnormalities increased. In case of intraperitoneal exposure, it has been observed that the number of micronucleus and nuclear abnormalities are more in comparison to dermal exposure. After long exposure to the chemical, appearance of red patches on the ventral side of the fish specimen has been recorded. With increase in time of exposure in intraperitoneal route, appearance of nuclear abnormalities and micronuclei increased. So in both dermal exposure and intraperitoneal exposure appearance of micronuclei and nuclear abnormalities occurred in fish specimen, which established the genotoxic effect of carbendazim. These results require further investigation of the interpretation of sensitivity and specificity of micronucleus test. Carbendazim toxicity can be observed in organisms of other species. Genotoxic effect of various pesticides has been studied previously in different fish species. Acute toxic effect of acephate on fresh water fish *Puntius sophore* and *Clarias batrachus* had been studied (Gavit *et al.,* 2016; Jagyanseni *et al.,*2023) Genotoxic effect of copper sulphate has been proven in previous studies in *Channa punctatus* (Jagyanseni *et al.,* 2024). The erythrocyte micronucleus test has been applied to different fish species to study the level of contamination of aquatic contaminants having mutagenic properties (Arslan *et al.,* 2017).

CONCLUSION

Hypertrophy of bacteria in aquatic ecosystems poses an increased risk of environmental pollution as cats and dogs of industrial and agricultural origin are highly raised, leading to severe concerns regarding genotoxicity in aquatic organisms, especially fish. Pollutants in fish; pesticides, metals, and other toxins can also cause genetic damage in fish, reflected as chromosome aberrations, DNA mutations and other genetic anomalies. Stocking fish with different genetics might compromise fish health, leading to lower survival and reproduction and increased disease susceptibility. Additionally, due to their pivotal role in various aquatic ecosystems, genotoxicity in fish could result in domino effect on the ecological balance and biodiversity. Strong energy

regulation and sustainable practices must stringently implement to mitigate pollution and safeguard fish populations' genetic viability. This can help ensure that aquatic ecosystems and the diverse species they support continue to thrive, and that the International aquatic ecosystems and the water system on the planet will continue to flourish. The study unequivocally shown that carbendazim had a clastogenic effect on *Channa punctatus*, which raises severe concerns regarding the use of this resource for agriculture as well as potential health risks for humans and other aquatic animals that depend on aquatic habitats. The variations in micronuclei rates among dangerous compounds and species suggest a connection between the chemical kinetics of toxins and the pace of the hemopoietic cycle. There is a link between genotoxic substances and gene alterations; if left unchecked, these pollutants could pose a threat to future generations. Contradictory results about the effects of the chemical need to be reconciled with additional research using a variety of test systems.

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Design and Development of IOT Based Automatic Irrigation System Using Arduino UNO

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ABSTRACT

The research paper deals with IOT based automatic irrigation system using Arduino UNO. In this research work we have designed a system which is going to measure various parameters of environment such as temperature, detect the presence of rain, soil moisture and humidity. Here Arduino Uno is used to control the entire system of sensor such as Temperature sensor, Rain sensor, Soil moisture sensor, Humidity Sensor, relays, fan, water pump and liquid crystal display. All the four sensors plays vital role in operating the fan and water pump. There are various conditions in which the fan and water pump turns ON or OFF. In the present system we have also interfaced liquid crystal display with the Arduino Uno. The LCD displays environment temperature, status of rain, soil moisture in percentage, humidity in percentage, and state of fan and water motor whether they are ON or OFF.

The purpose of designing such type of system is to automatically monitor the irrigation system, one can see the various parameters on single screen. The advantage of such system is that, we know the status of fan and water motor whether they are ON or OFF just from the LCD screen display. The fan and water motor is automatically turned ON or OFF according to predefined values of sensors so no human intervention is required.

Keyword- Arduino Uno, Temperature Sensor, Rain Sensor, Soil Moisture sensor, Humidity Sensor.

INTRODUCTION

India ranks second worldwide in farm outputs. As per the Indian economic survey 2020-21, agriculture employed more than 50% of the Indian workforce and contributed 20.2% to the country's GDP [1]. Trees, plants, crops in the field adds natural beauty to the surroundings and serves as food for humans and animals,

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they are also the source of oxygen for all the living being on the earth [2]. With the increase in population, the need for agriculture production is also going to rise and will result is increase in requirement of the amount of fresh water for irrigating the crops. Currently more than 80% of water consumption is utilized in Agriculture. The unplanned water usage may result in unnecessary loss of water with limited productivity. This problem can be solved by designing a system to make optimum use of water by avoiding water wastage, increased productivity without additional financial burden on farmers [3]. Since last few years' farmers have started using computers and mobile phones to update themselves with latest technologies used in agriculture and monitor their crop production effectively with the use of various latest technology. IOT based automatic irrigation system using Arduino UNO provides an advanced technology that facilitates optimum management of resources and water in rural and urban locations [4]. Multiple sensors such as temperature sensor using IC LM35, Rain Sensor using Logic State, Soil Moisture sensor using variable resistor, Humidity sensor variable sensor are used in this work. The information is collected from the various sensors and given to Arduino UNO for controlling the water motor and fan, with the addition of Internet of Things (IOT) module or Wifi chip the traditional irrigation system can be converted to smart irrigation system which will increase the agriculture output and make optimum use of water with reduced wastage.

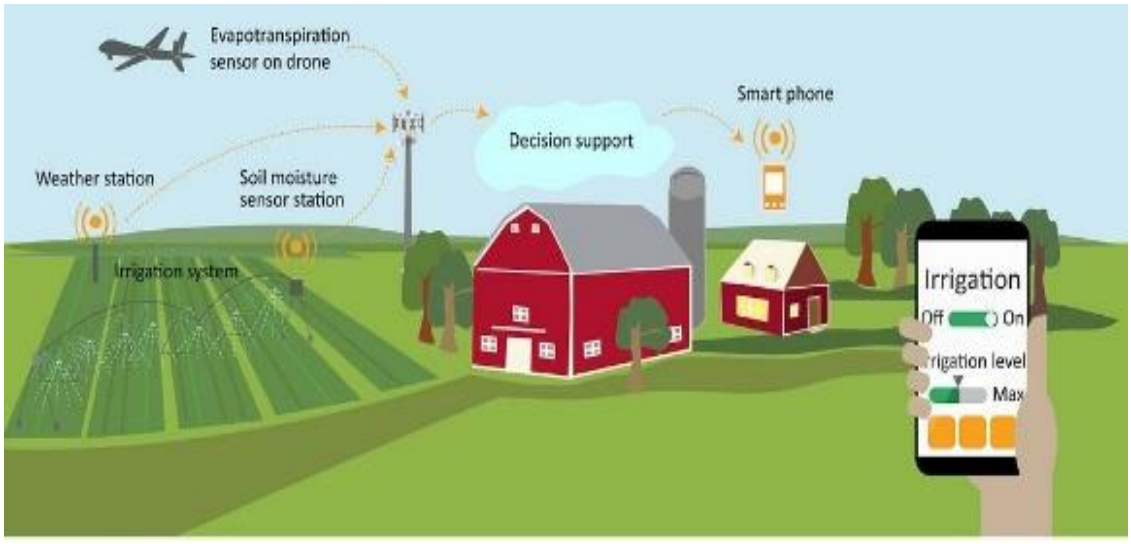

Figure 1: IOT based smart irrigation system

The research paper will illustrates how Arduino UNO will detect the temperature of atmosphere turn the fan on if temperature is greater than threshold value, turn the water motor on if the soil moisture is less than threshold value, detects the rain and regularly measures the humidity in the atmosphere. The measures values are displayed on LCD display as well as can be transmitted to remote location using IOT module or Wifi chip

METHODS AND MATERIAL

In order to check the working of present system, after its designing, construction and programming the temperature sensor detects the atmospheric temperature which gives signals to Arduino, the microcontroller controls the fan accordingly, the moisture sensor detects the moisture and gives it to controller, the controller controls the water motor accordingly, the rain sensor detects the presence of rain, signals it to microcontroller which is turn controls the water motor, the humidity sensor measures the atmospheric humidity. All the measured parameters are displayed on LCD display and can be transmitted to mobile device or website using IOT module or Wifi device.

2.1 SYSTEM OVERVIEW

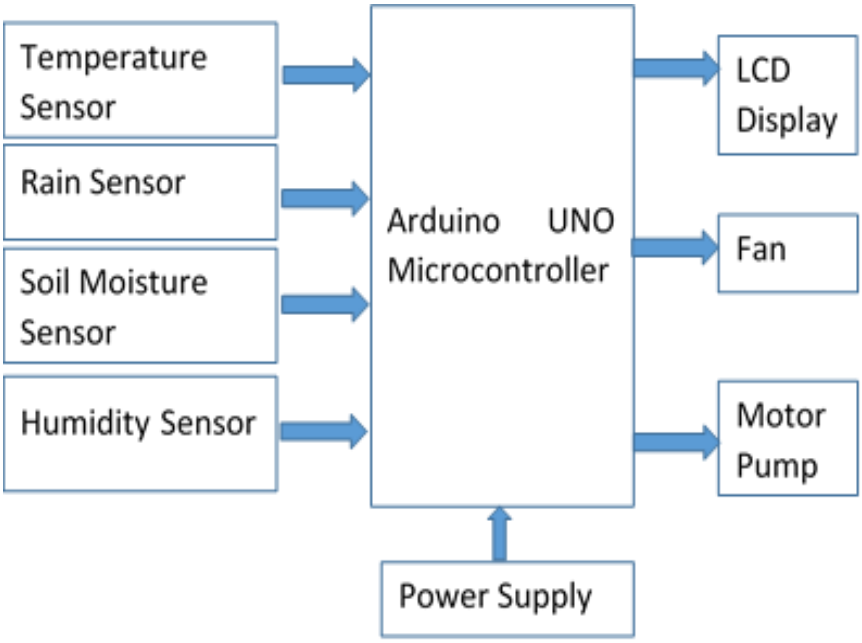

Figure 2: System Block Diagram

1. **Temperature Sensor LM35:** The LM35 series consists of high-precision integrated temperature sensors that produce an output voltage directly proportional to the temperature in degrees Celsius. Unlike temperature sensors calibrated in Kelvin, the LM35 eliminates the need for subtracting a constant offset to achieve Celsius readings. It offers high accuracy without requiring external calibration or adjustments, with a typical precision of ±0.25°C at room temperature and ±0.75°C over its full operating range of –55°C to 150°C. The sensor's wafer-level trimming and calibration ensure cost efficiency. Additionally, its low output impedance, linear response, and built-in calibration make it easy to integrate with measurement or control systems [5].

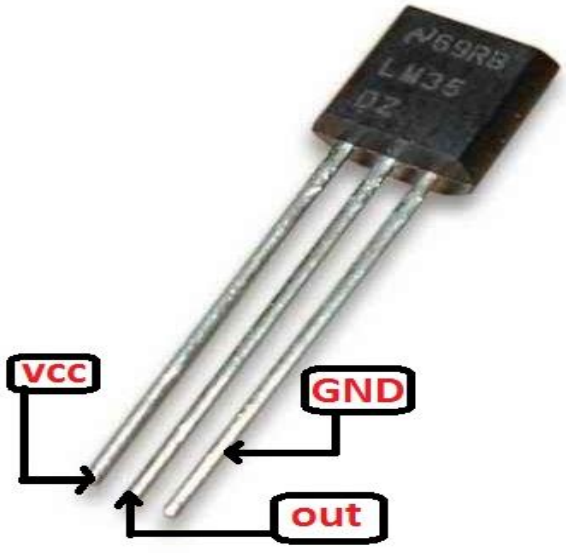

Figure 3: LM35 Temperature Sensor

2. Rain Sensor FC 37:

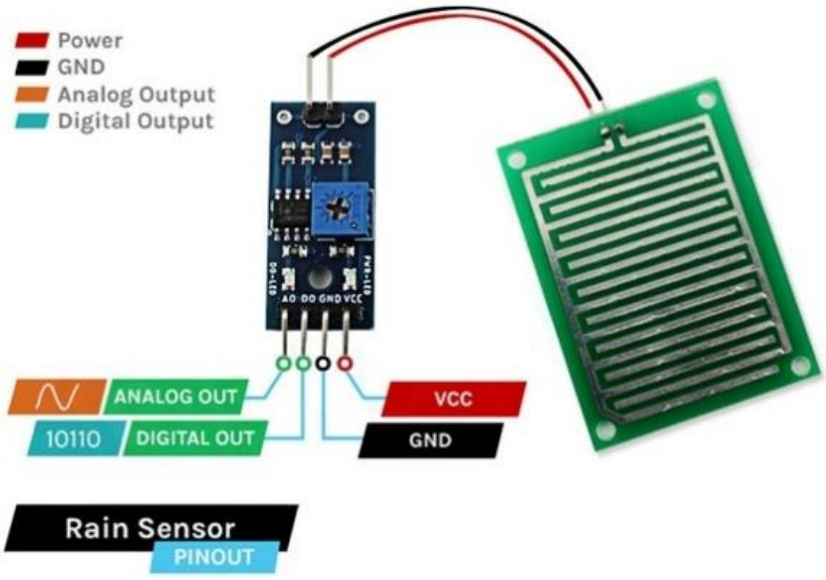

Figure 4: FC 37 Rain Sensor Module

VCC: is the power supply pin of the Rain Detection Sensor that can be connected to 3.3V or 5V of the supply. But do note that the analog output will vary depending upon the provided supply voltage.
GND: is the ground pin of the board and it should be connected to the ground pin of the Arduino.
DOUT: is the Digital output pin of the board, output low indicates rain is detected, and high indicates no rain condition.
AOUT: is the Analog output pin of the board that will give us an analog signal in between vcc and ground.
When the Rain Detection Sensor is interfaced with Arduino the LED indicator will remain off when no rain is detected and the LED indicator will turn on as soon as rain droplets falls on the module [6].

3. Soil Moisture Sensor SEN0114:

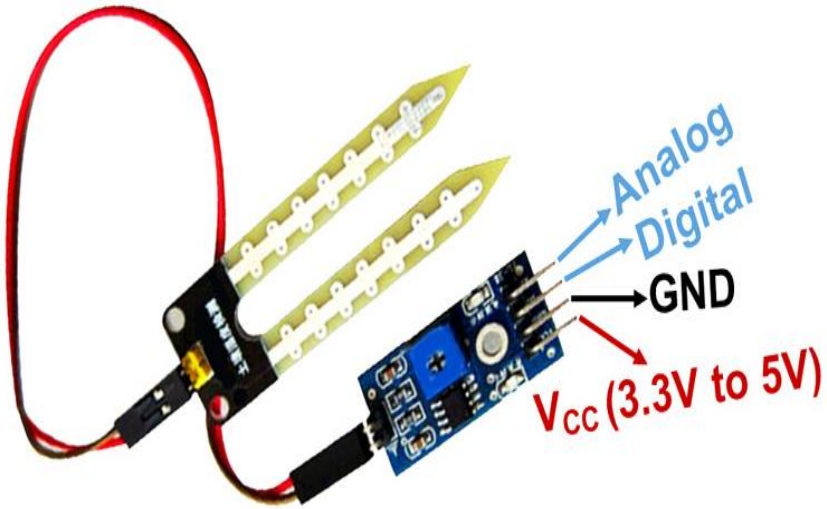

Figure 5: Soil Moisture Sensor

This module with a soil moisture sensor is used to recognize soil moisture. It measures volumetric water content in the soil and provides water levels as a result. The module has digital and analog outputs and potentiometers that adapt the thresholds [7].

Specifications:

Operating Voltage	3.3 V to 5 V DC
Operating Current	15 mA
Output Digital	0V to 5V
Output Analog	0V to 5V
LED	Indicate O/P and Power
PCB Size	3.2 cm x 1.4 cm

4. Humidity Sensor DHT11:

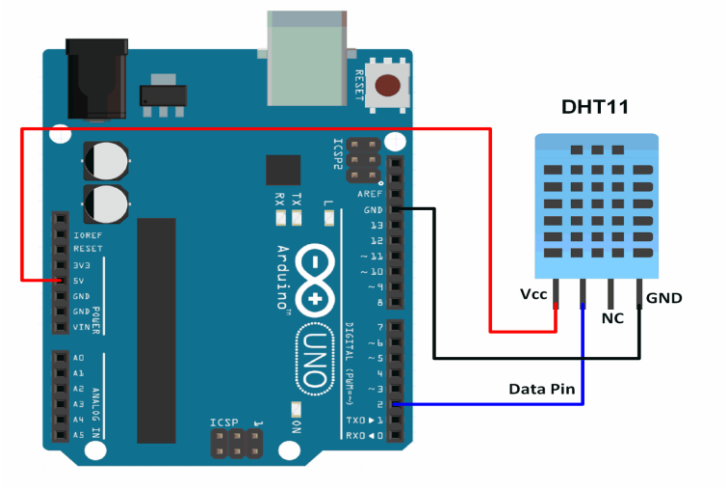

Figure 6: DHT 11 Humidity Sensor

The DHT11 is a cheap basic digital temperature and moisture sensor. This is a single wire digital moisture and temperature sensor, providing moisture and temperature values in the air through the wire protocol. The sensor provides temperature values in degrees Celsius (0-50°C) with relative air humidity values in percentage (20-90% RH). Uses the humidity resistant component and NTC temperature measurement components [8].

Pin Description:

Pin No.	Pin Name	Pin Description
1	VCC	Power supply 3.3 to 5.5 Volt DC
2	DATA	Digital output pin
3	NC	Not in use
4	GND	Ground

5. Arduino Uno:

A microcontroller board called Arduino UNO is built on the ATmega328P. It has 6 analogue inputs, a 16 MHz ceramic resonator, 14 digital input/output pins (six of which can be used as PWM outputs), a USB port, a power jack, an ICSP header, and a reset switch. It comes with everything required to support the microcontroller; to get started, just plug in a USB cable, an AC-to-DC adapter, or a battery [9].

Figure 7: Arduino Uno board

6. Relay:

Relays' primary purpose is to simultaneously serve as an ON and OFF switch. Relay is primarily used for switching, detecting, actuating, and other functions. From very tiny electronic circuits to very large high voltage circuits, relays are used for switching, protection, and sensing [10].

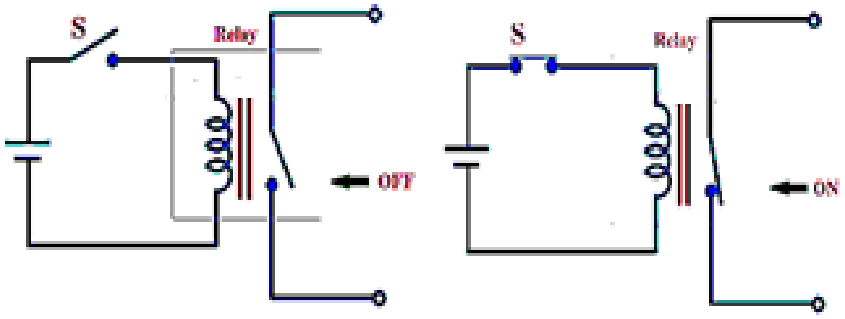

Figure 8: Relay Symbol

7. 20X4 LCD Display:

Liquid crystal display is referred to as LCD. It is a particular type of electrical display module used in a wide array of circuits and devices, including mobile phones, calculators, computers, TVs, and other electronics. These displays are mostly favored for seven segments and multi-segment light-emitting diodes. The main advantages of using this module are its low cost, ease of programming, animations, and unlimited ability to show custom characters, unique animations, etc [11].

Figure 9: 20X4 LCD

WORKING

The working of present system begins with the control of all the sensors, displays, motors and pump as per the signals received from Arduino UNO. The fan used in the system is used for cooling purpose, the fan is turned on as soon as the temperature of LM35 is rises greater than threshold value of 30 °C and the fan turns off as soon as the threshold value is less than 30 °C, the status of fan is shown on 20X4 LCD display. Another unit is the water pump used for watering the plants, it is controlled by soil moisture sensor. The water pump is turned on as soon as the soil moisture falls below threshold value of 40% and the pump turns off as soon as the soil moisture increases to 40%, the status of water pump is shown on 20X4 LCD display. Another sensor is the humidity sensor DHT 11, this sensor provides humidity and temperature values serially with one-wire protocol, the measured humidity is displayed on LCD display. Next sensor is the rain sensor which detects the presence of rain and controls the water pump. The pump is turned off as soon as the rain is detected and turn on as soon as the rain stops but with the condition that soil moisture should be less than 40% threshold. If we install IOT module or WiFi chip then we can transmit the various values displayed on LCD display on webserver or monitor the values on smart phone or check on the website using laptop or PC.

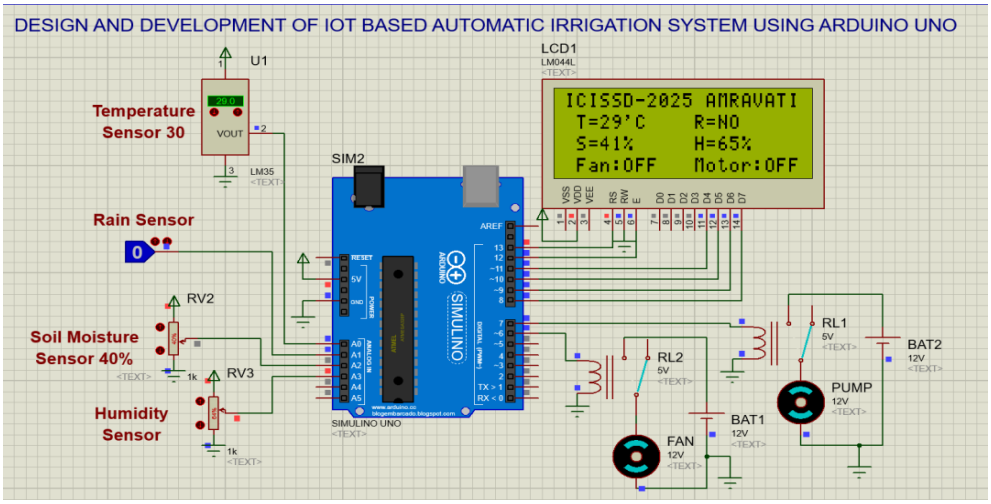

Figure 10: Complete schematic diagram

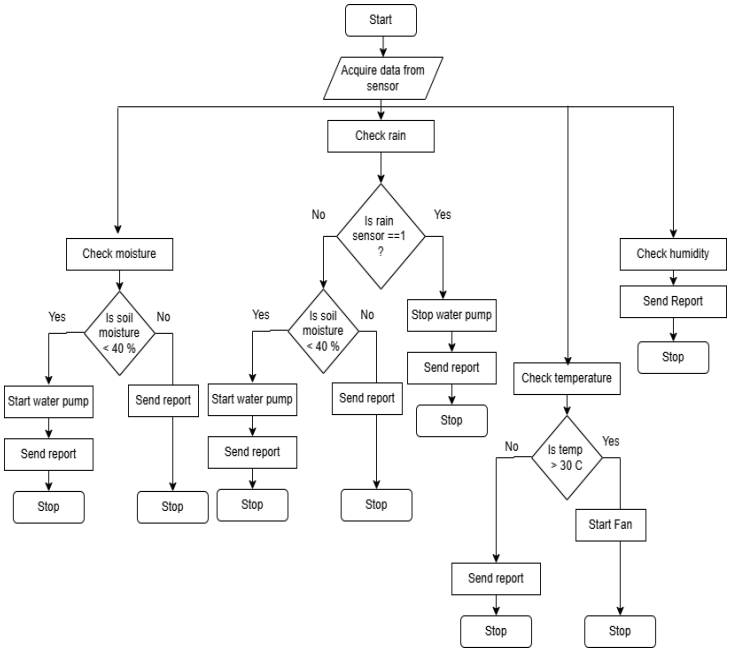

Figure 11: Flow chart

Above flow chart depicts the entire process of operations to be performed by the designed system. Various sensors such as temperature, rain, soil, humidity work under the control signals received from Arduino UNO, which in turn controls the fan and water pump. All the parameters of sensors and status of fan and water module are displayed on 20X4 LCD display and transmitted to website or mobile phone by using IOT module or WiFi Chip.

RESULT

In this paper we have designed system using Arduino UNO microcontroller board, Temperature sensor LM31, Rain Sensor FC 37, Soil Moisture Sensor SEN0114, Humidity Sensor DHT-11, LCD and relay. Designed system's objective is to detect the temperature, rain, soil moisture, humidity and microcontroller controls the fan and water motor according to inputs received from the various sensors. The output of various sensors and status of fan and motor is displayed on LCD display. The fan is turned on as soon as the temperature of LM35 goes above 30°C for the cooling purpose and the fan remains off until the temperature is below 30°C as shown in Fig below.

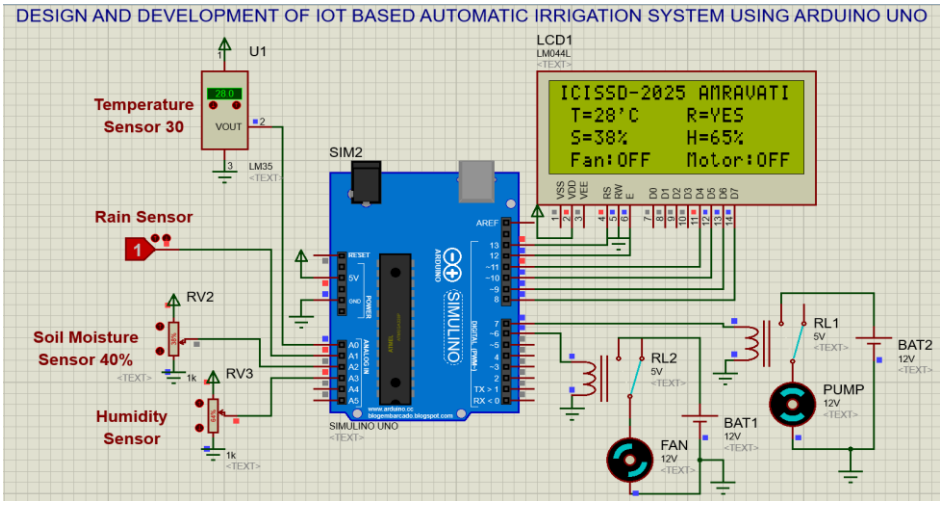

Figure 12: Temperature is 28°C, fan is OFF

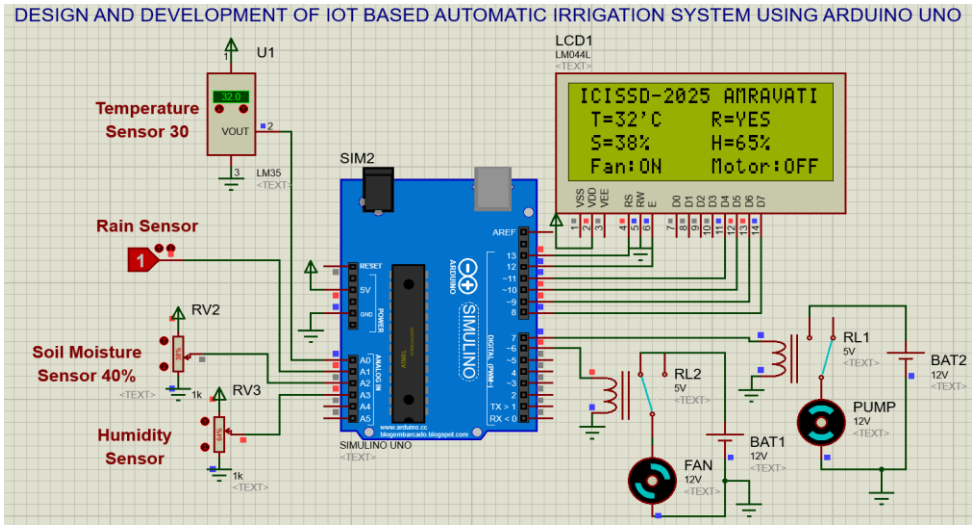

Figure 13: Temperature is 32°C, fan is ON

In case if the soil moisture is more than 40% of threshold value the water pump remains off as shown in fig below.

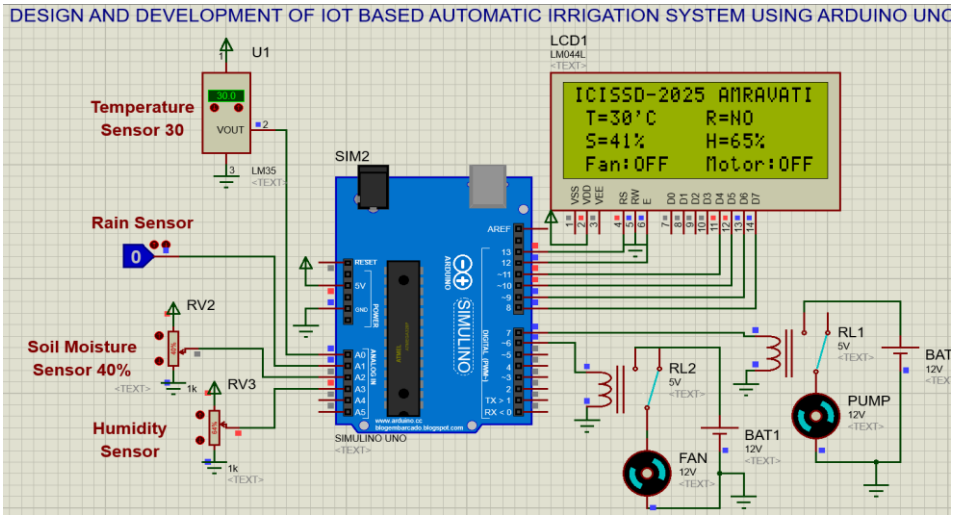

Figure 14: Humidity is 41%, motor is OFF

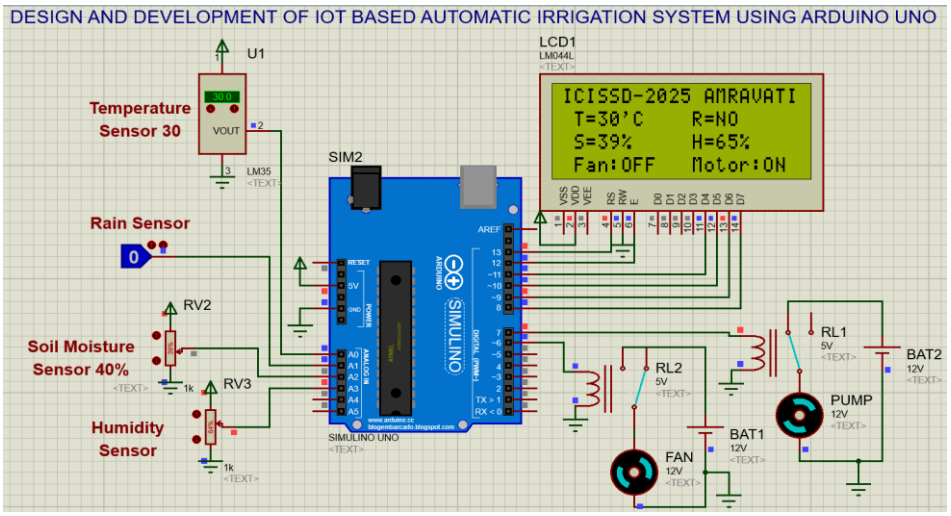

Figure 15: Humidity is 39%, motor is ON

In case rain sensor detects the rain the motor will remain off even though soil moisture is below 40% of threshold.

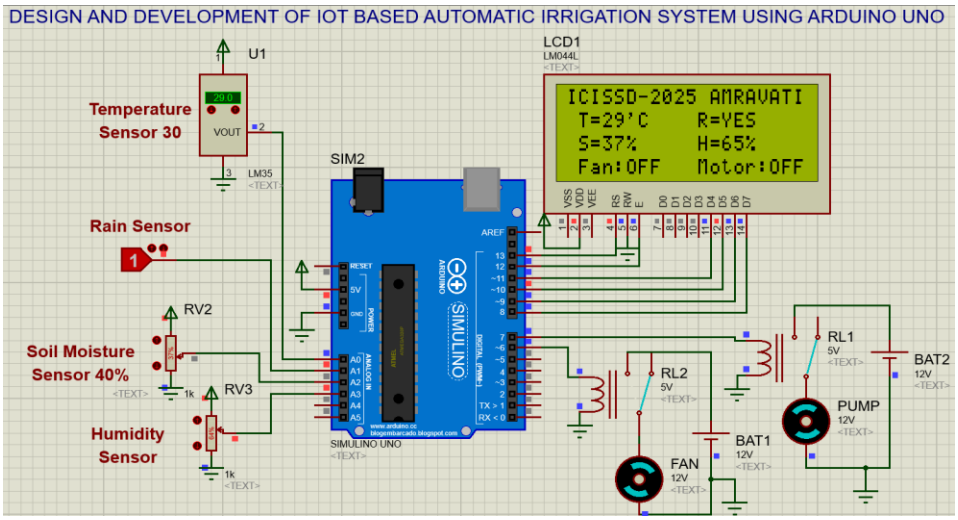

Figure 16: Motor OFF due to rain

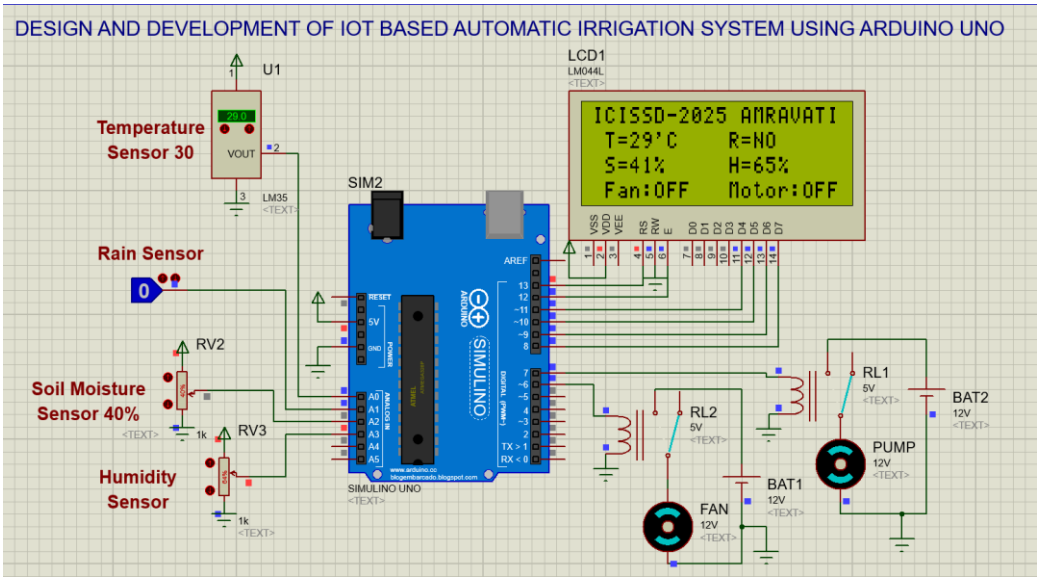

Figure 17: Use of humidity sensor

Another sensor, humidity sensor detects the humidity in the atmosphere and displays the sensor values on LCD display.

DISCUSSION AND CONCLUSION

The designed system of IOT based automatic irrigation system using Arduino UNO gives added advantages in water conservation and management in agriculture with optimum water usage and increase crop yield. The use of various electronic sensors helps in effective and real time tracking of environmental parameters and immediate solution. The designed system helps in real-time monitoring of environmental parameters to conserve water usage, resources and increase crop health and productivity. The use of IOT module helps in precise analysis of temperature, soil moisture, presence of rain, and atmospheric humidity. This leads to optimum usage of water for crops leading to less water losses and result in cost saving of farmers. The data received from the system helps in better decision making in irrigation strategies for future, type of crop selection and available resources management. The designed system provides promising solution for making optimum use of water, reducing wastage, and promoting effective use of environmental resources.

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Zooplankton Diversity of Shekhdari Dam Water in Warud Tahsil of Amravati District (M.S.)

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ABSTRACT

The study was carried out at Shekhdari dam in Warud tahsil of Amravati district belonging to state of Maharashtra. There was no back record found for diversity of zooplankton occurring in this dam. The analysis was taken into observation for the period of one year and five major groups of zooplankton were observed i.e., Rotifera, Ostracoda, Cladocera, Copepoda and Protozoa. Among them, most of the species belongs to Rotifera.

Keywords – Plankton, copepods, crustaceans, rotifera, Shekhdari dam, diversity, etc.

INTRODUCTION

Plankton include the free floating minute plant and animal organisms, that have very feeble locomotory organs and simply drift with the water currents. On the basis of size, plankton are divided into three kinds-macro-, micro-, and nano-plankton. The macro-plankton include organisms that are larger than 3 mm in size, and visible with the naked eye, such as larvae, mysids, salpa etc. The largest forms are also called 'megaloplankton'. The microplankton are forms below 3 mm in size, while the forms less than 60 micra in diameter are called nanoplankton. These latter can be collected by the finest mesh cloth and comprise of diatoms, protozoans and bacteria. Plankton are also classified as phytoplankton and zooplankton. Of these the phytoplankton includes organisms with chlorophyll such as Microcystis, Volvox etc., as well as non-photosynthetic plants like bacteria and fungi. It includes all the passively floating microscopic plants, diatoms and dinoflagellates. The zooplanktons are minute animals like the protozoans (radiolaria, foraminifera) rotifers, crustaceans like the copepods, ostracoda, amphipods, worms, eggs and larvae. The plankton may be of temporary nature (meroplankton). These consist of planktonic eggs and larvae, and are abundant during certain seasons only, depending upon the spawning habits of the parents. But due to considerable variation in the spawning time of different animal species, these plankton may be found during all seasons in small or large quantities. Planktons found throughout the year are called permanent holoplankton. Plankton show a number of adaptations to keep

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them floating in the surface water, and prevent sinking. For example, the cell is relatively large and becomes bladder-like, filled with a light fluid. Some are cylinderical hair-like, others are broad and flat like a ribbon, or may become branched with fine hairy projections.

Zooplankton plays an important role in aquatic ecosystem. They link the primary producers, phytoplankton with higher larger trophic level organisms. Zooplankton communities respond to a wide variety of disturbances including nutrient loading and also play a key role in the aquatic food chain. The zooplankton plays an integral role and serves as bioindicator and it is a well suited tool for understanding water pollution status. So this paper deals with the studies of zooplankton in lotic water of Shekhdari Dam. vital role in the food chain of fish as animal food, which supply amino acids fatty acids, vitamins (Akin-Oriola) 2003. Zooplankton is important aquatic organism occurring abundantly in all types of aquatic habits and plays a vital role in energy transfer in an aquatic ecosystem. It occupies an intermediate position in food web many of them feed upon bacteria and algae and in turn fed by numerous invertebrates, fishes and birds (Basu) 1996. There was no back record found about the zooplankton diversity of Shekhdari Dam in Warud tahsil of Amravati district, hence this task was undertaken. Zooplanktons are heterotrophic, minute aquatic organisms which play important role in food web. They are important link between primary producers and high tropic levels. Freshwater zooplanktons mainly contain protozoa, rotifers, cladocerans copepods, and ostracodes.

MATERIALS AND METHOD

The study site is located near the Gavankund village in Warud Taluka in Amravati district. (21°31'51"N 78°11'47"E). This dam is surrounded by open hills of Satpuda ranges. Official designation of Shekdhari dam irrigation Project is “Shekdhari Dam, D – 01383”. However loacal& popular name is ‘Shekhdari Lake/Shekhdari Talav’. It was constructed as parts of Irrigation Projects by the Government of Maharashtra in the year 1982. It is built on & impounds Shakti river. Nearest city to dam is Warud taluka, Warud in Amravati district of Maharashtra. The dam is an Earth fill dam. The length of dam is 730m (2395.01feet), while the height of the dam above lowest foundation is 30.36m(99.6062feet). Project has other type of spillway. Length of the spillway is 501.969m. The dam has ungated spillway. The dam’s catchment area is 3.51 thousand hecter. Maximum/Gross storage capacity is 5.204MCM. Live storage capacity is 4.54 MCM.

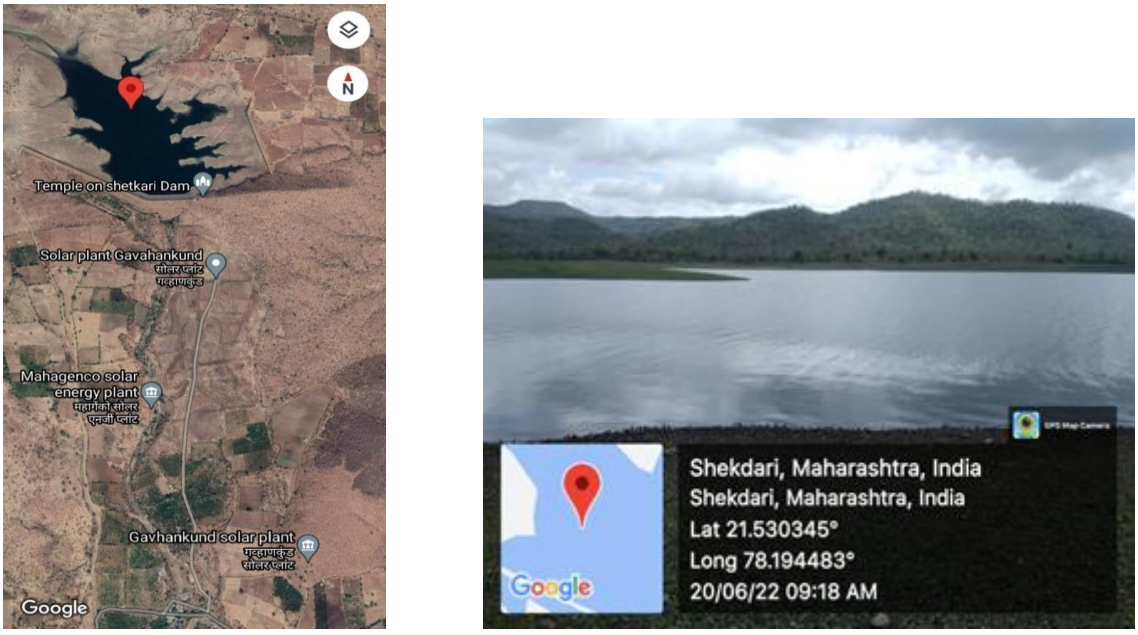

Fig., - Geographical location of study site

For the present investigation water samples were collected from the three sampling stations of Dam. The water was collected directly from each selected sampling station of Dam. The samples were transferred to the bottle and brought to the laboratory without disturbances. The water samples were collected by monthly intervals from the sampling stations for a period of one year (June 2021- June 2022) during morning hours. The zooplankton were collected by using zooplankton net and preserved with 5% of neutral formalin. Each planktonic replicate identified under the microscope with its standard identification and its monographs as well as keys which were suggested by APHA.

Senapati et al. (2011) studied the variation of phytoplankton diversity and its relationship with the physicochemical parameters of semi lentic water body Golapbag, West Bengal India Factors like nitrate, phosphate concentration support huge growth of Cyanophycean members and sometimes produces algal bloom. Plankton density reached its maximum level in monsoon time. All the physico-chemical parameters of the water were within the permissible limits and can be used for domestic, irrigation and pisciculture (Thirupathaiah et al. 2012).

Planktons, those are very sensitive and respond quickly to any changes in the environment which affects the plankton communities in terms of tolerance, abundance, diversity and dominance in the habitat. Therefore, it is observed that plankton act as pollution indicators to assess the pollution status of aquatic bodies (Onkarsingh and Sunil kumar, 2015). Zooplankton comprising of rotifers, cladocerans, copepods and ostracods are considered to be most important in terms of population density, biomass production, grazing and nutrient regeneration in any aquatic ecosystem. Their diversity and density is mainly controlled by availability of food as favorable water quality (Chandrasekhar and Kodarkar, 1997). According to Reid (1961), the plankton population on which the whole aquatic life depends directly or indirectly is governed by the interaction of a number of physical, chemical and biological conditions and the tolerance of the organisms to variations in one or more of these conditions. The water quality parameters and nutrient status of water play the most important role in governing the production of planktonic biomass.

OBSERVATION-

Through microscopic examination of water sample at different site of dam, following types of zooplankton were recorded and identified. The result showed monthly & seasonal variation in the diversity of planktons highest during March to June (summer season) & lowest during July to October (Monsoon season). Most frequently observed are the large size Cladocerans which moves by rowing action of their large size antennae in a series of jerks. Their bodies are enveloped by a translucent shell (bivalve carapace) because of which animal undergoes moulting periodically to shed their exoskeleton in order to grow, mature and reproduce. *Ceratopdaphnia* are abundant in water sample followed by rotifer. Increase in the population of zooplanktons during summer season probably due to evaporation of water molecule and increased in the level of organic material on which they feed. On contrary their low number during monsoon may be due to dilution of water body (due to the rainfall) and decreased level of organic matter.

Table no. 1 – List of some zooplankton found in Shekhdari dam

Sr. no.	Rotifera	Ostracoda	Cladocera	Copepoda	Protozoa
1	*Brachionus angularis*	*Cypris*	*Alonella*	*Cyclops*	*Arcella*
2	*B. calyciforus*	*Stenocypris*	*Ceratodaphnia*	*Diaptomus*	*Paramecium*
3	*B. candatus*	*Cyrinotus*	*Daphnia*	*Nauplius*	*Amoeba*
4	*B. rubens*	*Stenocypris fontinalis*	*Diaphanosoma*	*Neodiaptomus*	*Euglena*
5	*B.forficula*		*Simocephalus*	*Cyclops viridis*	*Vorticella*
6	*B. quadridentalus*			*Eucyclops agilis*	*Diffugia*
7	*B. falacatus*				
8	*B. bidentatus*				
9	*Keratella cochlearis*				
10	*K. tropica*				
11	*K. quadrates*				
12	*Filinia ovalis*				
13	*Asplanchna*				
14	*Rotarria*				
15	*Monostyla*				
16	*Lecane luna*				

RESULT AND DISCUSSION-

In the present investigation, zooplankton studied under five groups *that is* Protozoa, Rotifera, Cladocera, Copepoda and Ostracoda. The present study would give a preliminary knowledge on the diversity and productivity of zooplankton and the reasons for the variation in reservoir. This information can be utilized during the formulation of management measures to improve the productivity the reservoir. Among the five groups, maximum number of species belongs to Rotifera.

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Physicochemical and Ion Exchange Studies of Co- Polymer Derived From Polyaniline and Sulfanilic Acid Analysed With Ammonium per Sulphate

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ABSTRACT

A number of copolymers have been synthesizing by reacting aniline with Sulfanilic acid and ammonium persulphate as an oxidizing agent proved to be selective chelating ion exchange resin for certain metals. The present paper reports the synthesis, characterization and ion exchange properties of a copolymer. Ion exchange properties have been also studied for Fe2+, Cu2+, Ni2+, Co2+, Zn2+ ions. It was employed to study the selectivity of metal ion uptake involving the measurements of distribution of a given metal ion between the polymer sample and a solution containing the metal ion. The study was carried out over wide pH range and in a media of various ionic strengths. The PANA-SA co-polymer showed higher selectivity for Fe2+, Cu2+ and Ni2+ ions than for Co2+, Zn2+. The co-polymer synthesized was characterized by IR spectroscopy, XRD, UV spectroscopy.

Keywords: Polyaniline, Ion Exchange resin, The PANA-SA Co-polymer, pH

INTRODUCTION

Plastics are polymeric materials behaves insulator until recently. Conducting polymers a relatively new class of materials having interesting metallic properties was first reported in 1977, with the discovery of electrically conducting polyacetylene [1]. This was happened when a researcher accidentally added too much catalyst while synthesizing polyacetylene from acetylene gas, resulting in a shiny metallic like substance rather than the expected black powder. This shiny semi-conducting material was subsequently partially oxidized with iodine or bromine vapors resulting in electrical conductivity values upto 10^5 S cm^{-1} which is in the metallic range [2]. The importance of this discovery was recognized in 2000 when the Nobel Prize for Chemistry was awarded to the

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scientists Alan MacDiarmid, Alan Heeger and Hideki Shirakawa who discovered electrically conducting polyacetylene in 1977.

Since the discovery of polyacetylene, there has been much research into conducting polymers and many new conducting polymers have been synthesized. The most important, and common, of these are polypyrrole [3], polythiophene [4] and polyaniline [5]. There have been many potential applications suggested for these materials, including sensors [6-9], electrochromic devices [10-11] corrosion inhibitors [12-14], electrochemical actuators [15,16] electromagnetic shielding [17,18] polymeric batteries [19-21] and membrane separations [22-27]. This wide range of applications is possible due to the ability to alter the electrochemical, optical, chemical and mechanical properties of these polymers by changing the monomer and/or dopant incorporated into the polymer.

Conducting polymers as a class of materials have a number of properties in common, even though their structures can differ greatly. The chief property they have in common is the fact that, unlike traditional polymers, they conduct electricity. These polymers also possess a high degree of conjugation along the polymer chain [28]. This conjugation gives rise to the electrical conductivity as it allows the efficient transfer of electrons along the polymer backbone. However, this conductivity only exists when the polymer is in an oxidized state. The loss of an electron from a π-bond results in the formation of a radical cation or polaron charge carrier. Electrical conductivity arises from the delocalization of these charge carriers, which are capable of both inter- and intra-chain transfer. The positive charge that arises during the formation of the polaron charge carriers necessitates the incorporation of an anion into the polymer to maintain overall charge neutrality in a process known as doping. The anions that are incorporated can be anything ranging from small ions such as Cl^-, to more complex ions including proteins. The nature of the dopant has dramatic effects on the electrical, mechanical, physical and morphological properties of the polymer.

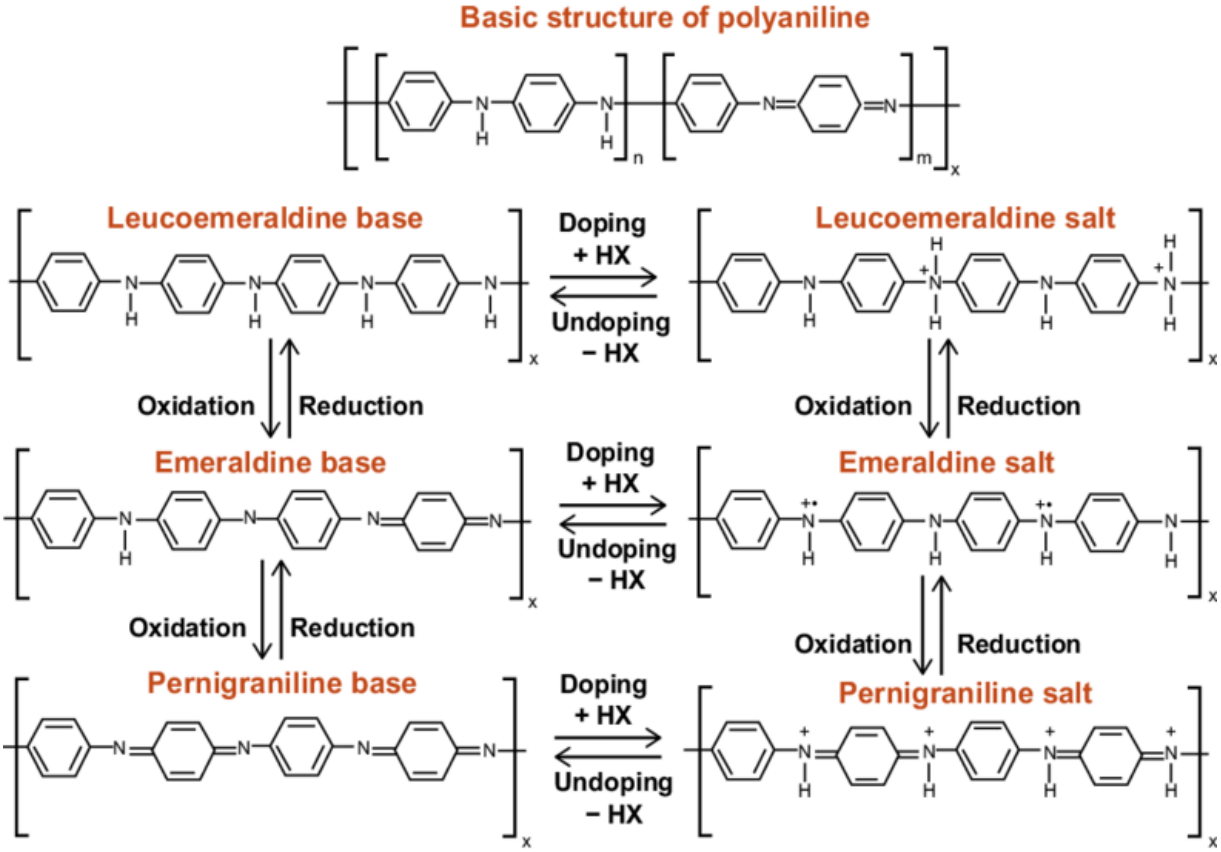


Figure 1: Different structure of Polyaniline

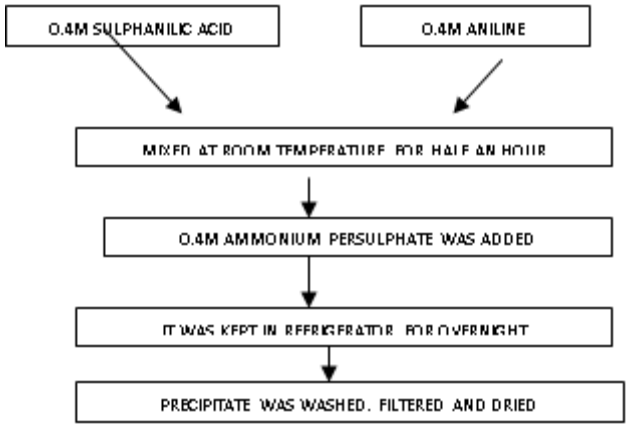
A. SYNTHESIS AND CHARACTERISTION

For the synthesis of co-polymer of aniline and sulphanilic acid, the chemicals with their source, molecular weight and purity are listed in

Table 1. The chemicals have been used as received (AR) grade. The detail of chemical used as

Chemicals	Acronym	Molecular weight	Purity	Source
Aniline	Ani	93.13	99.0	s.d. fine- Chem. Ltd
Ammonium persulphate	(NH4)2S2O8	228.2	99.0	s.d. fine- Chem. Ltd
Sulfanilic acid	C6H7NO3S	173.19	98.0	s.d. fine- Chem. Ltd

Synthesis by Chemical Method: Preparation of 0.4 molar aniline solutions, 0.8 molar of sulphanilic acid solution and 0.4 molar ammonium persulfate solutions was done. 0.8 molar a sulphanilic solution was dissolved in 100 ml of double distilled water. Add 0.4 molar solution of aniline to above solution. Both the solutions were stirred on a magnetic stirrer for half hour at room temperature. After complete mixing of both the solutions, ammonium persulphate which acted as an oxidant was added after 25 minutes, again stir for minutes and stop stirring. The solutions were kept in refrigerator overnight. Next day filter the solution on suction pump. Washed co-polymer with distilled water, then 50% methanol solution several times until the filtrate become colorless. Finally the product was dried in vacuum oven at 60^0c temperature for overnight. A greenish black salt of polyaniline was obtained. The graphical representation of the synthesis of co-polymer of polyaniline is shown in scheme.The procedure adopted for 1:1 proportion is adapted for other proportions such as 1:2 and 1:3 for Aniline to sulphanilic acid.

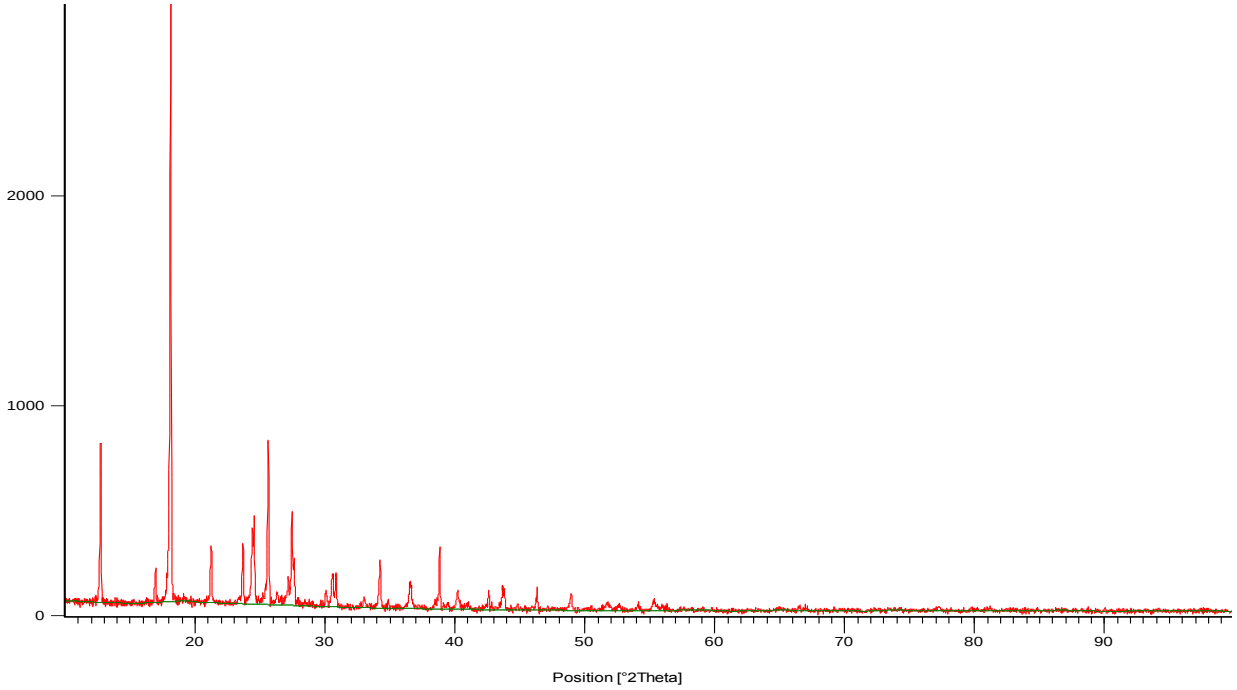


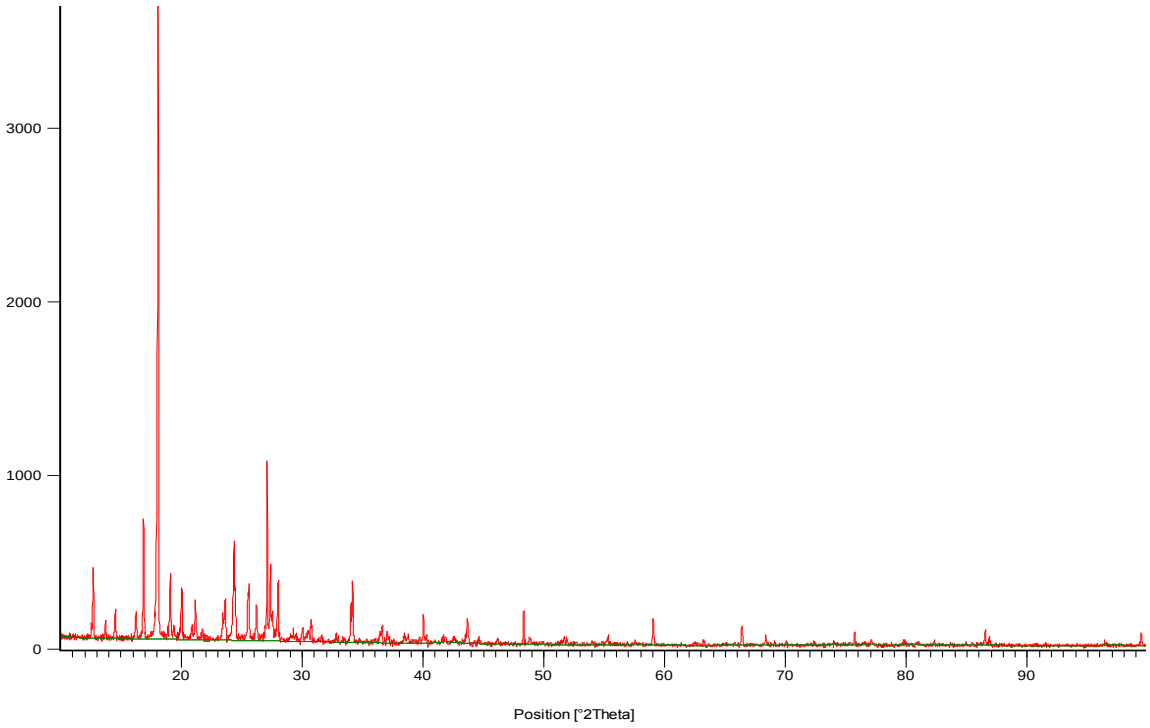
Flowchart of synthesis of co-polymer of Polyaniline and sulphanilic acid (1:1) by Chemical method

CHARACTERISATIONS:

XRD

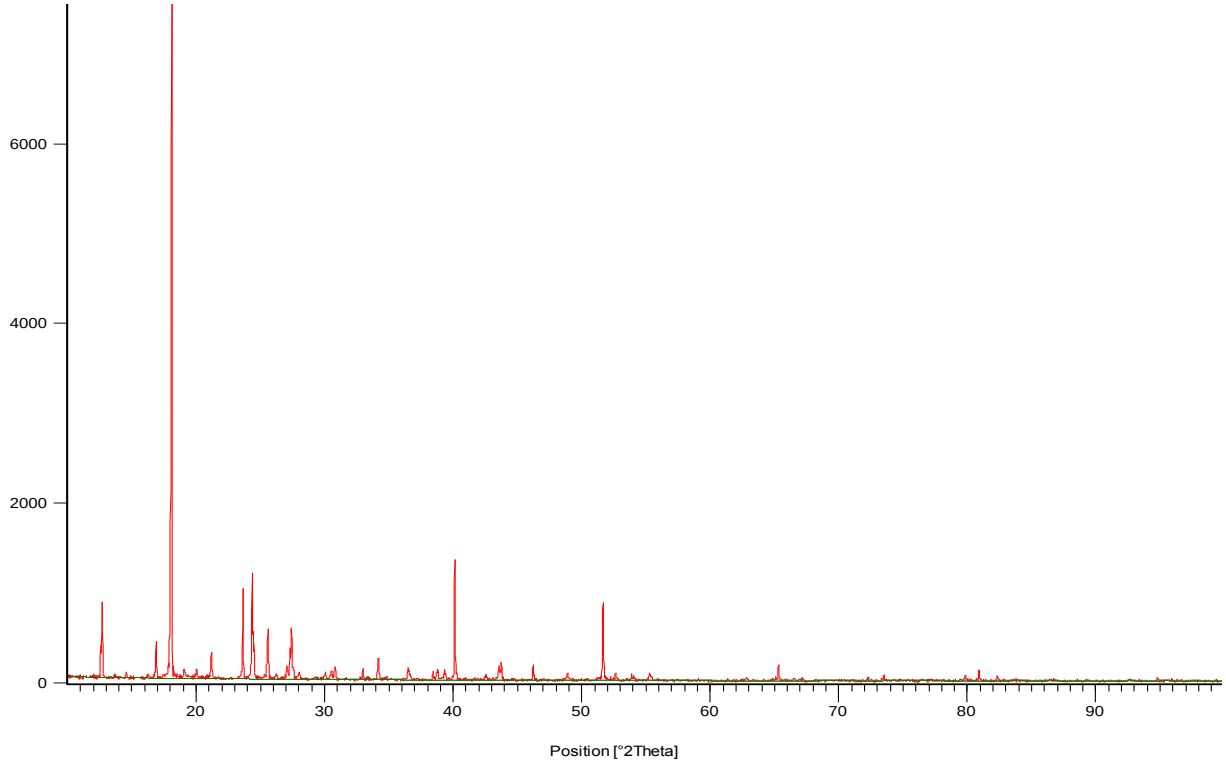
Physical characterization consists of spectroscopic analysis using fourier transform infra-red (ft-ir) and UV-visible spectrometer, thermal analysis (thermo gravimetric analysis), XRD, SEM, Electrical Conductivity, Ion Exchange and Adsorption and Electrochemical properties. As one can see in figure a to c (where the concentration of sulphanilic acid change) aniline doped with Sulphanilic acid having ratio 1:1, 1:2 and 1:3 shows crystalline nature. In addition, two broad bands observed at $2\theta=18^0$ and $2\theta=28^0$ which are ascribed to periodicity parallel and perpendicular to the polymer chains of PANI respectively. It is observed that as the concentration of sulphanilic acid increases the number of XRD peaks decreases may indicates the systematic orientation of molecule in a particular direction.

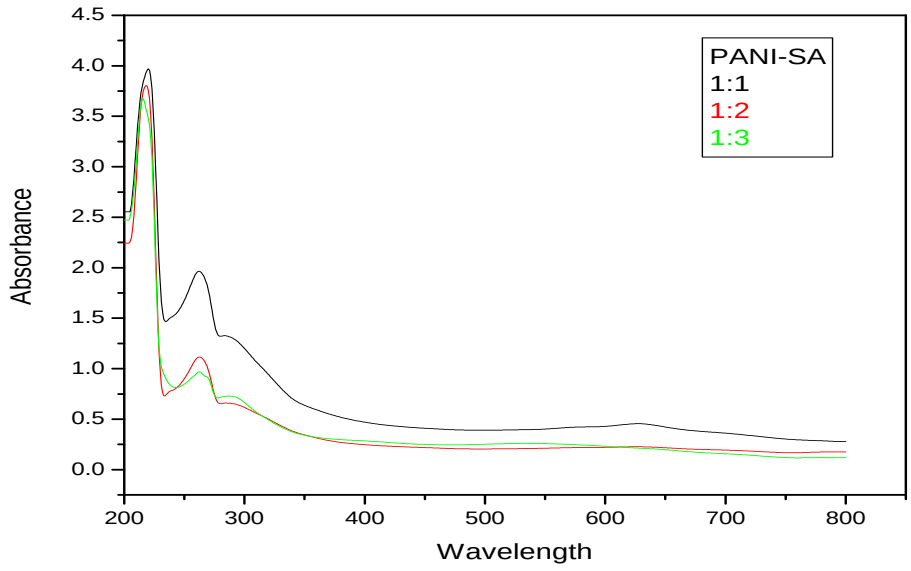




UV SPECTRA

The Uv-Vis Spectra of copolymer of polyaniline with sulphanilic acid shown in fig. prepared by chemical method exhibit more resemblance to the spectral features of aniline. The Spectrum of copolymer is dominated by two bonds: A strong absorption band at 270-360 nm and a broad band at 500-700 nm. According to the general practice of peak assignment, first peak is attributed to the Π-Π* transition of the benzenoid moieties in the copolymer linear structure or simply to the band gap of the copolymer [52]. The second peak closely resembles the benzenoid-quinoid transition in the copolymer [53-56]. To address the effect of monomer ratio in the synthesized copolymer, the polymerization was carried out in different ratios of sulphanilic acid to aniline.





UV-Visible spectra of copolymer of polyaniline with sulphanilic acid (1:1, 1:2, 1:3) by chemical method.

FT-IR

Figure (a to c) represents the FTIR spectra of co- polymer of polyaniline and sulphanilic acid. A broad band at 3441.86, 3472.80, 3448.64 and 3440.88 cm^{-1} in 1:1,1:2,1:3 prepared by chemical method and 1:1 prepared by hydrothermal method respectively assigned to the free N-H stretching vibrations and absorbed water. The band at 2946.91, 2883.70, 2943.12 and 2950.79 cm^{-1} in 1:1, 1:2, 1:3 prepared by chemical method and 1:1 prepared by hydrothermal method respectively shows the aromatic C-H stretching. The ring stretching vibration of quinoid (N=Q=N) was observed at 1575.38, 1575.38,1575.38 and 1574.91, cm^{-1} in 1:1,1:2,1:3 prepared by chemical

method and 1:1 prepared by hydrothermal method respectively. The characteristic peaks at 1400 cm^{-1} corresponds to benzenoid (N-B-N) in all four co-polymer was observed. The C-N stretching band of an aromatic amine appeared at 1318.17 cm^{-1} and 1299.40 cm^{-1} indicate the long chain length of the Polyaniline. The peaks at 1035-1040 cm^{-1} is caused by (S=O) stretching confirms the presence of sulphonate groups in all four co-polymer of polyaniline and sulphanilic acid. The S-O stretching peaks at 688.31 cm^{-1} and peaks at 633.61cm^{-1} represents C-S stretching vibration in all co-polymer of polyaniline and sulphanilic acid. The absorption band at 1040, 688, and 633 cm^{-1} in the FTIR spectra of PANI-SA co-polymer are constituent with the presence of $–SO_3H$ groups attached to the aromatic ring.

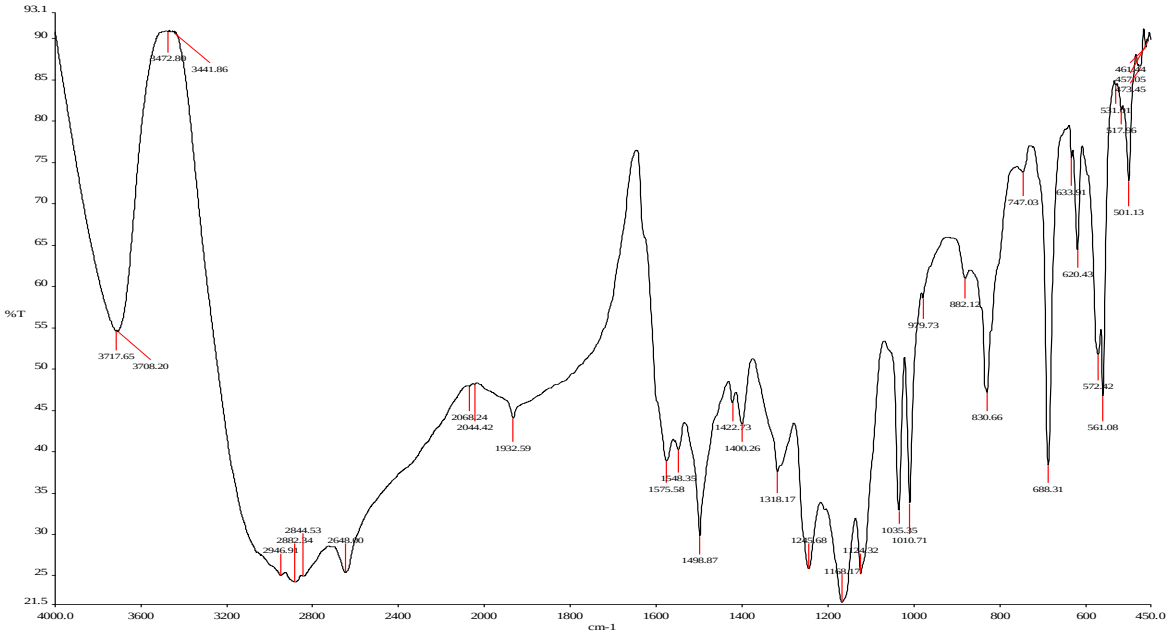


Fig.-a FT-IR spectra of copolymer of polyaniline with sulphanilic acid (1:1) by chemical method.

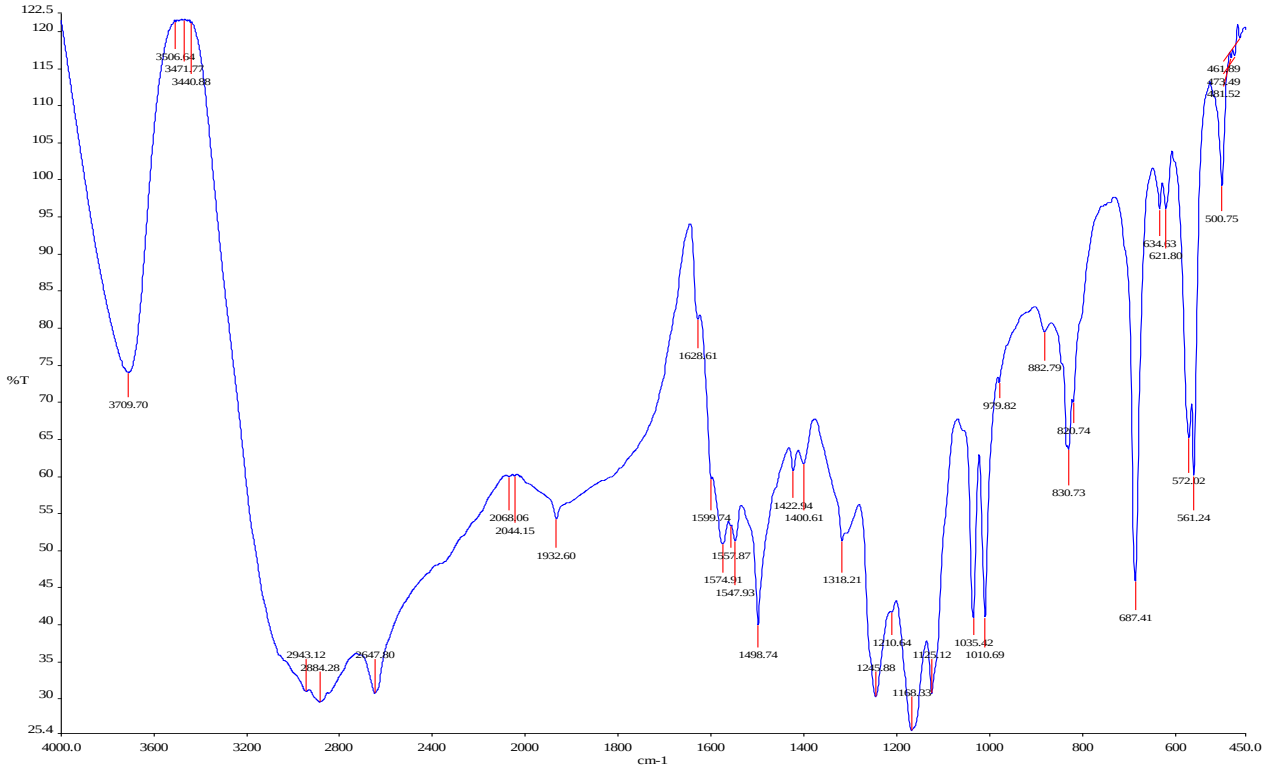


Fig. -b FT-IR spectra of copolymer of polyaniline with sulphanilic acid (1:2) by chemical method

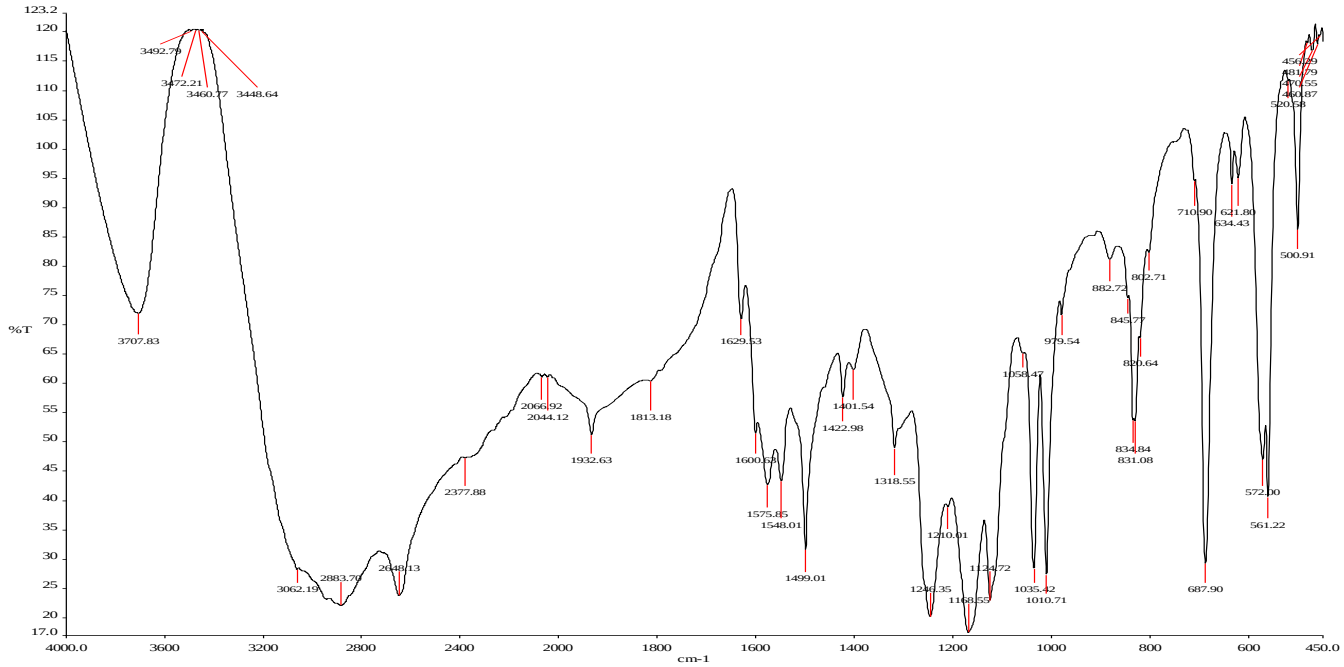


Fig.-c FT-IR spectra of copolymer of polyaniline with sulphanilic acid (1:3) by chemical method

SCANNING ELECTRON MICROSCOPY (SEM)

A scanning electron microscope (sem) is a type of electron microscope that produces images of a sample by scanning it with a focused beam of electrons. The electrons interact with atoms in the sample, producing various signals that can be detected and that contain information about the sample's surface topography and composition.

The morphological studies of copolymer of aniline and sulphanilic acid by SEM analysis were carried out at Cochin, the sample was percolated with platinum before scanning. The morphological study is very distinct and shows that there is variety of morphological feature observed in the copolymer. In the chemical method it is observed that as the concentration of sulphanilic acid increases in the copolymer the distinct morphology is observed. At 1:1 proportion there are no distinct morphological features of copolymer were observed and material is more aggregate form rather than distinct morphology. As the concentration of sulphanilic acid increases, that is for 1:2 proportions, the morphological feature was quite

distinct and aggregated globular morphology were observed. Further increase of concentration of sulphanilic acid that is for 1:3 proportions, the morphology is more distinct, and it is look like tubular or pipe like. It is observed that the aggregation of copolymer is less as compared to previews one. From the observation we assume that the presence of sulphanilic acid play an important role for the morphological feature of the copolymer.

In the hydrothermal method (Fig.-a to c) the morphological feature of polymer is completely distinct and tubular morphology was observed.

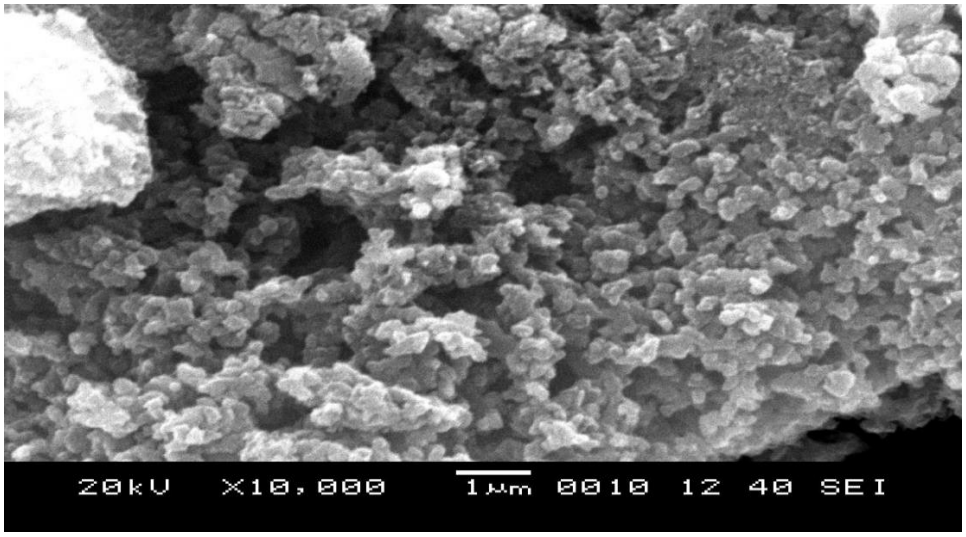


Fig.-A SEM images of 1:1 PANI-SA by chemical method

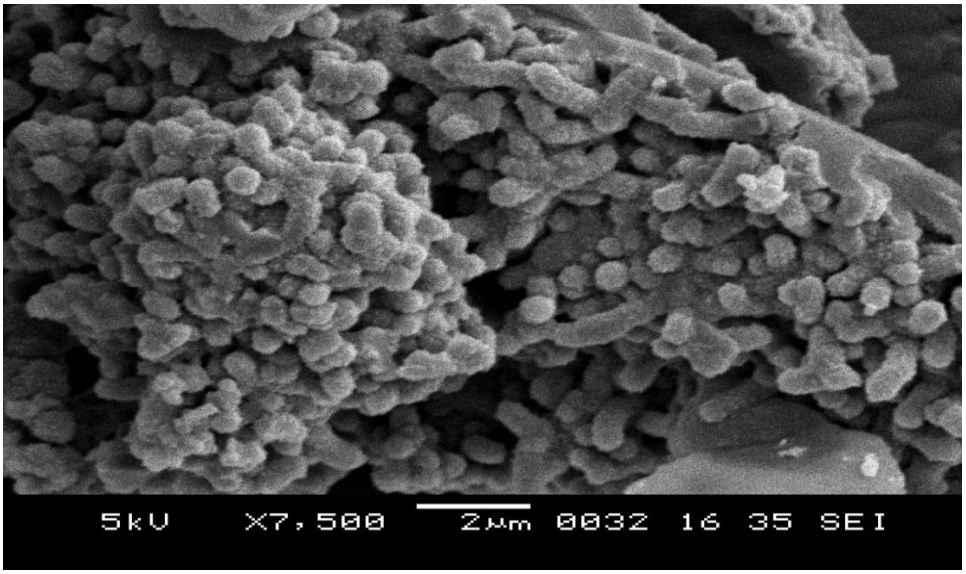


FIG.-B SEM IMAGES OF 1:3 PANI-SA BY CHEMICAL METHOD

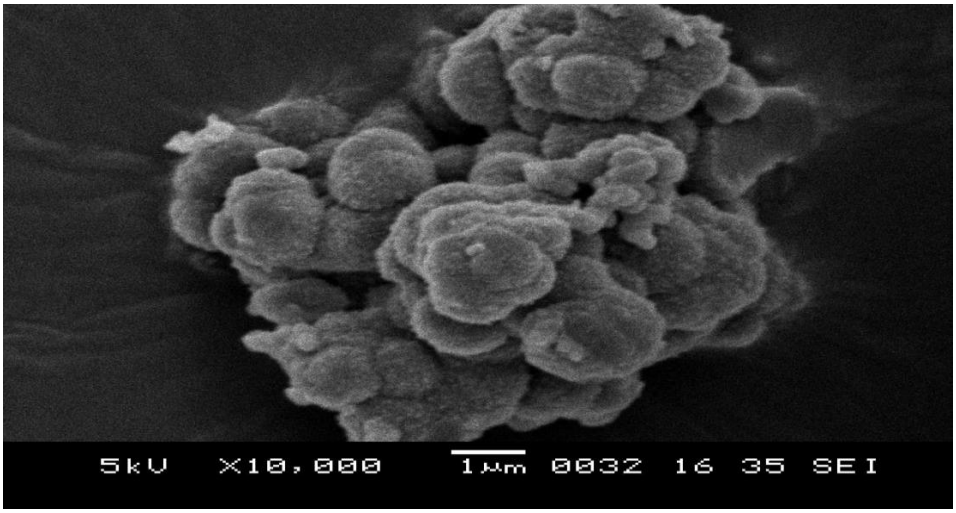


FIG. C- SEM IMAGES OF 1:2 PANI-SA BY CHEMICAL METHOD

APPLICATIONS:

TRANSITION METAL ION REMOVAL

The release of large quantities of heavy metals into the natural environment has resulted in a number of environmental problems. Toxic metals can be distinguished from other pollutants, since they are not biodegradable and can be accumulated in nature. They also cause various diseases and disorders when exceed specific limits [**57, 58**]. Zinc is one of the most important pollutants for surface and ground water. Because of its acute toxicity and non-biodegradability, zinc-containing liquid and solid wastes are considered as hazardous wastes [**59, 60**]. The nickel ion, compared with other heavy metals, is a more recalcitrant pollutant [**61**]. As it is widely used in many industrial processes, removal of nickel from wastewaters gains importance. Metal treatment industries containing nickel in discharged waters, frequently use nickel in its sulfate form [**62**]. This affects the decision of treatment method used for removal of nickel from wastewaters. Classical techniques of heavy metal removal from solutions include the following processes: precipitation, electrolytic methods, ion exchange, evaporation and adsorption [**63**]. Among these methods ion exchange receives considerable interest with high efficiency and low operational costs. The main advantages of ion exchange over chemical precipitation are recovery of metal value, selectivity, less sludge volume produced and the meeting of strict discharge specifications [**64**].

Analytical grade reagents were used in experimental studies. Nitrate salts of test metals ($Zn(NO_3)_2 \cdot 6H_2O$, $Cu(NO_3)_2 \cdot 6H_2O$ and $Ni(NO_3)_2 \cdot 6H_2O$ from Merck) were used for preparing certain concentrations of synthetic solutions. pH adjustments were carried out by using 0.1N HCl and 0.1N NaOH. Copolymer prepared by hydrothermal method was preferred as ion exchangers are durable, insoluble and compatible. UV3000$^+$ spectrophotometer was used for the determination of remaining metal concentrations in solutions. (Batch experiments were carried out in shaker. Testo pH-meter was used for pH measurements. The batch ion exchange experiments were performed in a wide variety of conditions including different pH, various resin dosages and agitation periods. Effects of each factor were determined keeping other variables constant. In the experiments 100 ml of synthetic solutions containing 100mg/L of Ni(II), Cu(II) and Zn(II) were added into flasks with different amounts of copolymer varying between 0.25 and 1.0 g. pH adjustments were made by using 0.1N sodium hydroxide and 0.1N hydrochloric acid. Solutions were shaked at 200 rpm for a predetermined period. Temparature was kept constant at 27 ◦C during batch tests. At the end of agitation time copolymer were filtered and metal contents of solutions were analyzed by spectrophotometer.

Hydrogen ion concentration is an important parameter affecting the ion-exchange process. This is partly because hydrogen ions themselves are strongly competing adsorbate and the solution pH influences the ionization of surface functional groups. In order to investigate the effect of pH on removal of nickel copper and zinc by copolymer 100ml of 100 mg/L metal solutions were used. Experiments were performed in the pH range 2–9. Constant copolymer amount (0.5 g) was added to all reaction bottles and solutions were agitated for 1 h at 200 rpm speed. Effect of pH on removal efficiency.

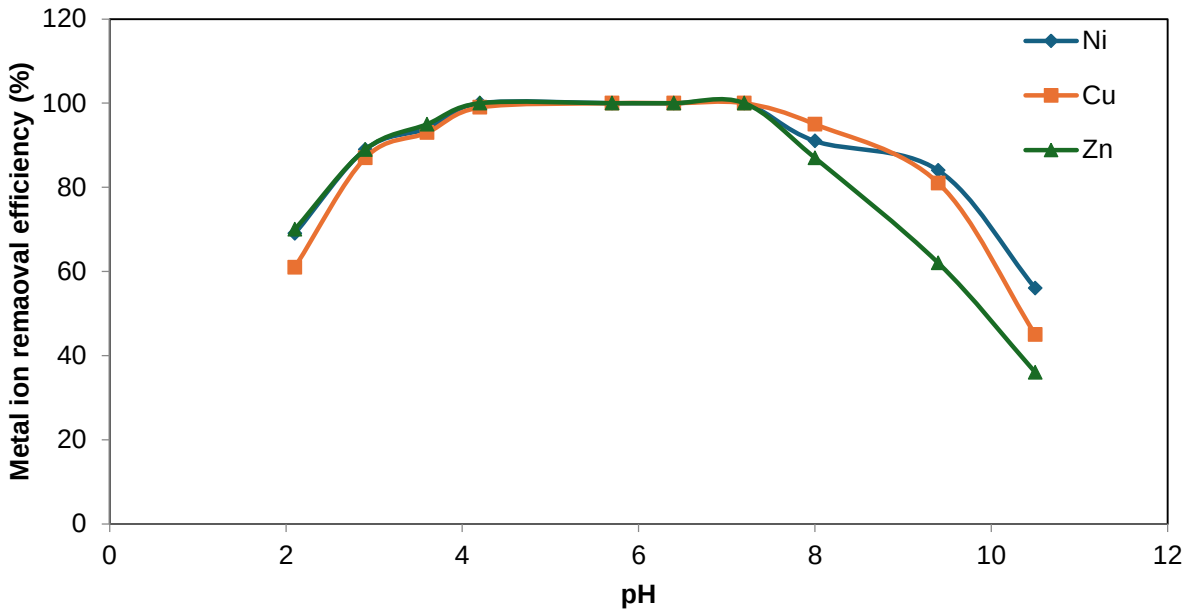


Fig. Effect of pH on Ni^{2+}, Cu^{2+} and Zn^{2+} ions

As seen from Fig that optimal uptake of Ni^{2+}, Cu^{2+} and Zn^{2+} occurred at pH ranges from 4 to 7. At high pH values, decrease in removal efficiency achieved by copolymer can be described with formation of metal hydroxide during reaction of Ni^{2+}, Cu^{2+} and Zn^{2+} ions with OH^-. In this state, hydrolysis accompanied by precipitation of metal hydroxides may occur. At lower pH may be a competitive reaction between H^+ ion and metal ion to exchange.

It was apparent that the adsorption percentage of metal ions increased with higher copolymer dosages and the removal efficiency of 100%was achieved by using 0.75g/100mL copolymer dosage for all metal ions. From fig, it was proved that increasing the amount of adsorbent provides higher removal due to formation of greater adsorption sites. Predetermined optimal values of pH and copolymer dosage were used for analyzing effects of time on removal process.

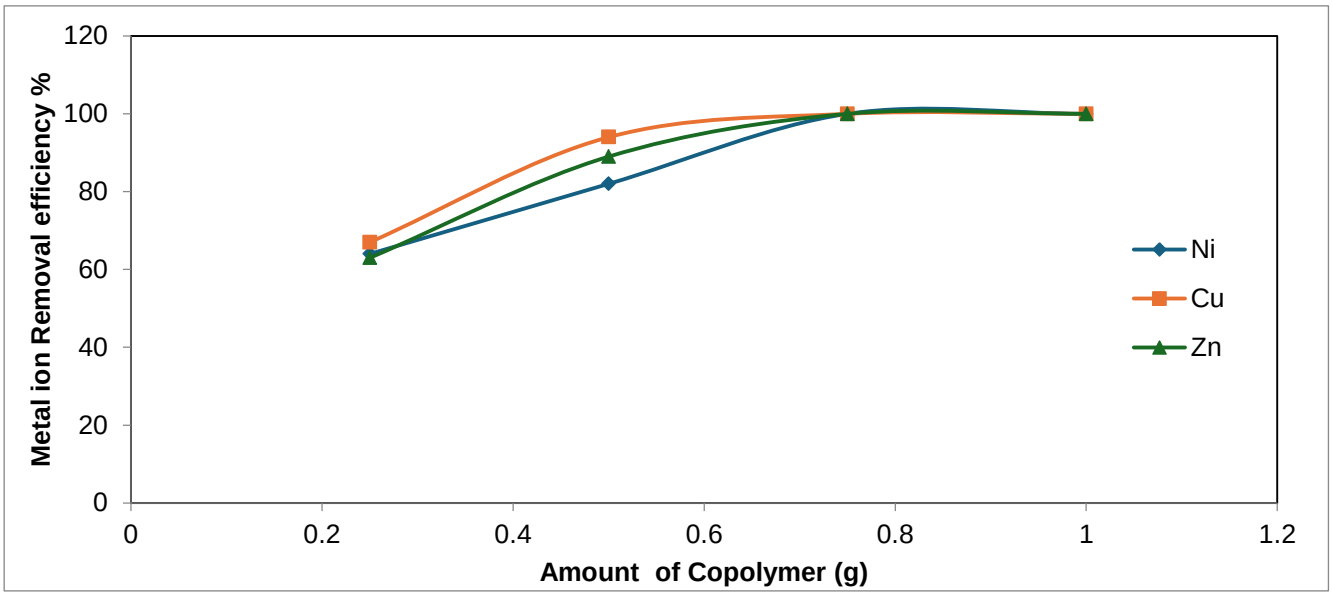


Fig.Adsorption of Ni, Cu, Zn ions on PANI-SA

The removal increases with time and attains equilibrium in 10 min for nickel, 12 min for Copper and in 15 min for zinc with initial concentrations of 100mg/L. It is clear that complete removal of nickel ions requires less residence time compared to copper and zinc.

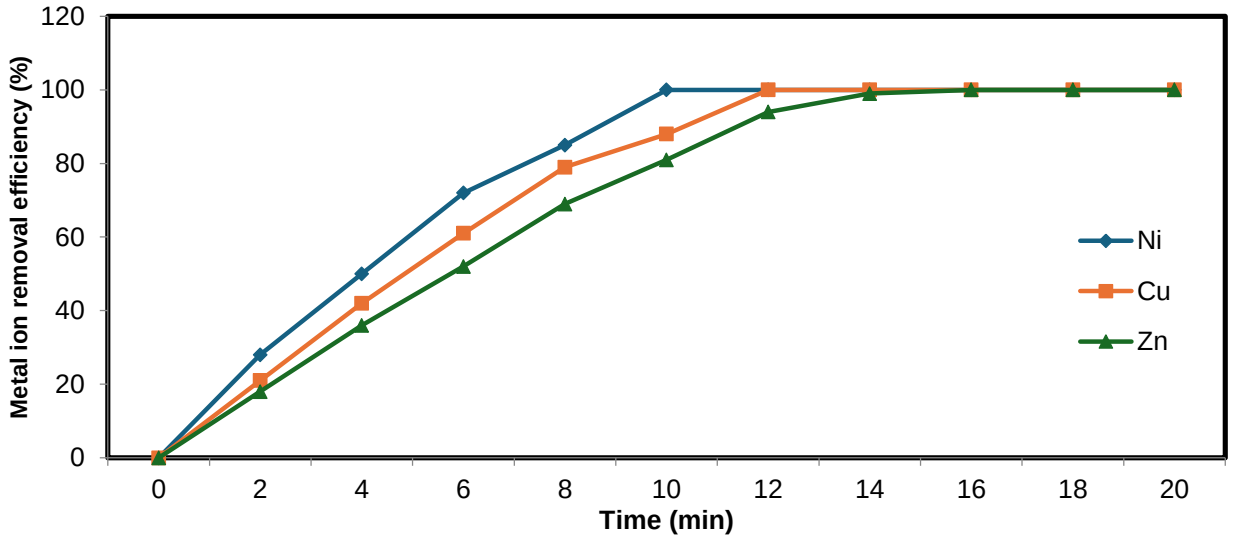


Fig. Dependence of removal efficiency of metal ions with agitation time

Result and discussion

Copolymer of sulphanilic acid and aniline was prepared for various proportions. In chemical method, the product was obtained for all proportions. The characterization of copolymer of polyaniline with sulphanilic acid is carried out by different techniques such as XRD, UV-Visible Absoption Spectroscopy, FTIR. When we apply the chemical method, it is observed that as the concentration of sulphanilic acid increases the number of XRD peaks decreases may indicates the systematic orientation of molecule in a particular direction. As we increases the concentration, the randomness in the structure may decrease. In a chemical method no much difference in the XRD spectra with change in the concentration of sulphanilic acid with reference to crystalanity is observed. We assume that the prepared copolymer has good ion exchange properties and hence it is used further for some environmental application Copolymer material was good enough to exchange the metal ion such as Ni^{2+}, Cu^{2+} and Zn^{2+} and order is $Ni^{2+}>Cu^{2+}>Zn^{2+}$.

Table-2 The comparative result of removal of metal ions with time are shown in following table.

Conclusion and Future prospect:

Sr. No.	Metal ion removal efficiency by co-polymer of PANI-SA	Time in min
1	Ni^{2+}	10
2	Cu^{2+}	12
3	Zn^{2+}	15

Copolymer of aniline and sulphanilic acid prepared by chemical method and it is suitable as a material for metal ion exchange. The material prepared in this study has remarkable properties and more study is required to understand the better chemistry.

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Spectroscopic and Antimicrobial Analysis of $Sr_xMn_{1-x}Fe_2O_4$ (X= 0.2 & 0.4) Nanoparticles Synthesized by Sol Gel Citrate Method for Wound Healing Therapy

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ABSTRACT

To explore the potential of spinel ferrite nanoparticles in wound healing therapy, a series of Sr-doped $MnFe_2O_4$ nanoparticles were synthesized by facile sol gel citrate method. The $MnFe_2O_4$ nanoparticles were doped with 0.2 and 0.4 % strontium (Sr) to evaluate and modify the optical, structural, elemental and antimicrobial properties. X-ray diffraction, Scanning Electron microscopy and EDS were studied to validate the structure, morphology and elemental composition and confirm the alterations in lattice parameters with crystalline size of around 30 nm due to doping of strontium (Sr). The lattice strain and dislocation plot was also studied. The presence of different chemical bond was confirmed using Fourier-transform infrared spectroscopy (FTIR) techniques. The decrease in band gap value (1.44-1.33eV) due to the incorporation of Sr3+ ions, were investigated through UV-Visible spectrum. To study the efficacy of synthesized Sr-doped $MnFe_2O_4$ nanomaterials in wound healing process the antimicrobial activity against various pathogenic strains were carried out, which demonstrated the effective inhibitory growth exhibiting notable antimicrobial activity. Due to all these multifaceted properties of Sr doped MnFe2O4 hold promise for biomedical applications especially in wound healthy therapy.

Keywords- Spinel ferrite, Sr-doped $MnFe_2O_4$, Antimicrobial, wound healing therapy, Lattice strain, and dislocation plot.

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INTRODUCTION

In science and technology, nanomaterials play a vital role in nanomedicine by giving a new approach to antibiotic resistance microbes. Because of the unique physical, chemical, mechanical and catalytic properties of the nanoparticles they can used in therapeutic tools to treat infections against microbes. Out of all types of nanoparticles, metal oxide due to its non-toxic effects of mammalian cells[1] are most widely used as antimicrobial agents. These nanoparticles due to their nano size permeate the bacterial cell to damage the cell membrane of microorganisms, which leads to inhibition of bacterial growth. Compared to other organic nanoparticles, metal oxide nanoparticles are more stable, durable, complex and less toxic and thus exhibits effective antimicrobial properties.

Due to high surface area, magnetic character, chemical stability and ability to interact with the biological systems, $MnFe_2O_4$ ferrite nanoparticles have been extensively studied. A well-known family of scientific material with high electrical resistivity, unique magnetic property and enhanced structural and morphological effectiveness which is recently been studied on a wide scale is Spinel ferrites. The general formula for cubic spinal structure-based ferrite is MFe_2O_4 (M= Zn, Mn, Co). The two distinct sites occupied by M^{2+} and Fe^{3+} ions in metal cations denotes tetrahedral and octahedral holes with FCC oxides (O^{2-}) . Ferrite nanoparticles have three different crystal structures like normal, inverse and mixed. The normal ferrite structure has M^{2+} in tetrahedral site and Fe^{3+} ions in octahedral site with general formula $(M^{2+})_A(Fe_2^{3+})_AO_4^{2-}$ while inverse spinel structure are inversely distributed with general formula[2], $(Fe_2^{3+})_A(M^{2+}Fe^{3+})_BO_4^{2-}$.

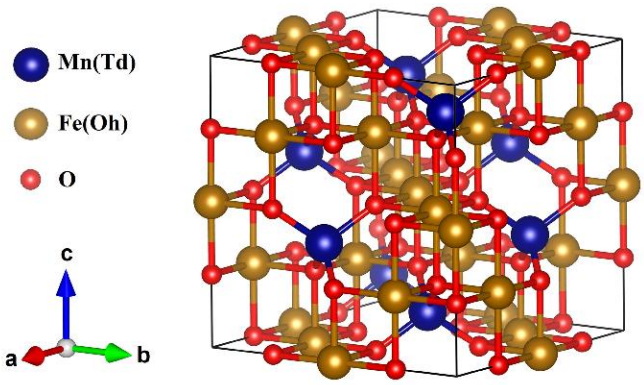


Figure 1 Crystal Structure of normal spinel $MnFe_2O_4$ nanoparticles

$Sr_xMn_{1-x}Fe_2O_4$ nanoparticles due to enhanced antimicrobial activity against gram positive, gram negative along with fungal strains makes them potential agent in **dressing and** wound healing therapy to treat infections due to the presence of Sr^{2+} ions. Wound healing involves the repair of damaged tissues in a complex physiological process. Due to presence of chronic wounds the cell gets damaged and antibiotic resistance increases and to recover this damaged cell antimicrobial agents plays a vital role and $MnFe_2O_4$ nanoparticles due to multifunctional properties have been extensively studied[3]. Doping the metal oxide ferrite nanoparticles with strontium ions improves the antimicrobial activity of the synthesized nanoparticles as it is a biocompatible metal ion with role in tissue regeneration and bone metabolism. When different concentration Sr is incorporated in $MnFe_2O_4$ nanoparticles it improves the magnetic properties and stimulates the bacterial growth. The Sr^{2+} ions have the ability to kill the bacterial by targeted heating and promoting the healing in infected wounds. These nanoparticles due to their magnetic properties generate localized heat and target the cancer cell and selectively kill these sensitive cells and thus we can say that Sr-doped $MnFe_2O_4$ nanoparticles can also be used in hyperthermia therapy[4,5].

EXPERIMENTAL DETAILS

2.1 Synthesis of Pure $MnFe_2O_4$ nanomaterials

The spinel ferrite pure $MnFe_2O_4$ nanoparticles were prepared by using the sol-gel citrate method. A stoichimetric mixture of manganese nitrate tetrahydrate ($Mn(NO_3)_2{\cdot}4H_2O$) and ferric nitrate nonahydrate ($Fe(NO_3)_3.9H_2O$) in the ratio of 1:2 was taken. To this mixture citric acid was added in the amount of 1:3 mole ratios to the metal ions of Mn^{2+} and Fe^{3+} present and thus the actual molar ration of the reaction mixture becomes 1:2:3. The mixture is dissolved in the ethylene glycol and was properly mixed. This mixture was then stirred on a magnetic stirrer continuously for 3 hours at 80°C to obtain a homogenous and transparent solution. The solution was further heated in a pressure vessel at 130^0 C for about 12 hours to form gel like solution. Then the gel is subjected to heat treatment at 350^0C in a muffle furnace to get the dried fine powder. The dried powder was then calcinated further in the range of 450^0C to 650^0C in order to improve the crystallinity of the synthesized $MnFe_2O_4$ nanoparticles.

2.2 Preparaion of ($Sr_xMn_{1-x}Fe_2O_4$) nanoparticles (x= 0.2, 0.4)

The nanocrystalline Sr doped Manganese ferrite nanoparticles ($Sr_xMn_{1-x}Fe_2O_4$) where (x= 0.2, 0.4) were prepared by using the sol-gel citrate method. A stoichimetric mixture of strontium nitrate ($Sr(NO_3)_2$), manganese nitrate tetrahydrate ($Mn(NO_3)_2{\cdot}4H_2O$) and ferric nitrate nonahydrate ($Fe(NO_3)_3 \cdot 9H_2O$) was taken in such a way that the molar ratio of Sr^{2+} and Mn^{2+} ions can match the actual ratio of $Sr_xMn_{1-x}Fe_2O_4$. To this mixture citric acid was added in equimolar amount of 1:1 ratio. Slowly add ethylene glycol so that this mixture gets dissolved in it. This mixture was then stirred on a magnetic stirrer continuously for 3 hours at 80°C to obtain a homogenous and transparent solution. The solution was further heated in a pressure vessel at 130^0 C for about 12 hours to form gel like solution. Then the gel is subjected to heat treatment at 350^0C in a muffle furnace to get the dried fine powder, which is free of organic components. The dried powder was then calcinated further in the range of 450^0C to 650^0C in order to improve the crystallinity of the synthesized Sr doped $MnFe_2O_4$ nanoparticles.

The synthesized nanoparticles was characterized using XRD which reveals that the nanoparticles calcinated at 650^0C exhibits better crystallinity and thus for further studies these samples were used. FTIR, UV, SEM and EDS were examined and antimicrobial studies were carried out to study the biomedical applications.

RESULT AND DISCUSSION

3.1 X-Ray Diffraction Analysis

XRD pattern of synthesized managnese ferrite and Sr doped managnese ferrite were obtained at room temperature. The scanning angle 2θ was varied from 20-80 degree. X-ray diffraction data were recorded by using Cu Kα radiation (1.5406 A^0) from a copper target which is the most common X-ray source for the measurement of XRD. To measure the average size of the nanoparticles a power XRD pattern was used. The crystallite size of prepared pure $MnFe_2O_4$ and Sr doped $MnFe_2O_4$ nanostructured was estimated using the full width at half maximum (FWHM) of the peaks by means of the Scherrer formula,

$$d = \frac{k\lambda}{\beta \cos\theta}$$

Where,

d is the average crystallite grain size

β is the full width half maximum(FWHM) in radian

θ is the Bragg angle

λ is the wavelength of X-rays which is 0.15406 nm for Cu target Kα radiation

k is shape factor[6] .

Furthermore, from the obtained XRD data different related physical properties such as lattice parameter, disslocation density (δ) and lattice strain (ε) of the synthesized nanospheres were also calculated and summarized. The calculation was carried out using the following equation,

$$D = \frac{0.9\,\lambda}{\beta .\ cos\,\theta} \qquad (1)$$

$$a^2 = \frac{\lambda^2}{4\,.\,sin^2\,\theta}(h^2 + k^2 + l^2) \qquad (2)$$

$$\delta = \frac{1}{D^2} \qquad (3)$$

$$\varepsilon = \frac{\beta\,.\,cos\,\theta}{4} \qquad (4)$$

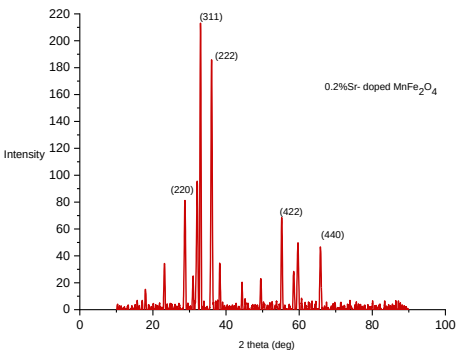
Where, a= lattice parameter

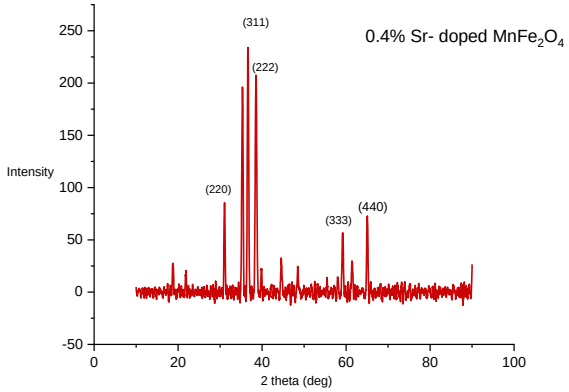
δ= dislocation density

hkl = Miller Index

ε= lattice strain

Figure 2 shows the X-ray diffraction pattern of pure and strontium doped $MnFe_2O_4$ nanoparticles with general formula $Sr_xMn_{1-x}Fe_2O_4$ (x= 0.2 and 0.4). The peaks obtained approximation between 23.4, 33.1, 49.52, 54.12 and 62.43 coordinate with (220), (311), (400), (422) and (440) out of which the main peak was marked at (311) and matched with the previous studies which at done by Setiadi *et al* , 2018[7]. The results indicate that the synthesized $MnFe_2O_4$ exhibits cubic spinel FCC structure. Doping does not affect the crystal structure and $MnFe_2O_4$ samples were substituted successfully by Sr^{2+} ions[8]. All the data matches with the JCPDS card No of 2101169, 1538523 and 9002330 for pure $MnFe_2O_4$, $Sr_{0.2}Mn_{1-0.2}Fe_2O_4$ and $Sr_{0.4}Mn_{1-0.4}Fe_2O_4$ respectively. The obtained crystalline size also gets reduced from 24.10nm to 23.35nm.





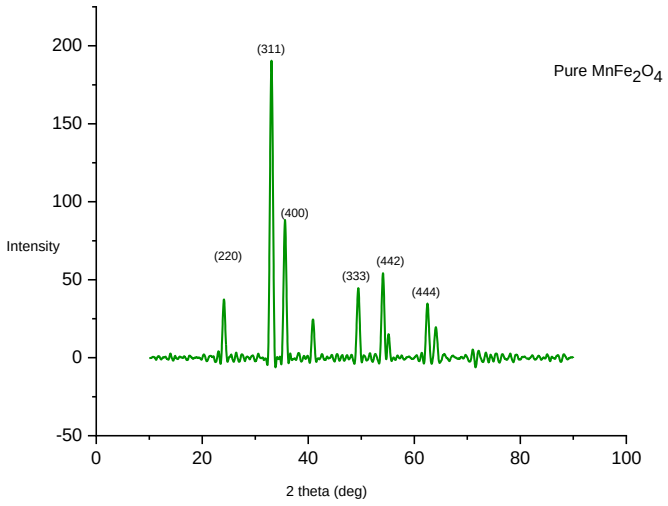


Figure 2.1 X-ray diffraction pattern of pure and strontium doped $MnFe_2O_4$ nanoparticles

The presence of defects in the crystalline solids is generally measured in terms of dislocation density (δ). When there is a strong interaction between the nuclei of atoms and delocalized electrons the formation of metallic crystals takes place. The stability of nanoparticles increases when the delocalized density rises. The delocalisation energy is measured in terms of 10^{15} lines/m^2 affirming the stability of synthesized nanoparticles. The dislocation energy for higher concentration doped nanoparticles is slightly higher as compared to other samples[9].

In present work, the other physical parameters like the dislocation density (δ) and lattice strain (ε) were also calculated using the equation 4. It was observed that in pure and doped $MnFe_2O_4$ nanoparticles the dislocation density (δ) increases from 1.722 x 10^{15} line/ m^2 to 1.83 x 10^{15} line/ m^2.The dislocation density versus the lattice strain graph was plotted for each samples to determine their correlation.

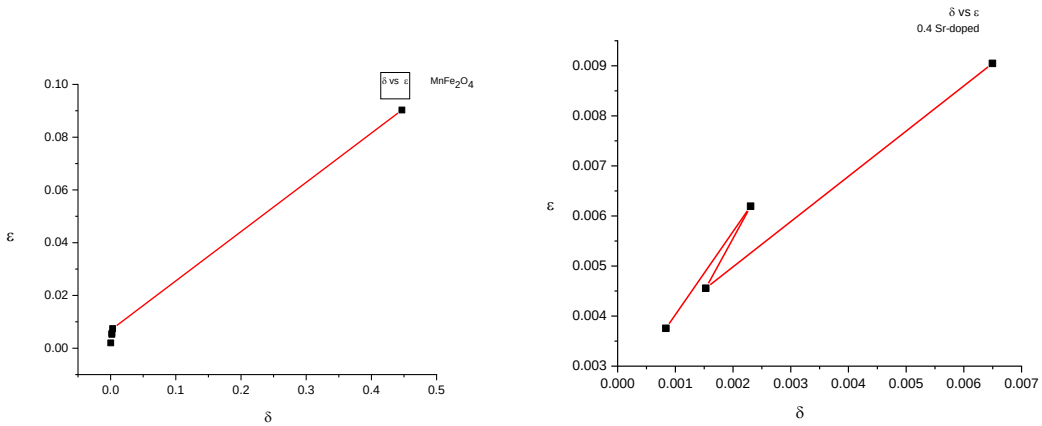


Figure 2.2 (δ) vs (ε) for pure and 0.4% Sr-doped $MnFe_2O_4$ nanoparticle

3.2 FTIR study

Figure 3 explains the FTIR analysis of pure and $Sr_xMn_{1-x}Fe_2O_4$ nanoparticles (x = 0.4) which was taken between the ranges of 400 – 4000 cm^{-1}. The absorption peak at high wave number of 522.71 cm^{-1} is the metal oxygen (M-O) range of stretching vibrations at site A while band at lower wave number of 480.28 cm^{-1} is the metal oxygen (M-O) bond at site B which confirms the formation of $MnFe_2O_4$ nanoparticles. The C- N=O bond absorption peak appears between 815.89 cm^{-1} to 860.25 cm^{-1} which leads to the formation of C-C ring. The stretching

vibration at 1228.66 cm^{-1} confirms the C-N bond formation. The bands in the range of 1340.53 cm^{-1} to 1458.18 cm^{-1} were the bands for C-H from methylene group. For C=O chemical bond the peak occurs in the range of 1600-1800 cm^{-1}. The stretching vibration at 3466.08 cm^{-1} attributes to the hydroxyl (O-H) bonding for N-H bond formation[10].

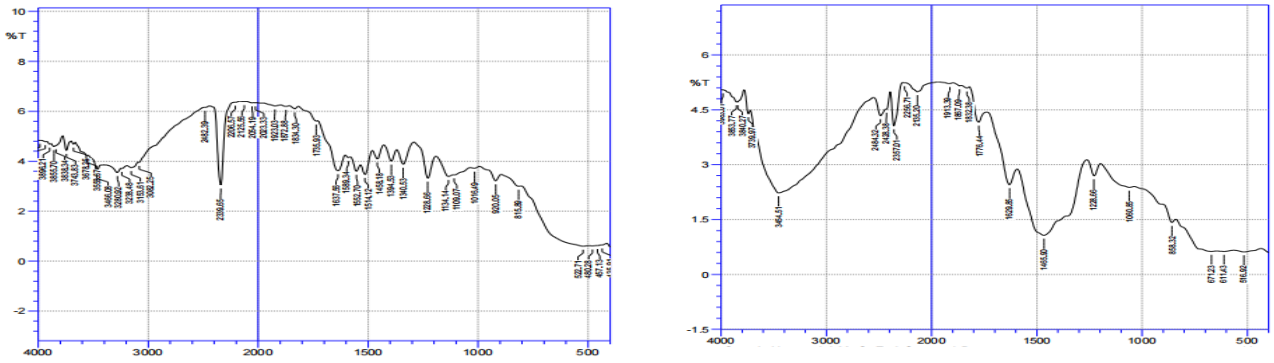


Figure 3 FTIR spectrum of Pure and 0.4% Sr doped $MnFe_2O_4$Nanoparticles

3.3 UV –Visible Analysis

The absorption spectra were recorded in the range of 200-500nm range. It was observed that, the absorption spectra of $MnFe_2O_4$ and $Sr_xMn_{1-x}Fe_2O_4$ (x=0.2 and 0.4) exhibited a strong absorption peak between 200-300nm which is shown in Figure 4. The spectra exhibit a shoulder-like structure due to presence of surface states in the absorption area. When the transition of electrons takes place from the valence shell of O-2p to conduction band of Fe-3d we get the absorption spectrum[11]. The optical band gap value was calculated by linear fitting of the curve and it was found that the band gap value increases from 3.58 eV to 4.67 eV after doping and this is due to lattice strain in the crystal and also the quantum confinement[12].

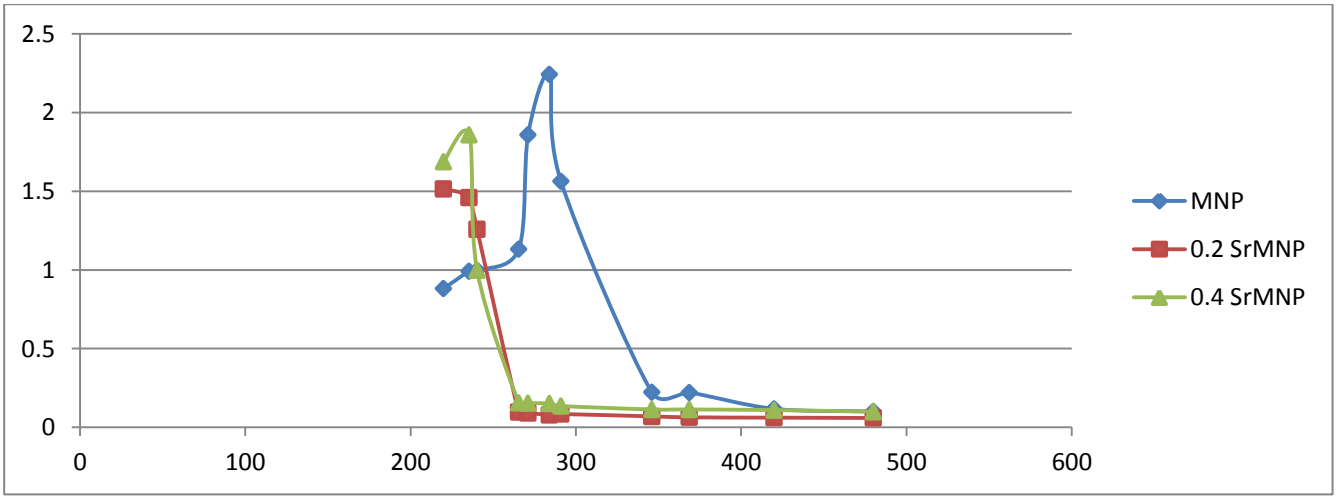


Figure 4 UV visible Spectra of pure and Sr doped $MnFe_2O_4$ nanoparticles

3.4 SEM with EDS Analysis

Figure 5.1 shows the FESEM images of pure and doped $Sr_xMn_{1-x}Fe_2O_4$ and nanomaterials. From the images it was observed that the synthesized pigments were uniformly distributed with spherical shape and some amount of agglomeration due to the blending nature of ferrite. The particle size, structure and morphology were somewhat similar for doped and undoped $MnFe_2O_4$ nanospheres. The evaluated particle size of the materials examined from XRD pattern was same when the particles were subjected to SEM analysis[13].

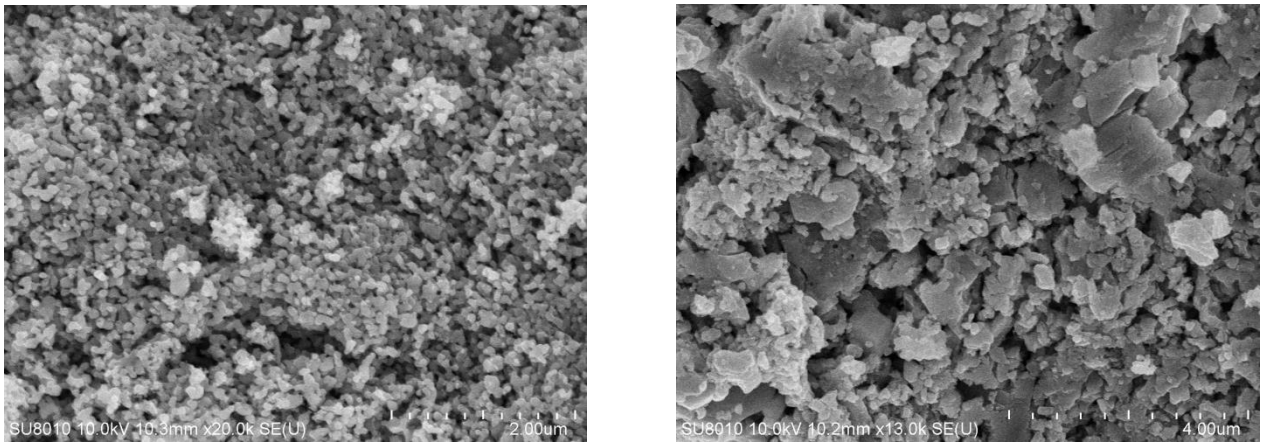


Figure 5.1 SEM images of pure and 0.4% Sr doped $MnFe_2O_4$ nanoparticles

Figure 5.2 shows the EDS images of pure and doped $Sr_xMn_{1-x}Fe_2O_4$ nanomaterials. From the images the presence of Mn, Fe mole ratio of the synthesized pigments was observed. For pure samples the peaks of Mn, Fe and O were observed while for $Sr_xMn_{1-x}Fe_2O_4$ doped particles the EDS spectra reveals the Mn, Fe, Sr and O metals[14]. From the EDS evaluation it was confirmed that the study of increasing Sr content has the impact on the manganese ferrite properties which also confirms the formation of pure and $Sr_xMn_{1-x}Fe_2O_4$ nanospheres.

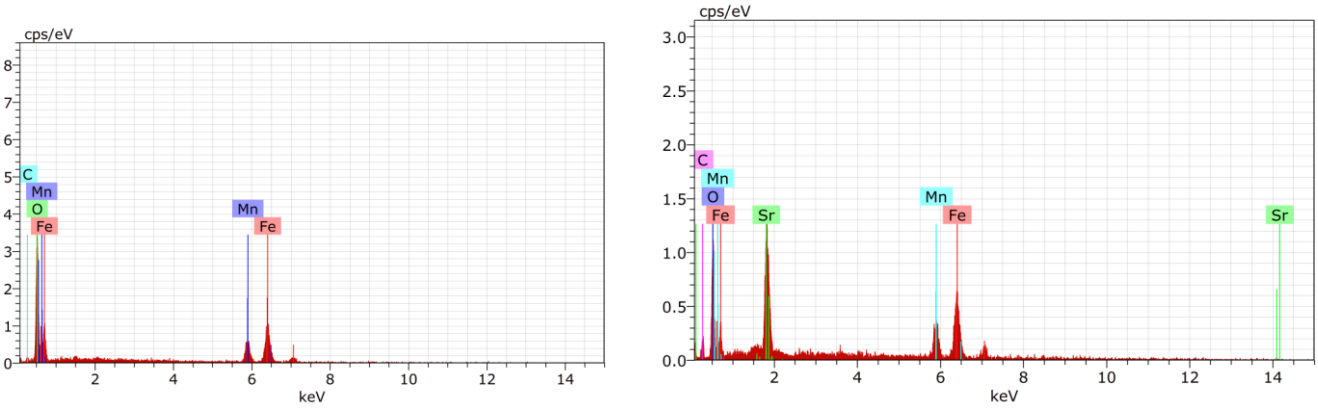


Figure 5.2 EDS Spectrum of pure and 0.4% Sr doped $MnFe_2O_4$ nanoparticles

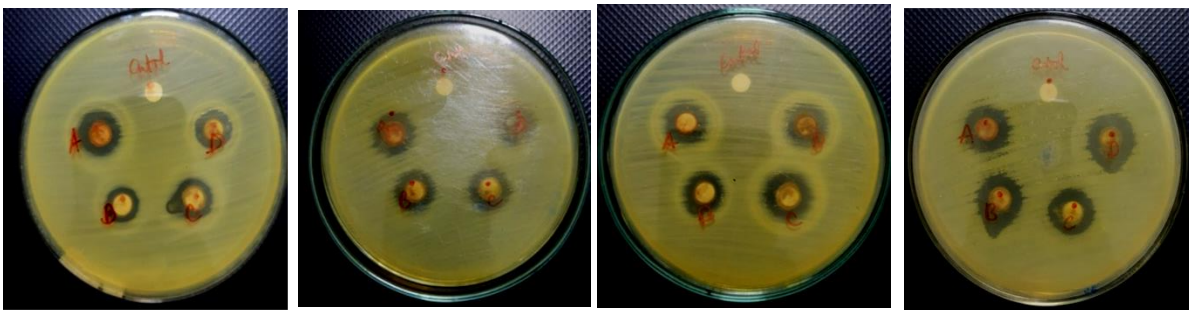
ANTIMICROBIAL APPLICATIONS

Due to potential application of $MnFe_2O_4$ nanoparticles in the biomedical field a lot of research is going on in this direction. Strontium metal increases the effectiveness of $MnFe_2O_4$ nanoparticles when it is added as dopant. The manganese ferrite nanoparticles have the ability to generate reactive oxygen species and thus it exhibits antimicrobial activity against various microorganisms which can include bacterial and fungal strains also against viruses. These nanoparticles damage the cell membrane and DNA of microorganism leading to their death. It has been observed in literature survey that spinel ferrite $MnFe_2O_4$ nanoparticles shows effective growth of bacteria against *Escherichia coli, Staphylococcus aureus, and E. faealis* where as fungal strain growth against *Candida albicans* can also be observed. [15,16].

4.1 Antibacterial Activity

The antibacterial activity of pure $MnFe_2O_4$ and doped $Sr_xMn_{1-x}Fe_2O_4$ and Sr_2FeNiO_6 nanoparticles were examined against four pathogenic strains *E. coli* (MTCC 118), *K. pneumoniae* (MTCC 109) (Gram negative), *S. aureus* (MTCC 1430) and *E. faecalis* (MTCC 2729) (gram positive). $MnFe_2O_4$ nanoparticles when doped with 0.2% and 0.4% strontium shows effective results when we compare it with undoped $MnFe_2O_4$ nanoparticles.

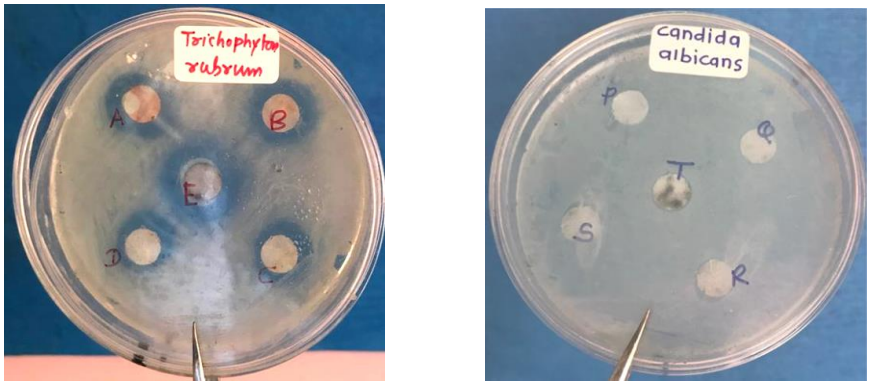
Strontium has the strong ability to interact with the cell membrane of bacteria and causing structural damage to the cell makes it a better antimicrobial agent as compare to other transition metals. And from all these findings we can say that Sr doped MnFe2O4 nanoparticles can be effectively used in antimicrobial therapy and wound healing process in various biomedical fields.



Zone of Inhibition for *E. coli*, *K. pneumoniae* , *S. aureus* and *E. faecalis*

4.2 ANTIFUNGAL ACTIVITY

The antifungal activity of pure and Sr doped $MnFe_2O_4$ along have been explored in this study. The doping of strontium in ferrite enhances their antifungal properties, as metal easily interacts with the fungal cell membrane causing damage to the fungal cell membrane and thus making them an important agent in biological and agricultural industry. The particle size of the synthesized nanoparticles also affects the antifungal activity as we know smaller the size larger is the surface area and then the interaction between the metal ion and fungal cell membrane can be increase, which results in enhancing the antifungal activity[17].



Antifungal activities of nanoparticles against *Trichophyton rubrum and Candida albicans fungal strains*

CONCLUSION

Nanoferrites of Sr doped $MnFe_2O_4$ were successfully prepared by sol gel citrate method and calcinated at 650^0C. The average crystalline size for pure, 0.4% Sr doped $MnFe_2O_4$ was found to be 24.10nm and 23.35nm respectively. FTIR confirms the chemical bonding and presence of different functional groups. The Optical band gap increases from 3.58 eV to 4.67 eV after doping calculated through Tauc plot. The SEM results confirm the formation of nanoparticle with surface morphologies. The EDS shows the presence of Mn, Fe, O, and Sr. The zone of inhibition against various pathogenic strains confirms that synthesized nanoparticles can be used in biomedial applications in wound Healing Therapy.

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Analysis of Micro Plastic in Contaminated Mahanadi River and Its Tributary Kathajodi River Water at Cuttack City, Odisha and Its Effect on Fish Species by Micronucleus Assay and Haematological Parameters Study

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ABSTRACT

As an unnecessary demand of modern life, a million tons of plastic waste releasing in to the environment it leads harmful effects on aquatic, soil ecosystem and polluting the environment. It contains synthetic polymers like polyethylene (PE), polypropylene (PP) polystyrene (PS), polyethylene terephthalate (PET) which have a dangerous quality to absorbed contaminants which leads to form a hazardous stressful environment for aquatic organisms. Specially fish which is the best indicator of aquatic pollution as they develop some damages in their body like hematological parameters change and formation of micronucleus. Micronucleus is the abnormal formation of nuclear fragments during cell division which occurs due to aquatic pollution and stress and its also affect the hematological parameters of the fish body. To study the pollutant level and its effect on fishes we covered the areas of Cuttack city from Lat.20.4642 Long 85.791489 to Lat. 20.452758° Long.85.873869° and collected water samples. Microplastics analysis done by evaporation method in the laboratory. Fish Labeo rohita and fish catla catla are taken as specimen as they widely used for human consumption. Blood sample collected from caudal region for the study of hematological parameters. And for the micronucleus assay Giemsa staining method was used. It results the damages in hematological parameters and formation of micronucleus as well as shows other DNA damages.

Keywords- Microplastic, Labeo rohita, catla catla, Hematological

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parameters, Micronucleus assay, DNA damage, Giemsa staining

INTRODUCTION

Cuttack city is surrounded by two beautiful rivers. Mahanadi and it's tributary katha Jodi which enhances the beauty of the city but unfortunately the industries which develops around the city release their waste in to the river and city sewage water also released to the rivers. which contains chemicals, polluted water and tons of plastic. Which affecting the river ecosystem and producing a very stress full environment. Microplastic particles may be very small in size but it absorbs contaminants which leads to further damage. Microplastics as an emerging pollutant pose a threat to water quality and freshwater ecosystems as they can contain harmful chemicals, such as phthalates or polybrominated diphenyl ethers, and have the ability to adsorb, absorb, and release persistent organic pollutants (Crawford and Quinn, 2017) it causes physical damage, organ damage and sometimes death.it affect the organisms in such a leave that they started forming abnormal nuclear fragments during cell decision. Microplastics (MP) are an emerging contaminant and ubiquitous within the environment. The primary microplastics are originated directly from industrial production, whereas secondary microplastics are formed due to the disintegration of larger plastic debris (Browne et al., 2011; Cole et al., 2011) The hematological profile of a fish cultivation can indicate its physiological status and health, so that hematology combined with other routine diagnostic methods could be used to identify and assess conditions that cause stress and/or diseases that affect production performance (Tavares-Dias and Moraes, 2004; Tavares-Dias and Moraes, 2006; Tavares-Dias and Moraes, 2007; Pavlidis et al., 2007) In marine and freshwater ecosystems, micronuclei counts have been widely employed to bio monitor wild areas with different levels of contamination, employing as marker species a variety of organisms, ranging from mussels (Mersch and Beauvais, 1997) to fish (Hayashi et al., 1998) Microplastic entering in to the body of aquatic organisms and affecting them , it damaging there hematological parameters like Hemoglobin ,RBC ,WBC , Lymphocyte, Monocyte and Neutrophil counts. It also combines with other harmful pollutants which leads to produce a very stress full environment for fishes which causing them formation of extra nuclear fragment during cell division which is known as Micronucleus. It's a life threatening abnormal health condition for aquatic organisms like fish.

Objective

To study the degree of microplastics present in river water by finding the extent of pollution in water of Mahanadi and its tributary river kathajodi and Hematological study as well as micronucleus assay to carry out the hematological and nuclear changes due to polluted river ecosystem.

Methodology

Study area

The study area covers Mahanadi and Kathajodi river of Cuttack city Odisha starting from Naraj area to till different 9 stations around the Cuttack city from Lat.20.4642 Long 85.791489 to Lat.20.452758° Long.85.873869°, It covers all city domestic drainage systems and other industrial drainages connected to the river.

Fish species

Fish species Labio rohita and Catla Catla are collected with proper precautions with average 500gm to 1200gm with proper precaution

Experimental methods

Water collection done from 9 different sites of the city pH varies from 5.3 to 7.9 collection done with use of bottles with precautions major and microplastics extraction done by evaporation methods. For fish species after collecting the fish, blood was collected by puncturing the caudal vein with heparinized disposable needle and stored per standard protocol. Hematological parameters study done to study the changes in hemoglobin, RBC, WBC, Lymphocyte, Monocyte, Neutrophil count due to pollution. Blood smear slides are prepared by Giemsa staining method to perform micronucleus assay to calculate the impact of water pollution on fish labeo rohita and catla catla.

RESULTS

Table 2(a)

Blood cells	S1	S2	S3	S4	S5	S6	S7	S8	S9
Hemoglobin(gr/dl)	3.3± 1.0	4.1± 0.1	8.1±2.2	5.9± 2.3	3.1± 1.2	6.2± 1.1	3.2± 0.1	6.1± 1.2	1.9± 1.1
RBC($^{x106\mu l}$)	1.9± 0.04	3.0± 00.3	8.1±2.2	1.6± 0.02	2.7± 0.01	5.5± 0.001	3.5± 1.2	2.3± 0.3	1.8± 0.3
WBC($^{x103\mu l}$)	15.1±4.3	29.0±0.1	23.1±2.3	21.3±0.1	41.2±0.1	29.1±0.1	19.1±0.8	18.2±0.2	27.2±0.5
Lymphocyte (%)	48.1±3.1	61.1±1.2	52.1±0.2	61.4±0.11	39.3±0.01	38.2±3.1	47.0±1.0	71.1±1.0	49.03±0.2
Monocyte (%)	4.1±1.1	6.1±0.2	4.1±1.1	1.2± 0.001	1.9± 0.1	3.1± 0.01	2.0± 0.1	2.3± 0.1	2.1± 0.1
Neutrophil (%)	0.09±0.03	0.17±0.09	0.21±0.2	0.17±0.1	0.18±0.5	0.29±0.3	0.41 ±0.5	0.21±0.2	0.28±0.3

Table 2 (a) shows the hematological parameters of fish labio rohita collected different stations of river.

Table 2(b)

Blood cells	S1	S2	S3	S4	S5	S6	S7	S8	S9
Hemoglobin(gr/dl)	9.2± 1.1	7.3± 0.1	9.1±3.3	7.6± 1.5	9.1± 2.1	3.2± 2.1	3.3± 3.0	7.1± 1.2	4.1± 2.0
RBC($^{x106\mu l}$)	1.9± 0.01	1.1± 00.3	4.1±1.1	3.6± 0.01	1.3± 0.02	6.5± 0.2	1.9± 2.0	6.3± 0.2	7.2± 0.1
WBC($^{x103\mu l}$)	21.1±5.4	18.0±0.1	28.1±1.6	27.3±0.2	41.2±0.9	21.1±0.5	25.1±0.5	21.6±0.2	26.2±0.3
Lymphocyte (%)	48.1±1.1	61.1±1.2	58.1±0.3	59.4±0.09	41.3±0.02	38.2±4.1	42.0±2.0	54.3±1.4	61.3±0.1
Monocyte (%)	4.1± 0.2	3.1± 0.2	5.1±00.1	1.2± 0.1	3.3± 0.2	6.1± 0.02	2.6± 0.2	1.9± 0.1	3.1± 0.2

Blood cells	S1	S2	S3	S4	S5	S6	S7	S8	S9
Neutrophil (%)	0.16±0.01	0.17±0.09	0.21±0.1	0.27±0.2	0.16±0.3	0.19±0.4	0.28±0.3	0.19±0.2	0.28±0.2

Table 2(b) shows the hematological parameters of fish catla catla collected from different stations of river.

Table 3

		S2	S3	S4	S5	S6	S7	S8	S9
Labio rohita	0.6± 0.09	0.2± 0.11	0.6± 0.1	0.9± 0.3	0.8± 0.2	0.8± 0.3	0.6± 0.2	0.2± 0.001	0.5± 0.2
Catla catla	4.1± 0.5	3.0± 0.5	4.2± 0.4	5.0± 0.2	2.4± 0.1	1.2± 0.9	4.5± 0.3	3.4± 0.2	3.2± 0.1

Table 3 represents micronucleus amount from study of 1000 cells of labio rohita and catla catla of different stations of river in control medium.

DISSCUSION

As table 2(a) and table2 (b)showing changes in hematological parameters which as the result of microplastic pollution in water and table 3 showing presence of micronucleus numbers study from 1000 number of cells which clearly indicates the suffering of aquatic organisms like fish due to stress full pollutes environment.

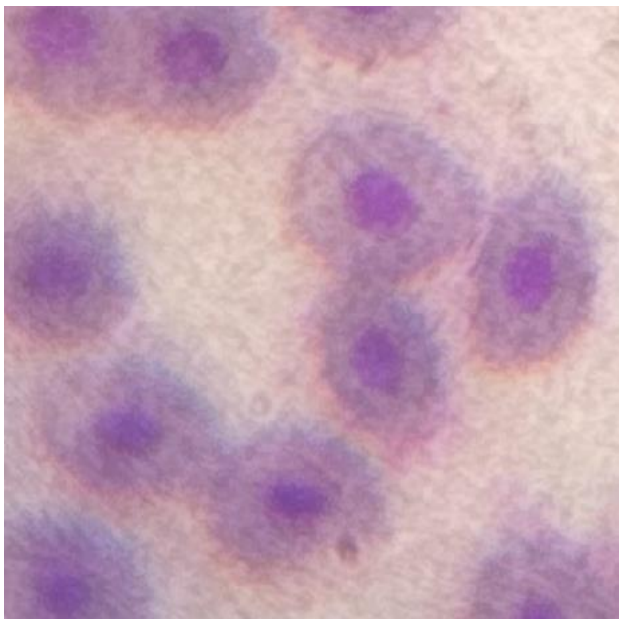

Figure showing micronucleus i

CONCLUSION

Fishes are best bio marker and here fish labeo rohita and catla catla showing changes in hematological paraments and formation of micronucleus which clearly showing the effect of pollutants as well as stress full environment on them. Our river ecosystem is go owing towards destruction which not only affecting them it also directly or indirectly affecting us. So, for a sustainable environment we should reduce the use of plastic products and careful towards our environment.

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Comparative Studies of Water and Salinity Stress on Mustard and Coriander Seeds

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ABSTRACT

The research aimed to explore the germination of seeds and the initial growth of seedlings for coriander and mustard under various stress conditions, particularly focusing on salt and water stress. The findings from the experiment illuminated how both plant species respond to environmental stressors and offered valuable perspectives on potential strategies to alleviate these stresses, thereby enhancing seedling growth and overall crop yield. Salinity and drought are significant stressors that negatively impact plant growth and productivity, making it essential to develop crops that can withstand these challenges. Typically, low temperatures lead to mechanical constraints, while salinity and drought primarily disrupt the ionic and osmotic balance within the cells. It is now well recognized that stress signals are initially detected at the membrane level by receptors, which then transmit these signals within the cell to activate stress-responsive genes that facilitate tolerance. Gaining insights into the mechanisms of stress tolerance, along with the myriad of genes involved in the stress signaling network, is vital for advancing crop improvement. Therefore, to enhance and maintain the productivity of mustard and coriander seeds, it is essential to comprehend and boost their salt tolerance. In this investigation, we analyzed the responses of mustard and coriander to salt stress.

Keywords- Drought, Germination, Salinity, Seedlings.

INTRODUCTION

Plants are constantly exposed to various environmental stresses that significantly affect their growth, development, and productivity. Among these stresses, water and salt stress stand out as major factors limiting plant growth and crop yield worldwide. Understanding how different plant species respond to these stresses is crucial for developing strategies to mitigate their negative impacts and ensure sustainable agriculture. Mustard

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(*Brassica juncea*) and coriander (*Coriandrum sativum*) are two widely cultivated plant species known for their culinary, medicinal, and economic significance globally. However, their growth and productivity are frequently challenged by environmental stressors, particularly water scarcity and soil salinity. As climate change continues to alter precipitation patterns and exacerbate soll salinization, understanding the physiological responses of these crops to water and salt stress is critical for ensuring agricultural sustainability and food security.Water stress, arising from insufficient soil moisture, adversely affects plant growth, development, and productivity by disrupting physiological processes such as photosynthesis, nutrient uptake, and metabolism. Conversely, salt stress, resulting from high levels of soluble salts in the soll, Imposes osmotic and lon toxicity effects on plants, leading to cellular dehydration, ion imbalance, and oxidative damage.Previous research has demonstrated that mustard and coriander exhibit varying degrees of tolerance to water and salt stress, with distinct morphological, physiological, and biochemical adaptations enabling them to withstand these environmental challenges. However, comparative studies directly comparing the physiological responses of these two species under water and salt stress conditions remains limited. Such comparative analyses are essential for elucidating species-specific stress tolerance mechanisms.

Therefore, this study aims to conduct a comprehensive comparative physiological Investigation of mustard and coriander under water and salt stress conditions. By examining their physiological responses, including water status, ion regulation, photosynthetic efficiency, osmotic adjustment, and antioxidant defence mechanisms, this research seeks to unravel the unique stress tolerance strategies employed by these two species. Additionally, the study aims to compare the effectiveness of these strategies between mustard and coriander and identify key physiological traits associated with stress resilience.

Material and Methodology

1) Seed Selection:

a. Source and Procurement: Obtained seeds of mustard (Brassica juncea) and coriander (Coriandrum sativum) from a reputable supplier known for providing high-quality seeds suitable for research purposes.

b. Quality Assurance: Inspected the seeds visually to ensure uniformity in size, shape, and color within each species. Conducted quality check by soaking seeds in water, damage seeds floats on water with a sample of seeds from each batch to assess viability. Discarded any seeds that show signs of damage .

c. Genetic Background: Choosed seeds from well-characterized cultivars or lines with documented genetic backgrounds to minimize genetic variability. Selected seeds that are known to exhibit typical responses to water and salt stress, based on prior research or breeding history.

d. Storage: Stored the seeds in a cool, dry environment away from direct sunlight to maintain their viability and vigor until the start of the experiment.

2) Plantation in Pots:

a. Preparation of Planting Containers: Used clean, sterilized pots or trays with drainage holes to prevent water logging. Filled the containers with a well-draining, nutrient-rich potting mix suitable for both mustard and coriander.

b. Sowing Seeds: Sowed the selected seeds at the recommended planting depth for each species, typically 1/4 to 1/2 inch deep. Spaced the seeds evenly to avoid overcrowding, ensuring each seedling has sufficient space for growth.

c. Labeling: Labeled each pot with the species name, treatment group (control, water stress, salt stress), and other relevant information to facilitate tracking and data collection.

d. Watering: Watered the planted seeds gently immediately after sowing to ensure adequate moisture for germination. Maintained consistent soil moisture throughout the germination and early growth stages to support seedling establishment.

3) **Regular Watering:**

- Watering Regimen: Developed a watering schedule based on the moisture requirements of mustard and coriander, considering factors such as soil type, temperature, and humidity. Watered the plants regularly, ensuring the soil remains evenly moist but not waterlogged.Adjusted the frequency and volume of watering as needed to prevent soil drying out or becoming overly saturated.

4) **Weekly Observation:**

a. **Data Collection:**Conducted weekly observations to monitor the growth and development of mustard and coriander plants.Recorded relevant parameters such as shoot height, leaf number, root development, and overall plant health.

b. **Stress Induction:**

- Introduced water stress by reducing watering frequency or maintaining the soil water level below optimal levels for a specified duration.
- For salt stress, gradually increased the concentration of saline solution applied to the soil or hydroponic system over time.

c. **Symptom Assessment:**

- Monitored plants for any signs of stress-related symptoms, such as wilting, yellowing of leaves, or stunted growth.Documented the severity and progression of stress symptoms over time to assess the impact of water and salt stress on mustard and coriander.
- By following these steps, I ensured the successful selection and planting of seeds, maintained optimal soil moisture conditions, and systematically observed the growth and responses of mustard and coriander plants to water and salt stress over time.

Observation and Result

1. **Germination Percentage:**Both coriander and mustard exhibited a decrease in germination percentage as the severity of stress increased. Salt stress, especially at higher concentrations, resulted in a notable reduction in germination rates for both species. Similarly, water stress conditions, whether due to overwatering or underwatering, led to decreased germination rates compared to the control.
2. **Plant Height and Number of Leaves:**Under optimal conditions (control), both coriander and mustard showed robust growth, characterized by taller plants with a greater number of leaves. However, under stress conditions, there was a consistent trend of reduced plant height and fewer leaves observed. This indicates that environmental stress negatively impacts seedling vigor and development, resulting in stunted growth and reduced foliage.
3. **Comparative Responses:** Coriander generally exhibited higher sensitivity to environmental stress compared to mustard. This is evident from the lower germination percentages and reduced growth parameters observed in coriander under salt and water stress conditions. Mustard, on the other hand, showed relatively better tolerance to stress, with higher germination rates and less severe growth inhibition.
4. **Effect of Specific Stressors:** Salt stress had a pronounced inhibitory effect on seed germination and seedling growth for both coriander and mustard. As the salt concentration increased, there was a corresponding decrease in germination percentage and growth parameters.Water stress, whether from

overwatering or underwatering, also adversely affected seedling growth. Overwatering resulted in signs of waterlogging stress, such as reduced vigor and yellowing leaves, while under watering led to delayed growth and reduced biomass accumulation.

I- Observation Table – Seed Germination under different condition

CONDITION	CORIANDER TOTAL NO. OF SEEDS SOWN	CORIANDER TOTAL NO. OF SEEDS GERMINATED	MUSTARD TOTAL NO. OF SEEDS SOWN	MUSTARD TOTAL NO. OF SEEDS GERMINATED
Control (Optimal watering)	10	09 - 90%	10	06 - 60%
Salt stress (20%)	10	-	10	05 - 50%
Salt stress (60%)	10	-	10	-
Salt stress (90%)	10	-	10	-
Water stress (Over watering)	10	02 – 20%	10	1 - 10%
Water stress (Under watering)	10	06 - 60%	10	5 - 50%

II Observation Table

CONDITION	Coriander Height of plant in week				Mustard Height of plant in week			
	1 week	2 week	3 week	4 week	1 week	2 week	3 week	4- week
Control (Optimal watering)	Germination	3.6 cm	10 cm	16 cm	6 cm	9.5cm	12 cm	20 cm
Salt stress (20%)	----	-----	-----	----	2.5 cm	4 cm	4.5 cm	6.5 cm
Salt stress (60%)	----	-----	-----	-----	------	------	-	
Salt stress (90%)	----	-----	-----	-----	------	------	-	
Water stress (Over watering)	Germination	1.5 cm	3.5 cm	4.5 cm	1 cm	1 cm	Dead	
Water stress (Under watering)	Germination	2.5 cm	6.5 cm	5.5 cm	2.5 cm	5.8 cm	8 cm	

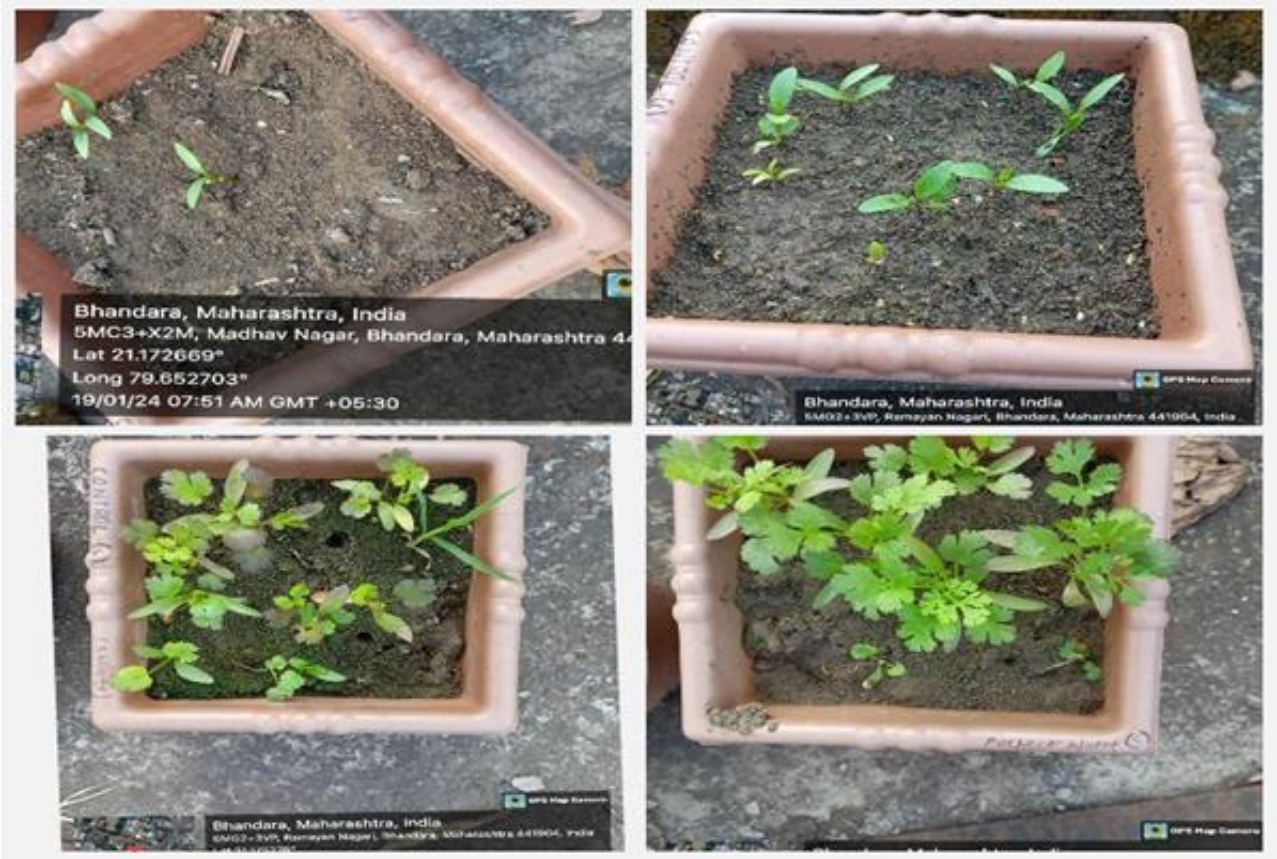

Fig-1-Corriander under Control

Fig-2 Mustard under Control

Fig- 3 Corrainder under watering

Fig- 4 under watering

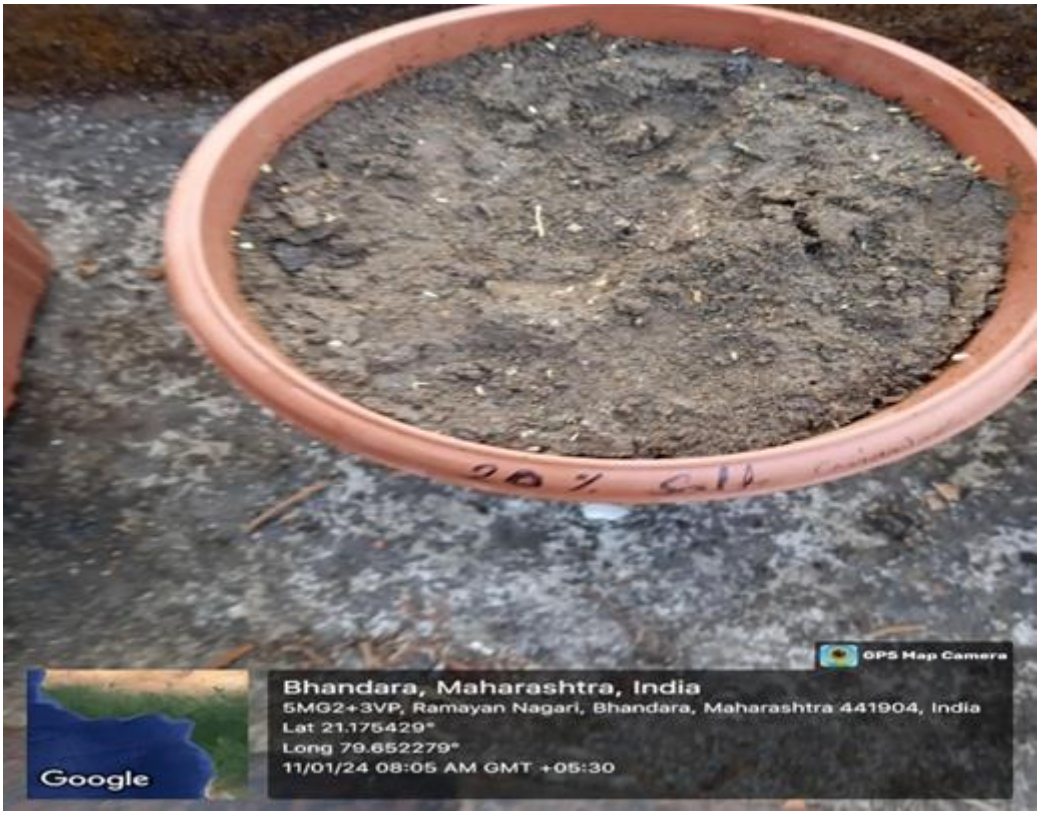

Fig -5-Corrainder under Salt Stress

Fig -6-Mustard under Salt Stress

Conclusion

The study aimed to investigate the seed germination and early seedling growth of coriander and mustard under different stress conditions, including salt stress and water stress. The results of the experiment shed light on the responses of both species to environmental stressors and provided insights into potential mitigation strategies to

improve seedling performance and crop productivity.Overall, the findings suggest that both corriander and mustard are sensitive to salt stress, with increasing salt concentrations leading to significant reductions in seed germination and seedling growth. Coriander exhibited higher sensitivity to salt stress. compared to mustard, highlighting species-specific differences in stress tolerance.Similarly, water stress, induced by overwatering or underwatering, adversely affected seedling growth in both coriander and mustard. Overwatering resulted in waterlogging stress, while underwatering led to reduced germination rates and delayed growth. Mustard demonstrated better tolerance to water stress compared to coriander, showing higher germination rates and less severe growth inhibition..Mitigation strategies, including exogenous application of plant growth regulators and microbial inoculation, showed promise in alleviating the adverse effects of environmental stress on seedling performance. Exogenous application of gibberellic acid and salicylic acid improved seed germination and early seedling growth in both coriander and mustard under stress conditions. Additionally, microbial inoculation with beneficial soil microbes enhanced stress tolerance and promoted seedling vigor, suggesting potential bio-based approaches for enhancing crop resilience to environmental stressors.In conclusion, the findings of this study contribute to the understanding of plant stress responses and provide valuable insights into the development of resilient crop varieties and sustainable agricultural practices. By implementing targeted mitigation strategies, such as the application of plant growth regulators and microbial inoculants, farmers can mitigate the impact of environmental stress on coriander and mustard cultivation, ultimately enhancing crop productivity and ensuring food security in the face of changing climatic conditions. Further research is warranted to explore the long-term effects of stress mitigation strategies and their scalability for practical implementation in agricultural systems.

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Monitoring Of Heavy Metals Concentration in Four Sites of Vena River Water, Hinganghat Dist. Wardha (Maharashtra)

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ABSTRACT

The current research aimed to monitor the heavy metal concentration in four sites of Vena river water, Hinganghat. In this area textiles, agro industries, pharmaceutical company, cotton mill, Swad Chai company, oil industry, paper mill, dall mill are located. Since these sampling sites received a lot of industrial effluents. Determination of heavy metals concentration was done with Inductively coupled plasma spectrometer. The concentration of heavy metals lead, chromium, cadmium, zinc, ferrous, arsenic, except nickel and copper is higher in site two, three and four due to nearby industries. Hence monitoring of heavy metals is necessary and it is necessary to do proper treatment before removal of industrial effluents in river water.

Keywords: Concentration, Heavy metals, Vena river, industries.

INTRODUCTION

Hinganghat is one of the tehsils of Wardha district, the town is located on the bank of Vena river, a tributary of the Wardha river which joins the big river Pranhita, which ultimately merges into Godavari river.[1]

Water is the basic necessity for the functioning of all life forms that exist on earth. This universal solvent is one of the major resources we have on this planet. It is impossible for life to function without water. After all, it makes for almost 70% of the earth. The human body needs water for the day to day survival. We may be able to survive without any food for a whole week but without water, we won't even survive for 3 days.

Lots of industries use water for various purposes like production, cleaning, cooling, etc. Many of the hazardous substances from industry are difficult to biodegrade and hence that accumulate in water sources. Thus, the lack consumption of contaminated water or effluent can cause serious health problems to water bodies.[2]

Hinganghat is one of the developing cities in the Wardha District. The average elevation of the city of Hinganghat is modest, at 215 (705ft) above sea level. The city's Vena River encircles the area on two sides.[3]

In this area textiles, agro industries, pharmaceutical company, cotton mill, Swad Chai company, oil industry, paper mill, dall mill are located. Since these sampling sites received a lot of industrial effluents.

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Therefore, monitoring heavy metal concentration is very important because of their toxicity and their bioaccumulation in living organisms.

METHODS AND MATERIALS

For the determination of heavy metals, the samples of water were collected from 4 stations such as Shalangadi, Smashanbhoomi, under bridge, Kawalghat shown in (fig.1, fig.2, fig.3, fig. 4 and fig. 5). Polyethylene bottles were used to collect surface water and ground water. Samples were collected between May and September, 2024. The samples were dried in the sun and taken to the Laboratory for storage in the refrigerated prior to digestion. Determination of heavy metals concentration was done with Inductively coupled plasma spectrometer.

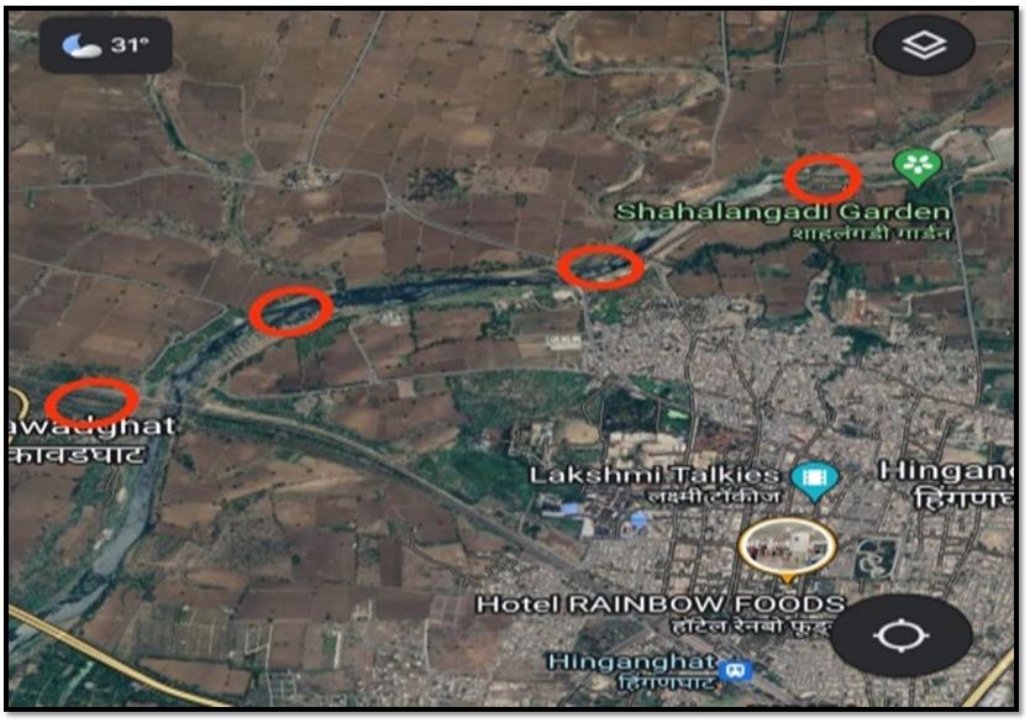

Fig. 5 Location of Four study site shown in satellite image of Vena river, Hinganghat (Arrow showing Under bridge and Showing Smashanbhoomi.)

RESULT AND DISCUSSION

The concentrations of heavy metals in the water of Vena River, from four locations are given in Table 1. The concentration of lead was found that high in site 2 and site 4. The concentration of copper found that below detection limit in site 1 and site 3. The concentration of chromium was found that higher in site 2. The concentration of cadmium was found that higher in site 2. The concentration zinc is higher in site 2 and site 4. The concentration of ferrous was found that higher in site 2 and site 4. The concentration of nickel was found that below detection limit. And concentration of arsenic was found that higher in site 2, site 3 and site 4. From above findings it is clear that the concentration of heavy metal was found higher in site 2 site 3 and site 4 due to nearby industries. And if that heavy metals consumed by water bodies like fishes it is very dangerous to their health also disturbed the food chain sometimes it imbalance the ecosystem. Hence monitoring of heavy metals is necessary and it is necessary to do proper treatment before removal of industrial effluents in river water.

TABLE I Concentration (mg/L) of heavy metals in the water of Vena River in Hinganghat at different stations.

Sites	Pb	Cu	Cr	Cd	Zn	Fe	Ni	As
S1	± 0.02	BDL	± 0.03	± 0.002	BDL	BDL	BDL	± 0.002
S2	± 0.026	± 0.005	± 0.021	± 0.007	± 1.32	± 0.15	BDL	± 0.038
S3	± 0.05	BDL	± 0.02	± 0.003	± 0.5	± 0.02	BDL	± 0.016
S4	± 0.034	± 0.1	± 0.05	± 0.005	± 0.15	± 0.08	BDL	± 0.019
WHO limits	0.05	1	0.05	0.005	5	0.3	0.1	0.01
SD	± 0.013	± 0.04922	± 0.00932	± 0.00222	± 1.31457	± 0.06752	0	± 0.01482

Fig. 1 Shmashan ghat

Fig. 2 Shalangadi

Fig.3 Under bridge

Fig. 4 Kawalghat

CONCLUSION

If heavy metals are consumed by water bodies, they can accumulate in aquatic organisms, leading to bioaccumulation and posing health risks to humans and other animals through the food chain, and potentially causing damage to ecosystems.

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Synthesis, Characterization and Antimicrobial Activities of some New Pyrimidine Derivatives

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ABSTRACT

Pyrimidines are important nitrogen containing six-member heterocyclic ring where two nitrogen atoms occupy 1st and 3rd position of the six-member ring. The pyrimidine derivatives exhibited extensive chemical and pharmacological properties. The structure of the pyrimidine ring is similar to benzene and pyridine, Pyrimidine derivatives are known to be biologically active compounds and substituted pyrimidines have shown wide range of biological activities. The present work synthesis of a series of substituted pyrimidine derivatives have been synthesized by the treatment of 1-(substituted-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (chalcones) were cyclised to substituted pyrimidine analogs by using urea / thiourea The newly synthesized substituted pyrimidine derivatives have been characterized by IR, 1HNMR and Mass spectral analysis and evaluated for their antibacterial and antifugal activities.

Keywords: 2-Hydroxychalcones, Urea, thiourea, Pyrimidine, Antimicrobial activity.

INTRODUCTION

Chalcone derivatives are considered as key starting materials for the syntheses of different classes of heterocyclic compounds such as pyrazolines, oxazoles, isoxazoles, benzothazepines, benzodiazepines and pyrimidines, etc.1-3 Among the heterocyclic compounds, Pyrimidine derivatives are valuable heteroaromatic compounds because of their wide spectrum of pharmacological applications such as antimalarial, anthelmintic, anticancer, antimicrobial anti-inflammatory activities.4-5 Pyrimidines are important nitrogen containing six-member heterocyclic ring where two nitrogen atoms occupy 1st and 3rd position of the six-member ring. The pyrimidine derivatives exhibited extensive chemical and pharmacological properties. The structure of the pyrimidine ring is similar to benzene and pyridine, Pyrimidine derivatives are known to be biologically active compounds and substituted pyrimidines have shown wide range of biological activities.6-7 The synthesized pyrimidine derivatives which have various biological activities including anticancer,8 antimicrobials,9-10

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anticonvulsants,11 antioxidants,12-13 anti-inflammatory,14-15 anti-HIV,16-17 anthelmintic screening 18 properties are one such area of study.

Heterocyclic derivatives involved nitrogen atoms occupies role in chemistry according for pharmacological application and therefor there are spectrum from research about pyrrole, imidazole and pyridine, which consider types important form heterocycles systems according to diverse pharmaceutical properties.19-20 Pyrimidines are six heterocyclic containing nitrogen atoms at 1, 3-positions within ring, are biologically active compounds.21-22 Depending on the divers' pharmaceutical applications of pyrimidine, we worked through this study on preparation of pyrimidine derivatives followed by a study of their biological activity. Therefore; our interest to synthesize some novel pyrimidine molecules and evaluated them as promising antimicrobial activity. In view of these observations, in the present investigation we report herein, a series of substituted pyrimidine derivatives have been synthesized by the treatment of 1-(substituted-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (chalcones) were cyclized to substituted pyrimidine analogs by using urea/thiourea The newly synthesized substituted pyrimidine derivatives have been characterized by IR, 1HNMR and Mass spectral analysis and evaluated for their antibacterial and antifungal activities.

MATERIALS AND METHODS

All the solvents and reagents were obtained from commercial sources and were used without further purification. The melting points were determined by Open Capillary method and are uncorrected. The mass spectra were obtained with a Shimadzu GC-MS spectrophotometer. The IR spectra in KBr were recorded on Shimadzu Spectrophotometer and 1H NMR spectra were recorded in DMSO on Avance 300 MHz Spectrometer using TMS as internal standard. The chemical shift values are expressed in part per million (ppm) downfield from the internal standard and signals are quoted as s (singlet), d (doublet), t (triplet) and m (multiplet). Thin-layer chromatography (TLC) was used to monitor the progress of all reactions and to check the purity of compounds by using ethyl acetate and petroleum ether as an eluent in the ratio of (3:7 v/v). All the newly synthesized substituted pyrimidine (2a-e) and (3a-e) compounds were tested for their antimicrobial activities by agar cup method and Poison plate method, respectively.

General method for the Synthesis of 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-ol (2a-e) derivatives.

An equimolar reaction mixture of 1-(substituted-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (1a-e) (Chlcones) and urea (0.001 mol) by using 10 ml of ethanol as a solvent, with 10ml of ethanolic NaOH, was refluxed for 7 to 8 hrs. The progress of the reaction was monitored by using TLC [eluent: ethyl acetate; petroleum ether (3:7)], after completion of reaction (checked by TLC). The reaction mixture was poured on crushed ice-cold water. The solid crude product obtained was filtered, washed with cold water, dried and recrystallized by using ethanol to get corresponding 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-ol compounds (2a-e) in 60-70 % yield.

General method for the Synthesis of 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-thiol (3a-e) derivatives.

An equimolar reaction mixture of 1-(substituted-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (1a-e) (Chalcones) and thiourea (0.001 mol) by using 10 ml of ethanol as a solvent, with 10 ml of ethanolic KOH, was refluxed for 17 to 18 hrs. The progress of the reaction was monitored by using TLC [eluent: ethyl acetate; petroleum ether (3:7)], after completion of reaction (checked by TLC). The reaction mixture was poured on crushed ice-cold water. The solid crude product obtained was filtered, washed with cold water, dried and

recrystallized by using ethanol to get corresponding 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-thiol compounds (3a-e) in 50-65 % yield.

Schemes: - Synthesized of 4-(substituted-phenyl)-6-(dimethylamino-phenyl)-1,6-dihydropyrimidine2-ol / thiol (2a-e) and (3a-e) derivatives.

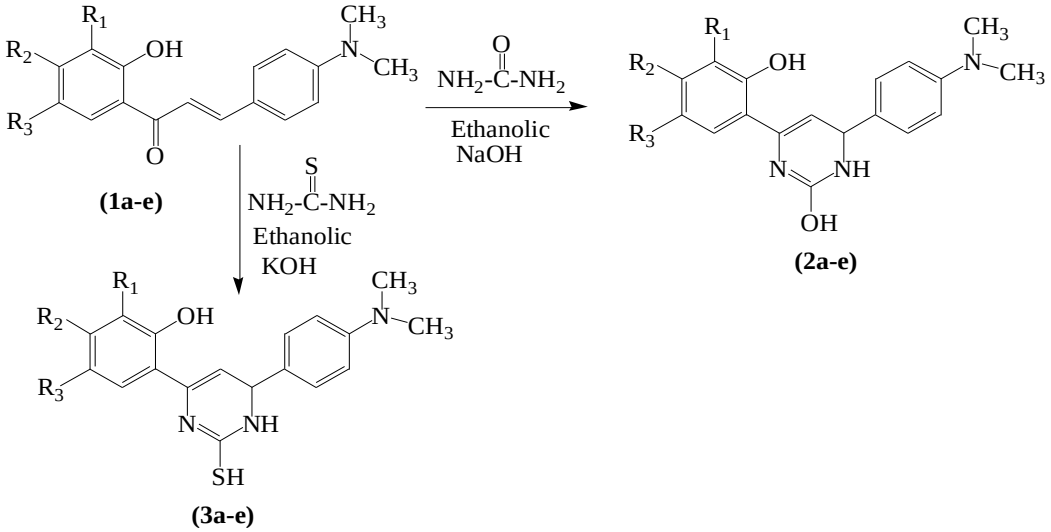

Table-1: Physical data of synthesized 4-(substituted-phenyl)-6-(dimethylamino-phenyl)-1, 6-dihydropyrimidine2-ol / thiol (2a-e) and (3a-e) derivatives.

Sr. No.	Entry	R1	R2	R3	Molecular Formula	Molecular weight	Yield in (%)	Melting Point 0C
1	2a	Br	H	CH3	C19H20N3BrO2	402	70	195-196
2	2b	I	H	Cl	C18H17N3IClO2	469	65	205-206
3	2c	Br	H	Br	C18H17N3Br2O2	467	60	185-186
4	2d	I	H	Br	C18H17N3IBrO2	514	65	202-203
5	2e	H	CH3	Cl	C19H20N3ClO2	357	70	198-200
6	3a	Br	H	CH3	C19H20N3SBrO	418	65	216-217
7	3b	I	H	Cl	C18H17N3SIClO	485	55	205-206
8	3c	Br	H	Br	C18H17N3SBr2O	483	65	212-213
9	3d	I	H	Br	C18H17N3SIBrO	530	50	185-186
10	3e	H	CH3	Cl	C19H20N3SClO	373	65	207-208

A. Antibacterial activity

All the synthesized 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine (2a-e) and (3a-e) compounds were assessed for their antibacterial and antifungal activities against four different strains of bacteria such as E. coli, S typhi, S. aureus and B. subtilis and four fungi like Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme and Aspergillus flavus. The test for antibacterial activity was carried by agar cup method 23-24 (cup size 8 mm) with nutrient agar as medium whereas antifungal activity was carried out by using potato-dextrose agar (PDA) medium by same agar cup plate method. All synthesized compounds were dissolved in DMSO and used as control concentration of each test compound was 100µg/ml. The experiments were performed in triplicate in order to minimize the errors. Zone of inhibition were recorded

after incubation at 37 0C for 24 hrs, zone of inhibition produced by each compound was measured in mm. After incubation plates were observed for the zone of inhibition of bacterial growth around the agar cup. Results were recorded by measuring the zone of inhibition in millimeter (mm) using zone reader. All the newly synthesized pyrimidine compounds were evaluated for their antibacterial activity against the selected four different pathogens, such as E. coli, S. typhi, S. aureus and B. subtilis. The 2c and 3a of substituted pyrimidine compounds show maximum activity against E. coli while compounds 2a, 2e, 3b and 3d does not show activity against E. coli. The synthesized compounds of pyrimidine 2a and 2e and 3c showed maximum activity against S. typhy and compounds 2d, 3e shows moderate activity against S aureus. The compounds 2c and 3b showed significant activity against S. aureus as compared with standard drugs.

Table No. 2: Antibacterial activity data of 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine (2a-e) and (3a-e) derivatives.

Sr. No.	Entry	molecular formula	Antibacterial activity (Zone of Inhibition in mm)			
			Escherichia coli	Salmonella typhi	Staphylococcus aureus	Bacillus subtilis
1	2a	C19H20N3BrO2	--	15	--	14
2	2b	C18H17N3IClO2	11	13	--	--
3	2c	C18H17N3Br2O2	13	--	22	14
4	2d	C18H17N3IBrO2	12	--	17	13
5	2e	C19H20N3ClO2	--	16	18	--
6	3a	C19H20N3BrSO	13	16	18	17
7	3b	C18H17N3IClSO	--	--	22	15
8	3c	C18H17N3Br2SO	12	15	20	12
9	3d	C18H17N3IBrSO	--	12	--	--
10	3e	C19H20N3ClSO	12	--	18	15
+ve Control DMSO			-ve	-ve	-ve	-ve
Penicilline			12	20	34	22

(-- = No Antibacterial activity)

B. Antifungal activity

The antifungal activity of substituted pyrimidine compounds was screened against four plant pathogenic and mold fungi, such as Aspergillus niger, penicillium chrysogenum, Fusarium moneliforme and Aspergillus flavus. The antifungal activities of the synthesized substituted pyrimidine (2a-e) and (3a-e) derivatives were assessed by poisoned plate method.25-26 Griseofulvin (100µg/disc) was used as standard drug for the antifungal test. Potato Dextrose Agar (PDA) was used as basal medium for test fungi. The compound 100 µg were mixed with sterilized potato dextrose agar (PDA) medium at 40 0C of the rate 100 mg/mL PDA. The medium was poured in sterilized Petri-plates and allowed solidified PDA media and then incubated at 30 0C for 72 hours. The growth of fungal area was measured in mm after 4 days of incubation at 30 0C. A control set was maintained using only PDA with DMSO as growth medium. Results were measured as the growth of fungi (does not show antifungal activity), reduced growth of fungi (to observed moderate antifungal activity), and no growth of fungi (antifungal activity observed in the area). All synthesized substituted pyrimidine compounds were evaluated for their antifungal activity against the four different pathogens Aspergillus niger, Penicillium chrysogenum,

Fusarium moneliforme and Aspergillus flavus. The antifungal activity of some substituted pyrimidine compounds showed good activity against four pathogens.

Table No. 3: Antifungal activity data of 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-ol/thiol (2a-e) and (3a-e) derivatives.

Sr. No.	Entry	molecular formula	Antifungal activity (Zone of Inhibition in mm)			
			Aspergillus niger	penicillium chrysogenum	Fusarium moneliforme	Aspergillus flavus
1	2a	C19H20N3BrO2	-ve	RG	-ve	-ve
2	2b	C18H17N3IClO2	-ve	-ve	-ve	-ve
3	2c	C18H17N3Br2O2	-ve	-ve	RG	RG
4	2d	C18H17N3IBrO2	-ve	RG	-ve	-ve
5	2e	C19H20N3ClO2	RG	-ve	RG	RG
6	3a	C19H20N3BrSO	RG	-ve	-ve	-ve
7	3b	C18H17N3IClSO	-ve	RG	-ve	-ve
8	3c	C18H17N3Br2SO	-ve	-ve	RG	RG
9	3d	C18H17N3IBrSO	RG	RG	-ve	RG
10	3e	C19H20N3ClSO	RG	-ve	RG	-ve
+ve Control DMSO			+ve	+ve	+ve	+ve
-ve Control (Griseofulvin)			-ve	-ve	-ve	-ve

[+ve = No growth (Antifungal activity absent), RG = Reduced Growth (more than 50 % but less than 90 % i. e. Moderate Activity), -ve = No Growth (Antifungal Activity Observed 90 %)]

RESULTS AND DISCUSSION

In the present work a series of some novel 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-ol/thiol (2a-e) and (3a-e) derivatives were synthesized by cyclization of corresponding 1-(substituted-phenyl)-3-(4'-dimethylamino-phenyl)-prop-2-en-1-one (1a-e) (2-HydroxyChalcones) and urea/thiourea. The uses of different chalcones for the synthesis of pyrimidine derivatives have been investigated. The presence of halogen group in different position of benzene ring of the chalcone and the use of urea/thiourea resulted in synthesis of pyrimidine derivatives with significantly high yield. All these products of pyrimidine derivatives didn't give pink coloration with concentrated H2SO4 solution. The structures of newly synthesized compounds have been confirmed by IR, 1H NMR and Mass spectral, and their spectral data are resembled with the reported values. The IR spectrum of compound 2a exhibited peaks due to group -C=N, at 1610 cm-1. The 1H NMR spectrum shows characteristic peaks at δ 2.45 [1H, (s, NH)], δ 4.56 [1H, =C-H) and δ 4.56 [1H, (d, pyrimidine -C-H), and δ 6.4-6.8 [1H, pyrimidine =C-H)], δ 2.0-2.2 [1H, Pyrimidine-C-OH], δ 5.0-5.2 [1H Ar-C-OH] and the pick of CH3 group shows at δ 2.1-2.2 (s, 3H, CH3) and dimethylaminine shows at δ 2.85-3.0 (s, 6H, -N(CH3). And also the 3a molecule shows pick of pyrimidine-thiol δ 1.48 [1H, (s, -SH)], these observations are in agreement with the spectral data reported by different researcher.27-28 All the newly synthesized pyrimidine derivatives were evaluated for their antibacterial activity against the selected four different pathogens, such as E. coli, S. typhi, S. aureus and B. subtilis.The 2c and 3a of substituted pyrimidine compounds show maximum activity against E. coli while compounds 2a, 2e, 3b and 3d does not show activity against E. coli. The synthesized compounds of pyrimidine 2a and 2e and 3c showed maximum activity against S.

typhy and compounds 2d, 3e shows moderate activity against S aureus. The compounds 2c and 3b showed significant activity against S. aureus as compared with standard drugs. All the newly synthesized compounds were evaluated for their antifungal activity against the four different pathogens Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme and Aspergillus flavus. The antifungal activity of some pyrimidine compounds showed good activity against four pathogens.

Spectroscopic data of synthesized compounds

4-(3-Bromo-5-methyl-2-hydroxy-phenyl)-6-(4'-dimethylamino-phenyl)-1,6-dihydropyrimidine- 2-ol (2a): Yield: 70% M P: 195-196 C0 IR (KBr) cm-1: 3385 cm-1 (O-H str.), 3068 cm-1 (Ar C-H str.), 1610 cm-1 (C=N str), 3245 cm-1 (N-H str.) and 958 cm-1 (C-Br str.); 1HNMR (DMSO): δ 2.1-2.3 (s, 3H, CH3), δ 2.85-3.0 (s, 6H, -N(CH3)2), δ 6.8-7.8 (m, 6H, Ar-H), δ 2.45 [1H, (s, NH)], δ 4.56 [1H, (1H, pyrimidine –C-H)], δ 6.4-6.8 [1H, (pyrimidine =C-H)], δ 2.0-2.2 [1H, pyrimidine-C-OH] ,δ 5.0-5.2 [1H Ar-C-OH] MS (m/z): 402 (M+1)

4-(3,5-dibromo-2-hydroxy-phenyl)-6-(4-dimethylamino-phenyl)-1,6-dihydropyrimidine-2-ol (2c): Yield: 60% M P: 185-186 C0 IR (KBr) cm-1: 3400 cm-1 (O-H str.), 3085 cm-1 (Ar C-H str.), 1608 cm-1 (C=N str), 3258 cm-1 (N-H str.) and 948 cm-1 (C-Br str.); 1HNMR (DMSO): δ 2.85-3.0 (s, 6H, -N(CH3)2), δ 6.8-7.8 (m, 6H, Ar-H), δ 2.38 [1H, (s, pyrimidine NH)], δ 4.58 [1H, pyrimidine –C-H], δ 6.5-7.0 [1H, pyrimidine =C-H)], δ 2.0-2.2 [1H, pyrimidine-C-OH] ,δ 5.0-5.3 [1H Ar-C-OH] MS (m/z): 467 (M+1)

4-(5-Chloro-4-methyl-2-hydroxy-phenyl)-6-(4-dimethylamino-phenyl)-1,6-dihydropyrimidine-2-ol (2e): Yield:70% M P:199-200 C0 IR (KBr) cm-1: 3412 cm-1 (O-H str.), 3086 cm-1 (Ar C-H str.), 1608 cm-1 (C=N str), 3248 cm-1 (N-H str.) and 785 cm-1 (C-Cl str.); 1HNMR (DMSO): δ 2.0-2.3 (s, 3H, CH3), δ 2.85-3.0 (s, 6H, -N(CH3)2), δ 6.8-8.0 (m, 6H, Ar-H), δ 2.48 [1H, (s, pyrimidine NH)], δ 4.56 [1H, pyrimidine –C-H], δ 6.50-6.8 [1H, pyrimidine =C-H], δ 2.0-2.2 [1H, pyrimidine-C-OH], δ 5.0-5.3 [1H Ar-C-OH] MS (m/z): 357 (M+1)

4-(3-Bromo-5-methyl-2-hydroxy-phenyl)-6-(4'-dimethylamino-phenyl)-1,6-dihydropyrimidine- 2-thiol (3a): Yield: 65% M P: 216-217 C0 IR (KBr) cm-1: 3405 cm-1 (O-H str.), 3105 cm-1 (Ar C-H str.), 1617 cm-1 (C=N str), 3345 cm-1 (N-H str.) and 954 cm-1 (C-Br str.); 1HNMR (DMSO): δ 2.1-2.3 (s, 3H, CH3), δ 2.85-3.0 (s, 6H, -N(CH3)2), δ 6.6-7.8 (m, 6H, Ar-H), δ 2.55 [1H, (s, pyrimidine NH], δ 4.50 [1H, pyrimidine –C-H], δ 6.50-6.8 [1H, pyrimidine =C-H], δ 1.45 [1H, (s, pyrimidine-SH)], δ 5.1-5.3 [1H Ar-C-OH] MS (m/z): 418 (M+1)

4-(3,5-dibromo-2-hydroxy-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-thiol (3c): Yield: 65% M P: 212-213 C0 IR (KBr) cm-1: 3410 cm-1 (O-H str.), 3106 cm-1 (Ar C-H str.), 1612 cm-1 (C=N str), 3252 cm-1 (N-H str.) and 935 cm-1 (C-Br str.); 1HNMR (DMSO): δ 2.85-3.0 (s, 6H, -N(CH3)2), δ 6.8-7.8 (m, 6H, Ar-H), δ 2.52 [1H, (s, pyrimidine NH], δ 4.55 [1H, pyrimidine –C-H], δ 6.50-6.8 [1H, pyrimidine =C-H], δ 1.48 [1H, (s, pyrimidine-SH)], δ 5.0-5.3 [1H Ar-C-OH] MS (m/z): 483 (M+1)

4-(5-Chloro-4-methyl-2-hydroxy-phenyl)-6-(4'-dimethylamino-phenyl)-1,6-dihydropyrimidine-2-thiol (3e): Yield: 65% M P: 207-208 C0 IR (KBr) cm-1: 3412 cm-1 (O-H str.), 3105 cm-1 (Ar C-H str.), 1610 cm-1 (C=N str), 3258 cm-1 (N-H str.) and 795 cm-1 (C-Cl str.); 1HNMR (DMSO): δ 2.0-2.3 (s, 3H, CH3), δ 2.85-3.0 (s, 6H, -N(CH3)2), δ 6.8-8.0 (m, 6H, Ar-H), δ 2.55 [1H, (s, pyrimidine NH], δ 4.52 [1H, pyrimidine –C-H], δ 6.50-6.8 [1H, pyrimidine =C-H], δ 1.45 [1H, (s, -SH)], δ 5.0-5.3 [1H Ar-C-OH], MS (m/z): 373 (M+1)

CONCLUSION

In the present work a series of some novel 4-(substituted-phenyl)-6-(4'-dimethylamino-phenyl)-1, 6-dihydropyrimidine-2-ol/thiol (2a-e) and (3a-e) derivatives using simple experimental procedure with high yield, relatively short reaction time and low cost. All the synthesized compounds were screened for their antibacterial and antifungal activities. From the result of antibacterial 2c and 3a compounds show maximum activity against E. coli while compounds 2a, 2e, 3b and 3d does not show activity against E. coli. The

synthesized compounds of pyrimidine 2a and 2e and 3c showed maximum activity against S. typhy and compounds 2d, 3e shows moderate activity against S aureus. The compounds 2c and 3b showed significant activity against S. aureus as compared with standard drugs. The antifungal activity of some pyrimidine compounds showed good activity against four selected pathogens. The presence of halogen and –N-(CH3)2 groups were found responsible for increasing antimicrobial activity.

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Synthesis and Spectral Characterization of Some Bromo-Substituted Chalcones by Conventional Method

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ABSTRACT

The synthesis of bromo-substituted chalcones were carried out by the reaction of 2-hydroxy-3-bromo-5-methyl acetophenone with different aromatic aldehydes. The newly synthesized chalcones were characterized by elemental analysis, IR and H1NMR spectral studies.

Keywords: Chalcones, aromatic aldehyde, IR, H1 NMR.

INTRODUCTION

Chalcones are a vital class of flavonoid precursors, characterized by an α,β-unsaturated ketone system that imparts significant biological and synthetic versatility. Among them, 2-Bromo Chalcone has garnered considerable attention due to its unique structural properties and potential pharmacological applications. The introduction of a bromine atom at the 2-position enhances its reactivity, making it a valuable intermediate in the synthesis of bioactive compounds, particularly in medicinal chemistry and material sciences. The conventional Claisen-Schmidt condensation method remains one of the simplest and most efficient approaches for synthesizing chalcones. This paper explores the synthesis and spectral characterization of bromo-substituted chalcones.

MATERIALS AND METHODS

The chemicals and solvents used were of highest purity purchased commercially from Merck, S.D. Fine and Alfa Aesar Company Ltd. The melting points of all the synthesized compounds were recorded by Thiele's melting point apparatus as uncorrected values. The elemental analysis was carried out on Thermo Scientific CHNS elemental analyser. IR spectra were recorded on a Shimadzu instrument using KBr pellets. ^{1}H NMR

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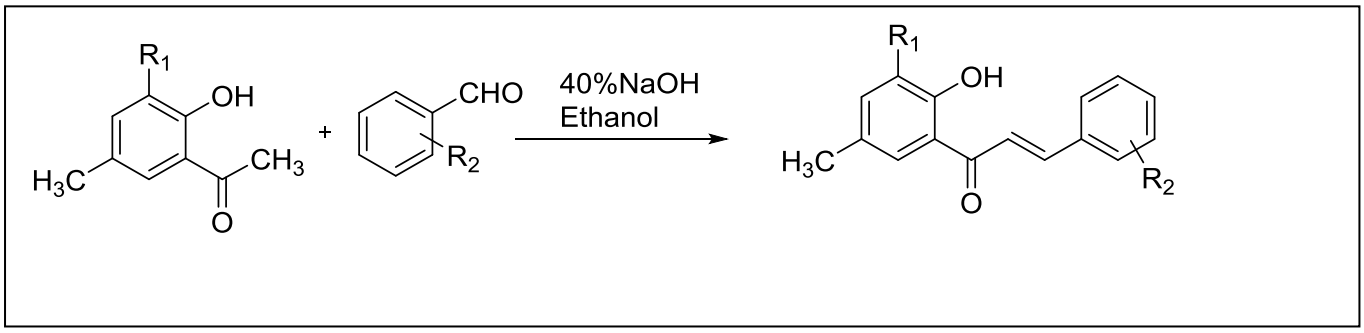
spectra were scanned by Brucker at 400 MHz using DMSO-d6 as solvent and TMS as an internal reference. ^{13}C NMR spectrum of a sample was recorded on same instrument at 100 MHz. Experimental procedure for synthesis of 3-(substituted)-1-(2-hydroxy-5-methyl-3-bromo phenyl)prop-2-ene-1-ones.

Synthesis of Chalcone derivatives:

2-hydroxy-5-methyl acetophenone (2) / 2-hydroxy-3-bromo-5-methyl acetophenone (3) (0.01mol) was dissolved in a suitable solvent and aromatic heterocyclic aldehyde (0.01mol) was added with constant stirring at room temperature. Then NaOH solution was added to reaction mixture which was stirred for 24 hrs at room temperature. Finally, the reaction mixture was pored into crushed ice and neutralized with HCl. The product separated out, was filtered washed with water, dried, and recrystallized from alcohol to give chalcone. All products satisfy the IR and 1H NMR spectroscopic data. M.P. and % yield of product 4a-b and 5a-b are given in a table no.1 The name of synthesized chalcones entitled below

- 1-(2-hydroxy-5-methyl phenyl)- 3-(2-chlorophenyl)- prop-2-en-1-one (4a)
- 1-(2-hydroxy-5-methyl phenyl)- 3-(3-chlorophenyl)- prop-2-en-1-one (4b)
- 1-(2-hydroxy-5-methyl-3-bromophenyl) -3-(2- chlorophenyl)- prop-2-en-1-one (5a)
- 1-(2-hydroxy-5-methyl-3-bromophenyl) -3-(3- chlorophenyl)- prop-2-en-1-one (5b)



R_1= H, -Br and R_2= 2-chloro benzaldehyde and 3-chloro benzaldehyde

Schematic procedure for synthesis of chalcone derivatives

Table 1: Physical Data of synthesized compound (4a-b and 5a-b)

R_1.	R_2	Product	M.P.	% yield
H	2-chloro benzaldehyde	4a	115°C	84%
H	3-chloro benzaldehyde	4b	102°C	74%
Br	2-chloro benzaldehyde	5a	122°C	69%
Br	3-chloro benzaldehyde	5b	98°C	72%

Result and discussion:

The condensation of substituted acetophenone 2 and 3 with substituted aromatic aldehyde in ethanolic alkali yielded chalcones which were purified by recrystallization in ethanol. All products were characterized by IR and H-NMR spectroscopy.

- **1-(2-hydroxy-5-methyl phenyl)- 3-(2-chlorophenyl)- prop-2-en-1-one (4a)**

IR(KBr, cm-1): 3350(Hydrogen bonded -OH), 3082.25 (-C-H stretch in aromatic), 2926.01 (-C-H aliphatic), 1083.99 (-C-O stretching), 786.96 (-C-Cl stretching), 1705 (C=O starching).

1-HNMR($CDCl_3$): 7.9 (m,4H, Ar) . 5.8 (d, 1H), 4.7 (s, 1H), 2.47 (s, 3H, CH_3), 2.6 (s, 1H).

- **1-(2-hydroxy-5-methyl phenyl)- 3-(3-chlorophenyl)- prop-2-en-1-one (4b)**

IR(KBr, cm-1): 3350(Hydrogen bonded -OH), 3082.25 (-C-H stretch in aromatic), 2926.01 (-C-H aliphatic), 1083.99 (-C-O stretching), 786.96 (-C-Cl stretching), 1705 (C=O starching)

1-HNMR($CDCl_3$): 7.9 (m,4H, Ar) . 5.8 (d, 1H), 4.7 (s, 1H), 2.47 (s, 3H, CH_3), 2.6 (s, 1H).

- **1-(2-hydroxy-5-methyl-3-bromophenyl) -3-(2- chlorophenyl)- prop-2-en-1-one (5a)**

IR(KBr, cm-1): 3348(Hydrogen bonded -OH), 3080.25 (-C-H stretch in aromatic), 2900.01 (-C-H aliphatic), 1183.99 (-C-O stretching), 780.96 (-C-Cl stretching), 745.72 (-C-Br stretching), 1710 (C=O starching)

1-HNMR($CDCl_3$): 7.9 (m,4H, Ar) . 5.8 (d, 1H), 4.7 (s, 1H), 2.47 (s, 3H, CH_3), 2.6 (s, 1H).

- **1-(2-hydroxy-5-methyl-3-bromophenyl) -3-(3- chlorophenyl)- prop-2-en-1-one (5b)**

IR(KBr, cm-1): 3348(Hydrogen bonded -OH), 3080.25 (-C-H stretch in aromatic), 2900.01 (-C-H aliphatic), 1183.99 (-C-O stretching), 780.96 (-C-Cl stretching), 745.72 (-C-Br stretching), 1710 (C=O starching).

1-HNMR($CDCl_3$): 7.9 (m,4H, Ar) . 5.8 (d, 1H), 4.7 (s, 1H), 2.47 (s, 3H, CH_3), 2.6 (s, 1H).

CONCLUSION:

We have synthesized number of various chalcone derivatives (4a-b and 5a-b). The reaction conditions were established and found to be reproducible. These derivatives may exhibit various pharmacological activities.

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Preparation of Maleinized Coconut-Linseed Oil (MCLO) By Conventional Method and its Application in the Formulation of Liquid Detergent

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ABSTRACT

Coconut-linseed oil has found wide application in the coatings, cosmetics & detergents. India is the largest exporter of coconut-linseed oil in the world.35-55% of the seed content is a valuable drying oil with many industrial applications. In the present study, modification of coconut-linseed oil through the malenization of coconut-linseed oil carried out with the use of maleic anhydride to form malenized coconut-linseed oil. In this method of addition of unsaturation compound to the unsaturated part of the oil molecule, thus increasing its complexity and heat reactivity. The product obtained from maleic addition is known as the adduct which when neutralized with inorganic alkali, ammonia gives water miscible oils. Their solubilized oils may be used for different applications like cosmetics, detergents etc. The application of malenized coconut-linseed oil has been done in the formulation of liquid detergent Liquid detergents prepared by this resin with acid slurry in different proportions are giving excellent results in comparison with that of commercial products. This research was undertaken to develop products which are based on naturally available raw materials specifically not of petroleum origin. This is an attempt to make the novel products useful for society and to reduce percentage of non-renewable product usage in day to day life thus solving problem of environmental pollution to some extent and thus favor eco-friendly products technology.

Keywords: Coconut-linseed oil; Malenized Coconut-linseed oil; Liquid Detergents; Maleic anhydride.

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INTRODUCTION

A laundry detergent composition generally comprises six groups of substances: surfactants, builders, enzymes, bleaching agents, fillers and other minor additives such as dispersing agents, fabric softening clay, dye-transfer inhibiting ingredient, and optical brighteners. Laundry detergents and, household and personal-care products account for over half the use of surfactant[1]. Therefore, the demand of the detergent industry is a driving force for the development of related chemical industry and chemical engineering which involve synthesis and production of surfactants and polymer builders.

Literature Review on malenized oil based on various vegetables oil as Polymeric Surfactants for Detergent Compositions is given below.

K. Maynil, Gogte B.B[2], developed a novel Malenized oil based on neem oil, used it as a base for liquid detergents. In this process neem oil was Malenized to yield a useful product and was converted to polymeric surfactant by neutralizing it with potassium hydroxide. The detergent has shown appreciable reduction of surface tension at different concentrations.

S. Petkar and Gogte B.B[3], Synthesized Malenized vegetable oil for the production of liquid detergents. Linseed oil was used; the Malenization reaction was carried out at maximum temperature of 225°C using 10% of maleic anhydride. The synthesized Malenized oil was then used for study of replacement of petroleum active ingredient from various liquid detergents.

B.W. Phate and B.B.Gogte[4] in their research paper named "Novel Polymer based Surfactants" suggested that Novel Castro alkyd polymer based liquid detergent sample is compared with commercially available sample. It is observed that prepared polymer shows excellent results for foam volume, surface tension and stain removal tests.

Anshuman M. Bhagwat[5] has used Rosinated alkyds as partial replacement of linear alkyl benzene sulphonate. The alkyd resins are based on coconut-linseed oil, Maleic anhydride and glycerol. The compositions based on a combination of LABS with alkyd polymer are giving clear and homogeneous liquid detergent product and they have equivalent performance compared to commercial samples in respect of cleaning and stain removing. In fact some compositions are better than commercial samples.

B.W. Phate and B.B. Gogte[6] developed a liquid detergent based on alkyd polymers. This polymer introduced as 50% replacement of conventional active agents, LABS. Detergents were analyzed for physicochemical properties like surface tension, foaming, detergency etc. The above properties were compared with commercial detergents.

Zhang and Moarang[7] have developed a liquid detergent composition containing coconut-linseed oil fatty acid ester. The household liquid detergent useful in food and cooking utensil cleaning, contains 0.5 - 5 wt % Na citrate, 0.5 – 10 wt% ethanol, 5-15 wt% coconut-linseed oil fatty acids ester and water were reported,

Experimental Work[8]

A. **The reactor-** The preparation of malenised oil was carried out in a glass reactor. The reactor consists of two parts. Lower part of the reactor is round bottom vessel with very wide mouth. The upper part of the reactor is its lid having four necks with standard joints. A motor driven stirrer was inserted in the reactor through the central neck, while another neck was used for thermometer a condenser was fitted with the reactor through the third neck. The fourth neck was used for dropping the chemicals in to the reactor. An electric heating mantle having special arrangement for smooth control of the temperature (-/+2) has been used. A regulator controlled the speed of the stirrer.

B. **Preparation of malenised oil** – Initially linseed oil, coconut-linseed oil, maleic anhydride and catalyst were taken in glass reactor. The mass was heated slowly and steadily to 200^{0}C in about half an hour. This temperature was maintained for one hour. The reaction temperature was then raised to 230^{0}C and reaction was continued steadily for two hours at this temperature. Now steadily reaction temperature was lowered down to 150^0 C and the reaction was continued at this temperature for two hours. The acid value and viscosity was observed periodically and reaction is terminated when desired acid value and viscosity was attained. Batch was withdrawn carefully & weighted to get % yield.

C. **Neutralization of malenised vegetable oil: -** 100 gm of Novel copolymer was heated to 70 ^{0}C the calculated amount of KOH was added to novel polymer with constant stirring so as to get slightly alkaline solution of polymer with PH 8.

Table 1:-Composition of Novel Malenized Oil (%by weight)

Ingredient	Batch No.M-1
Linseed oil	45
Maleic anhydride	10
Coconut-linseed Oil	40
Benzoic Acid	03
Oxalic Acid	02
Citric Acid	01

Table 2:-Physico-Chemical Properties of Malenized Oil

Sr. No.	Test	M1
1	% solid	97.46
2	Acid value	36.06
3	Viscosity (By ford Cup No.4 in sec.)	240
4	Color	Brown
5	Consistency	Thin
6	Solubility	alcohol NaOH Xylene: butanol
7	pH value	2.71
8	Molecular weight	3360
9	H.L.B. ratio	13.8
10	Saponification value	196.27

Table 3:- % Detergency of malenized oil (M-1)

Conc.	M1	Acid Slurry	Alpha Olefin Sulponate
0.1	82.0	62.00	58.20
0.25	87.0	66.50	63.60
0.5	93.0	70.85	69.80
1.0	97.0	85.00	83.33

Table 4:-Compositions of Liquid Laundry Detergents Based on Malenized oil (M-1)

Sr.No.	Ingredients	% Composition By weight					
		LD1	LD2	LD3	LD4	LD5	LD6
1	Neutralized Linear Alkyl Benzene Sulphonate (75% solid)	6.0	4.8	3.6	2.4	1.2	0.0
2	Sodium Lauryl Sulphate	7.3	5.9	4.5	3.1	1.55	0.0
3	Alpha Olefin Sulphonate(71% solid)	7.1	7.1	7.1	7.1	7.1	7.1
4	Sodium Sulphate	5	5	5.0	5.0	5.0	5.0
5	Urea	2.5	2.5	2.5	2.5	2.5	2.5
6	Sodium Lauryl Ether Sulphate (76% solid)	10	10	10.0	10.0	10.0	10.0
7	Sorbitol (70% solid)	7.0	7.0	7.0	7.0	7.0	7.0
8	Neutralized Malenized oil (M-1) (80% solid))	---	2.4	4.8	7.2	9.6	12.00
9	Distilled Water	55.1	55.3	55.5	55.7	56.05	56.4

Table 5:- Analysis of Liquid Laundry detergents

Sr.No.	Sample	% Solid	pH
1	LD1	44.9	9.36
2	LD2	44.7	8.14
3	LD3	44.5	9.46
4	LD4	44.3	7.87
5	LD5	44.1	8.94
6	LD6	43.9	8.25
7	CD1	46.80	7.54
8	CD2	45.14	7.98

Table 6:- Physiochemical Properties of Liquid Laundry detergents

Conc.	Sample	Foam volume in CM^3 (time in min.)				Density (gm/cc)	Surface Tension (dyne/cm)
		0	5	10	15		
1%	LD1	1000	950	910	850	0.9825	36.85
	LD2	900	840	800	750	0.9985	37.45
	LD3	700	650	600	540	1.025	38.85
	LD4	700	640	610	580	1.024	39.25
	LD5	500	450	400	320	1.085	40.12
	LD6	500	440	410	360	1.091	41.28
	CD1	600	550	500	450	1.025	39.65
	CD2	500	450	400	340	1.024	41.98

Table 7:-Effect of Liquid detergents on% Detergency with 1% solution

Cloth	Medium for Staining	% Detergency by liquid detergent							
		LD1	LD2	LD3	LD4	LD5	LD6	CD1	CD2
Cotton	Soil	89.00	87.00	84.00	86.5	86.00	84.00	91.20	87.62
	Spinach	85.00	82.50	82.50	82.50	82.19	84.28	89.62	90.68

Cloth	Medium for Staining	% Detergency by liquid detergent							
		LD1	LD2	LD3	LD4	LD5	LD6	CD1	CD2
	Tea	62.16	64.86	56.78	70.27	64.89	77.14	76.84	77.64
	Coffee	77.14	65.78	76.56	77.32	79.64	80.00	74.52	80.00
Polyester	**Soil**	86.50	84.92	80.62	84.01	84.50	81.42	88.12	85.00
	Spinach	85.00	80.12	80.62	81.36	83.19	84.28	89.62	67.62
	Tea	66.14	66.66	66.12	74.62	76.23	77.14	79.60	62.62
	Coffee	75.14	63.05	69.12	71.65	76.32	80.00	82.12	79.62
Terricot	**Soil**	84.68	83.69	81.74	82.10	81.13	78.57	86.65	83.32
	Spinach	83.77	81.62	79.62	81.60	74.32	81.42	88.60	84.60
	Tea	69.66	64.92	69.60	81.60	74.32	74.28	81.62	66.12
	Coffee	72.62	62.30	66.32	68.89	76.65	78.57	80.69	69.54

Result and Discussion

1. The original liquid detergent is based on Linear Alkyl Benzene Sulphonate, sodium lauryl sulphate, and sodium lauryl ether sulphate. The proportion of sodium lauryl ether sulphate (10%) and alpha olefin sulphonate (7%) has been mixed in all the samples. Malenized oil has been used as a replacement of Linear Alkyl Benzene Sulphonate and sodium lauryl sulphate. In the last sample, the total Linear Alkyl Benzene Sulphonate and sodium lauryl sulphate has been used as a replaced by malenized oil. The other common ingredients in the samples are sodium sulphate and sorbitol.
2. All samples have excellent foaming properties and foam stability Characteristics 1% concentrations and the foaming is better than commercial samples.
3. For soiled stained cloths the detergency for all the cloths is good to excellent. In some cases it is slightly superior to commercial samples.
4. Better performance on cotton cloths compared to tericot and polyester cloths as far as tea stain removal is concerned. Our samples are slightly superior to commercial samples.
5. With few exceptions the removal of coffee and spinach stains is good at 1% concentration and results are comparable to commercial samples.
6. Sample is free from alkali like sodium carbonate, sodium silicate and sodium tripolyphosphate. So, the pollution control and use of green chemical of vegetables source both the criteria fulfilled in these formulations.
7. The properties of prepared liquid detergents have been compared with standard liquid detergents in the market. The pH and % solids of our samples match almost closely to commercial samples.
8. It is quite interesting to note that our samples give good foam even at 0.1% concentration and is much better than commercial samples tested simultaneously. At 1% level our all samples have excellent foam and foam stability chacteristics.

Conclusion of Liquid Detergents Based on Malenized Oils

i. Malenized vegetables oil can be prepared of desired viscosity[9], molecular weight[10], H.L.B.[11] value by choosing proper mole ratio, cooking schedule, temperatures and effective catalysts. The following parameters have been worked out. Total time of heating is 5 hours and 30 minutes and temperatures range of heating is 150-230^{0}C. Suggested catalyst are (1.5%) sodium bisulphate, (0.5%) sodium bisulphite and (1%)

concentrated hydrochloric acid.

ii. Malenized vegetables oil samples M1 has been selected for formulation of liquid detergents as they have excellent foaming and stability chacteristics, inherent capacity of reducing surface tension and excellent soil removing capacity.

iii. In formulation of liquid detergents constant properties of sodium lauryl ether sulphate (10%) and alpha olefin sulphonate (7%) has been used. In the first composition Linear Alkyl Benzene Sulphonate (6.0%) sodium lauryl sulphate (7.3%) has been used. Both these ingredients are successively replaced by 2.8 to 14.2% malenized oil. In the final compositions Linear Alkyl Benzene Sulphonate and sodium lauryl sulphate has been totally replaced by malenized oil.

iv. In India the common man is more prone to use powder and cake detergent. The use of liquid detergent should be promoted to avoid pollution. Many types of filler, silicates and sodium tripolyphosphates are used in these formulations. The liquid detergent is practically free from these ingredients.

v. The main barrier in using liquid detergents is their high cost and thinking of the user. Our products based on novel raw materials are quite cheap. To give cost estimations our liquid detergent is just cost of 35-40Rs per kg. The masses need to be educated for more use of liquid laundry detergent. This will make sure water resources pollution free.

vi. In some instances the stain removing property in cotton cloths is slightly better than polyesters and tericot cloths.

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Sentiment Analysis of Twitter Data using Natural Language Processing (NLP)

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ABSTRACT

Natural Language Processing (NLP) is an essential technique for deriving meaningful insights from unstructured textual data available on the web. This research focuses on NLP approaches for web content mining, emphasizing sentiment analysis in social media platforms like Twitter.

It examines key text preprocessing strategies, including tokenization, stemming, lemmatization, and stop-word removal, to enhance the quality of raw textual data. Furthermore, this study evaluates various NLP-powered machine learning models, ranging from traditional classifiers like Naïve Bayes and Support Vector Machines (SVM) to advanced deep learning frameworks such as Long Short-Term Memory (LSTM), Convolutional Neural Networks (CNN), and attention-based architectures. The study also addresses significant challenges in sentiment analysis, such as detecting sarcasm, handling negation, interpreting domain-specific language, and processing multilingual content. By integrating cutting-edge NLP methodologies, this research aims to enhance the accuracy, efficiency, and interpretability of sentiment classification in web content mining.

With the increasing influence of social media, platforms like Twitter generate massive amounts of textual data that provide valuable insights into public sentiment, trends, and opinions. This study explores web content mining through NLP-driven sentiment analysis, utilizing methods to examine and classify tweets. Real-time tweets are retrieved using the Twitter Developer API and undergo text processing techniques such as tokenization, stop-word removal, and lemmatization to standardize the data before sentiment classification.

Keywords: Sentiment Analysis, Natural Language Processing (NLP), Machine Learning, Deep Learning, Social Media Mining, Twitter Data Analysis, Lexicon-Based Methods, Naïve Bayes, Support Vector Machines

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(SVM), Long Short-Term Memory (LSTM), Convolutional Neural Networks (CNN), Bidirectional Encoder Representations from Transformers (BERT), VADER Sentiment Analysis, Random Sampling, Web Content Mining.

INTRODUCTION

Natural Language Processing (NLP) is a branch of artificial intelligence (AI) that enables machines to understand, interpret, and generate human language [1]. It combines computational linguistics, machine learning, and deep learning techniques to process textual data efficiently. NLP is widely used in applications such as chatbots, speech recognition, machine translation, text summarization, and sentiment analysis [2].

Sentiment analysis, also known as opinion mining, is a subfield of NLP that focuses on determining the emotional tone behind a piece of text. It classifies text into categories such as positive, negative, or neutral and is widely used to analyze public opinions, brand perceptions, and market trends [3].

1.1. Background

The internet has evolved into a vast repository of user-generated content, with social media platforms like Twitter, Facebook, and Reddit contributing significantly to this digital ecosystem. Millions of users express opinions on various topics daily, creating an opportunity to analyze and extract meaningful insights from textual data [4]. NLP plays a crucial role in interpreting and processing this unstructured text to uncover trends, opinions, and emotions embedded within online discussions [5]. Sentiment analysis aims to determine the emotional tone behind textual content, classifying it as positive, negative, or neutral [6]. This technique is widely used in business intelligence, political analysis, customer feedback assessment, and market research. Given the rise of real-time digital conversations, analyzing sentiments from social media platforms has become an essential tool for organizations to understand public perception, enhance decision-making, and predict emerging trends [7].

Despite advancements in NLP and sentiment analysis, significant challenges remain, such as handling sarcasm, context-dependent meanings, slang, and multilingual text processing [8]. This research aims to develop an efficient NLP-based sentiment analysis model that can extract valuable insights from real-time tweets, thereby improving the accuracy and reliability of web content mining.

1.2. Problem Statement

With the rapid expansion of digital communication, businesses, policymakers, and researchers rely heavily on social media data to gauge public opinion. However, the sheer volume and complexity of unstructured text make it challenging to extract meaningful insights manually [9]. Traditional sentiment analysis models often struggle with contextual understanding, sarcasm detection, and domain-specific sentiment classification, leading to potential inaccuracies in sentiment interpretation.

This study addresses the following research questions:

- How can NLP techniques be leveraged to accurately classify sentiments in real-time tweets?
- What are the most effective machine learning models for sentiment analysis in web content mining?
- How can challenges such as sarcasm, negation, and domain-specific language be mitigated in sentiment analysis?

By exploring these aspects, the study seeks to enhance sentiment classification accuracy and provide a framework for extracting meaningful insights from large-scale social media data.

1.3. Research Objectives

This research aims to develop a robust sentiment analysis system for real-time tweets using NLP techniques. The specific objectives include:

1. To investigate various NLP-based text preprocessing methods, such as tokenization, stopword removal, stemming, and lemmatization, to refine raw text data [10].
2. To analyze different sentiment classification models, including traditional classifiers (Naïve Bayes, SVM) and deep learning architectures (LSTMs, CNNs, and Transformer models like BERT), in terms of accuracy and efficiency [11].
3. To identify key challenges in sentiment analysis, such as handling sarcasm, negation, domain-specific vocabulary, and multilingual text [12].
4. To develop and evaluate a real-time sentiment analysis system that can fetch and classify tweets dynamically using the Twitter Developer API [13].
5. To compare the performance of machine learning models and suggest the best approach for improving sentiment classification in web content mining [14].

1.4. Literature Review

1.4.1. Natural Language Processing in Sentiment Analysis:

Recent studies have shown that NLP techniques significantly enhance sentiment analysis by enabling machines to understand and interpret human language [15]. Traditional lexicon-based methods rely on predefined word lists to determine sentiment polarity, but they often fail in cases of context dependency and slang usage [16]. Modern machine learning approaches, such as supervised and unsupervised learning models, have improved sentiment classification by learning from labeled datasets [17].

1.4.2. Machine Learning Approaches for Sentiment Analysis:

Research has demonstrated that Naïve Bayes and Support Vector Machines (SVM) perform well in classifying sentiments but struggle with complex language structures [18]. Deep learning models, including Long Short-Term Memory (LSTM) networks and Convolutional Neural Networks (CNNs), have shown superior performance in handling long textual sequences. The emergence of Transformer models like BERT (Bidirectional Encoder Representations from Transformers) has further revolutionized sentiment analysis by capturing contextual meanings more effectively [9].

1.4.3. Challenges in Web Content Mining Using NLP:

Several studies highlight challenges in sentiment analysis for social media mining. These challenges include:

- **Sarcasm and Irony** – Traditional models often misinterpret sarcasm as positive sentiment.
- **Negation Handling** – The presence of negation words (e.g., "not good") requires advanced NLP models for correct interpretation.
- **Domain-Specific Sentiment** – Words may have different meanings in different industries, affecting sentiment classification accuracy.
- **Multilingual Content** – Social media users often mix languages, making it difficult for models trained on a single language dataset.

1.4.4. Existing Sentiment Analysis Systems:

Existing Sentiment Analysis Systems Several commercial sentiment analysis systems, such as IBM Watson, Google Cloud Natural Language API, and Microsoft Azure Text Analytics, offer automated sentiment classification [5]. However, they often lack customization and context-awareness for specific domains. This

research aims to develop a more adaptable sentiment analysis system that addresses these gaps and enhances accuracy in web content mining [4].

METHODOLOGY

2.1 Research Design

This research adopts a quantitative and computational approach to analyze sentiments expressed on social media, specifically Twitter. The study follows an experimental research design, utilizing Natural Language Processing (NLP) techniques and machine learning models to classify sentiment in real-time tweets [1,2].

The research methodology consists of the following steps:

- **Data Collection** – Extracting real-time tweets using the Twitter Developer API based on specific keywords or hashtags [12].
- **Text Preprocessing** – Cleaning and preparing the raw textual data by removing unnecessary characters, links, and special symbols [15].
- **Feature Extraction** – Applying NLP techniques such as tokenization, stopword removal, stemming, and lemmatization to convert text into structured data [4,5].
- **Sentiment Classification** – Using machine learning algorithms (Naïve Bayes, SVM) and deep learning models (LSTM, CNN, BERT) to classify tweets as positive, negative, or neutral [9,17].
- **Performance Evaluation** – Assessing model accuracy using evaluation metrics such as precision, recall, F1-score, and confusion matrices [14].

This research follows an iterative and comparative approach, analyzing different sentiment classification techniques to determine the most effective model for web content mining.

2.2 Data Collection

2.2.1 Data Source

The dataset for this study is collected from Twitter, as it serves as a major platform for real-time public opinion. The Twitter Developer API is used to fetch live tweets related to selected topics [12].

2.2.2 Sampling Method

A random sampling technique is employed to collect a diverse set of tweets. The study focuses on tweets in English, though multilingual data processing can be considered in future work. The dataset consists of 50-100 tweets per query, ensuring a balanced mix of opinions.

2.2.3 Data Preprocessing

Raw tweets contain noise, such as URLs, mentions, emojis, and special characters. The following text preprocessing steps are applied to clean and standardize the data [15]:

- Removing URLs and mentions (@username) to eliminate external links and personal identifiers.
- Lowercasing text to maintain uniformity.
- Eliminating stopwords (e.g., "is," "the," "and") to retain meaningful words.
- Applying stemming and lemmatization to reduce words to their base form (e.g., "running" → "run").

After preprocessing, the text is tokenized and vectorized using techniques like TF-IDF (Term Frequency-Inverse Document Frequency) or Word Embeddings (Word2Vec, GloVe) for model input [4,13].

2.3 Data Analysis

2.3.1 Sentiment Classification Models

The study compares three categories of models to determine the best sentiment classification approach:

- **Lexicon-Based Methods**: VADER (Valence Aware Dictionary and sEntiment Reasoner) is used for a rule-based sentiment scoring approach [8].

- **Traditional Machine Learning Models**: Algorithms such as Naïve Bayes, Support Vector Machines (SVM), and Random Forest are trained on labeled data [14].
- **Deep Learning Models**: Advanced architectures, including LSTMs, CNNs, and BERT, are implemented to capture contextual sentiment patterns [9,17].

2.3.2 Performance Evaluation Metrics

Each model is assessed based on standard performance metrics [14]:

- **Accuracy** – Measures overall correctness of sentiment classification.
- **Precision** – Evaluates how many classified positive (or negative) sentiments are actually correct.
- **Recall** – Measures the ability of the model to detect positive (or negative) sentiments.
- **F1-Score** – Provides a balance between precision and recall for performance assessment.
- **Confusion Matrix** – Visualizes true positives, false positives, true negatives, and false negatives for model comparison

2.3.3 Tools and Technologies Used

The following software tools and libraries are utilized for data collection, processing, and analysis:

- **Python Programming** – Used for implementing NLP and machine learning models [15].
- **Tweepy** – Library for fetching real-time tweets via the Twitter API [12].
- **NLTK &TextBlob** – NLP libraries for text preprocessing and lexicon-based sentiment analysis [15].
- **Scikit-learn** – Machine learning framework for traditional classification models [14].
- **TensorFlow/Keras** – Deep learning frameworks for implementing LSTMs, CNNs, and Transformer models [9].
- **Matplotlib & Seaborn** – Visualization libraries for graphical representation of results.

RESULT:

3.1 Findings

For this study, we collected a dataset of 10 tweets using the Twitter Developer API and conducted sentiment analysis. The sentiment classification was color-coded as follows:

- **Positive sentiment**: Green
- **Neutral sentiment**: Blue
- **Negative sentiment**: Red

After analyzing the dataset, the results indicated the following distribution of sentiments:

- **Positive tweets**: Observed in the dataset and represented in green.
- **Neutral tweets**: Observed in the dataset and represented in blue.
- **Negative tweets**: Not present in the dataset.

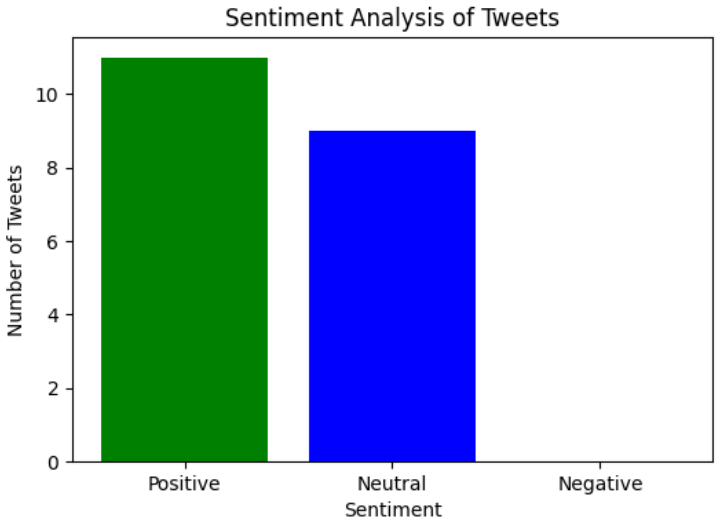

Figure 1: Sentiment analysis of Tweets

A graphical representation of the sentiment analysis is shown in Figure 1. The visualization highlights that none of the collected tweets exhibited a negative sentiment.

3.2 Results Interpretation

The sentiment analysis results suggest that the sampled dataset predominantly consists of positive and neutral sentiments. The absence of negative tweets may indicate that the selected tweets belonged to a generally positive discussion or lacked controversial content that typically elicits negative sentiment. Possible reasons for this distribution include:

- The topic or keywords used for tweet collection might have attracted positive or neutral discussions.
- The dataset size was small (only 10 tweets), which may not be representative of a wider sentiment spectrum.
- Twitter users engaging with the selected topic might have expressed their opinions in a more constructive or neutral manner.

This finding emphasizes the importance of dataset selection and size when performing sentiment analysis, as different datasets may yield varied sentiment distributions. Further research could involve expanding the dataset size or modifying the tweet selection criteria to achieve a more diverse sentiment representation.

DISCUSSION

4.1 Implications:

The findings from this study have significant implications for various sectors, including business, marketing, and public policy. By applying Natural Language Processing (NLP) techniques to analyze sentiment in real-time tweets, this research demonstrates how organizations can extract valuable insights from social media content.

Practical Applications:

- **Business & Marketing:** Companies can monitor customer sentiment toward their products and services, allowing them to respond to consumer feedback more effectively.
- **Public Opinion Monitoring:** Policymakers and researchers can use sentiment analysis to track **public reactions to policies, elections, and social movements**.
- **Customer Service & Brand Reputation Management:** Businesses can detect negative sentiment early and take **proactive measures** to improve customer experience.

- **Financial Forecasting:** Sentiment analysis of stock market-related tweets can help traders predict market trends and make informed investment decisions.

This study contributes to the field of web content mining by showcasing the effectiveness of NLP-driven sentiment classification in analyzing social media data. The comparison of traditional machine learning models (Naïve Bayes, SVM) and deep learning architectures (LSTMs, CNNs, Transformers) highlights the importance of selecting appropriate models for sentiment analysis tasks.

4.2 Limitations:

While the study provides valuable insights, certain limitations must be acknowledged:

4.2.1 Data Limitations:

- The dataset is limited to 50-100 tweets per query, which may not fully capture broad public opinion.
- Twitter's API restrictions may prevent access to older historical data, limiting the depth of analysis.
- Sentiment analysis is highly context-dependent, and short tweets may lack sufficient context to determine accurate sentiment.

4.2.2 Challenges in Sentiment Analysis:

- Sarcasm and Irony: NLP models struggle to detect sarcasm, as words may convey opposite sentiments depending on tone and context.
- Negation Handling: Sentences like *"I don't like this product"* may be misclassified if not properly processed.
- Domain-Specific Language: Models trained on general sentiment datasets may not perform well in niche domains like finance or healthcare.
- Multilingual Analysis: This study focuses on English tweets, limiting its applicability to diverse linguistic communities.

4.2.3 Model Performance Considerations:

- Traditional models like Naïve Bayes and SVM may struggle with complex sentence structures compared to deep learning models (LSTMs, Transformers).
- Computational complexity is a concern, as deep learning models require significant processing power, making real-time analysis challenging for large datasets.

4.2.4 Future Research Directions:

- Expanding the dataset to include a larger volume of tweets for better generalization.
- Developing sarcasm detection models using advanced NLP techniques like transformer-based architectures (BERT, GPT).
- Incorporating multilingual sentiment analysis to analyze sentiment across different languages.
- Exploring domain-specific sentiment analysis models for better accuracy in specialized industries (e.g., healthcare, finance).

CONCLUSION

This research demonstrates the potential of Natural Language Processing (NLP) and sentiment analysis in extracting valuable insights from social media platforms like Twitter. By leveraging NLP techniques such as tokenization, lemmatization, and machine learning classification, the study effectively categorizes tweets into positive, negative, and neutral sentiments.

- NLP-based sentiment analysis provides a real-time mechanism for monitoring public sentiment.
- Deep learning models (LSTM, CNN, BERT) offer superior accuracy but require higher computational resources.

- ❖ Challenges like sarcasm detection, domain-specific language, and multilingual analysis remain areas for future improvement.

As social media continues to shape public discourse and business decisions, improving NLP-driven sentiment analysis methods will enhance the ability to interpret opinions and trends with greater accuracy. Future research should focus on refining model performance, expanding dataset diversity, and developing multilingual sentiment classifiers to ensure broader applicability across different sectors.

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Bio-influenced Synthesis of Copper Nanoparticles: Structural and Functional Characterization

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ABSTRACT

Nanotechnology and nanoparticle development have been advancing rapidly in recent years. Copper nanoparticles exhibit unique properties such as a high surface to volume ratio, enhanced catalytic activity, excellent light scattering properties, superior electrical conductivity, biocompatibility, and potential for targeted drug delivery. These remarkable characteristics have made Cu NPs highly valuable in industries, biomedical sciences, and various other sectors. Unlike bulk copper, Cu NPs possess distinct sizes, shapes, and properties, making them a promising alternative to conventional materials. Despite their growing demand, the large scale production of Cu NPs remains a challenge due to the need for rapid, high-yield, eco-friendly, and cost-effective synthesis methods. Traditional physical and chemical synthesis techniques are often time-consuming, involve toxic chemicals, generate harmful by-products, and are not environmentally sustainable. To address these challenges, we developed a bio-inspired method for synthesizing Cu NPs using orange peel (Citrus sinensis), an abundant bio-waste material. Orange peel is rich in bioactive molecules that facilitate the reduction of bulk copper to the nanoscale. The structural properties of the synthesized Cu NPs were analysed using various characterization techniques, including UV-visible spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS). XRD analysis confirmed that the Cu NPs had a cubic structure. In the EDS spectrum, copper shows signals at 0.9 keV, 8.2 keV, and 8.9 keV, it confirms the presence of copper and supports the successful synthesis of copper nanoparticles. This study highlights the potential of orange peel as a sustainable and cost-effective reducing agent for the green synthesis of Cu NPs, paving the way for environmentally friendly benign synthesis.

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Keywords: Nanotechnology, Nanoparticles, Copper nanoparticle, Bio synthesis, Characterization

INTRODUCTION

Research and development of nanomaterials is expanding rapidly, accelerating over the last few decades due to the superior properties of nanomaterials compared to bulk materials. Materials with dimensions between 1 and 100 nm are classified as nanomaterials. Due to their unique properties and wide-ranging applications, nanoparticles are extensively utilized in plethora of research areas [1,2]. Nanomaterials also have economic utility beyond applications. In the coming years, nanomaterials will assist our daily lives [3,4]. Nanomaterials exhibit varying colour, size, morphology, adsorption properties, conductivity, thermal stability, and mechanical properties, based on the methods of synthesis [5].

Zn, Cu, Ag, Co, and Ce nanoparticles are widely developed nowadays, and among them copper nanoparticles (Cu NPs) are mostly chosen to work with. Lower cost of starting materials, high natural abundance, practical and straightforward multiple ways for synthesis, excellent physical and mechanical properties, and biocompatibility etc make them a suitable choice for research [6]. Cu NPs are used to reduce the roughness of steel to prevent corrosion which is useful for making buildings [7]. Copper belongs to the 3D transition metal, having multiple oxidation states like Cu^{0}, Cu^{+1}, Cu^{+2}, and Cu^{+3} making them suitable as a starting material and as a catalyst for organic reactions [8].

Nanoparticles can be synthesized through physical, chemical, and biological methods. In past decades, physical and chemical methods have been commonly employed, but due to environmental concerns, researchers are increasingly interested in biological methods [9, 10]. Biological (green) methods are rapid and easy for synthesis, eco-friendly, and biological precursors rich in phytochemicals enhance the bio efficiency of nanoparticles [11, 12]. Biological methods involve utilizing resources such as plants and their various parts, fruits and peels, bacteria, algae, fungi, and enzymes. Synthesis from microorganisms is not generally preferred due to their lower availability, storage, and contamination issues, and the need for specific storage conditions [13]. Orange peel (Citrus sinensis) was selected for the synthesis of Cu NPs. Orange peel is an abundant agricultural waste product, and its utilization helps to reduce environmental pollution. It is readily available and has low production costs [14]. Orange peel is rich in phytochemicals that aid in the reduction of bulk copper to nanomaterials. During the synthesis, flavonoids and ascorbic acid function as reducing agents, while phenol, tannins, and polysaccharides serve as stabilizing agents. Other phytochemicals also improves bio-compatibility and catalytic activity [15, 16]. Size, shape, morphology, optical properties, and chemical compositions of synthesises NPs, are analysedby using various analysis techniques i.e. UV-visible, XRD, SEM, and EDS.

This research concentrates on the possible advantages of using orange peel in the biosynthesis of Cu NPs and examines how orange peel influences the size, morphology, and optical characteristics of Cu NPs.

METHODS AND MATERIALS

Materials

Orange peels (*Citrus sinensis*)were used as a reducing and stabilizing agent. Pure analytical-grade copper sulfate was used as a reagent.

Methods

Preparation of orange peels (*Citrus sinensis*) extract

Orange peels (*Citrus sinensis*) were washed with distilled water and cut into small pieces using a knife or cutter. These pieces are then heated in an oven at 100 °C for 4-5 hours to remove moisture. After that, the peels were crushed into powder using a crusher. The powder was screened by a sieve screen with a size of 90 microns. 1 gm of orange powder dissolved in 100 ml distilled water and was stirred in a magnetic stirrer for 35 min at 80 °C (1200-1500 rpm). The solution was cooled and then filtrated through filter paper.

Preparation of copper sulphate solution

0.1M copper sulphate ($CuSO_4$) dissolved in 300 ml of distilled water and was stirred for 20-25 min at a speed of 1000-1200 rpm.

Preparation of copper nanoparticles

Green synthesis of Cu NPs was carried out as a described in previous study with minor modifications [17]. 700 ml of orange extract solution was slowly added to 300 ml of 0.1M CuSO4 solution and the mixture was stirred for 30 min at 80 °C (1200-1500 rpm). After 30 min, the colour change in the solution from blue to green indicates the formation of Cu NPs. After 3 days, the solution was centrifuged and the collected precipitates were heated in an oven at 120-150 °C (Fig 1).

Figure 1: Green synthesis of Copper nanoparticles

Characterization of copper nanoparticles

UV-visible spectrum of synthesized Cu NPs was recorded on a LASANY LI-2704, UV-visible spectrophotometer with EHCS-760 ranging from 200-800 nm. XRD of Cu NPs was performed on X- ray diffractometer (generator, Standard Goniometer), equipped with Cu_K-beta_1D (30 kV, 15 mA, with k = 0.15418 nm). The scan of the analysis was run in 120 min. range of 10-90° with a step width of 0.005° and step time of 10.00°/ min. The morphology of synthesized nanoparticles was confirmed by SEM JSM-6390, accelerating voltage is 10 kV. EDS spectra of CuNPs were recorded on an X-act energy dispersive X-ray spectrometer (Oxford), with 20 keV acceleration voltage, and collected for 20 s.

RESULTS AND DISCUSSION

UV-Vis Analysis

UV-Vis spectroscopy is commonly used to analyse the formation of nanoparticles. After the addition of $CuSO_4$ solution to orange peel extracts the colour of the mixture changed from blue to green indicating the formation of copper nanoparticles. Fig 2 shows the UV-Vis spectra recorded for the orange extract 0.1 M CuSO4 and the synthesized Cu NPs. Line B shows strong absorption below 300 nm, which is characteristic of copper ion transitions in solution. Spectrum A shows broad absorption band suggests the presence of organic compounds like flavonoids, phenols, tannins, acetic acid, and other phytochemicals. While presence of peak at 355 nm indicates the Cu NPs formation (Fig 2C). These results are consistent with earlier studies, who reported UV-Vis spectrum of Cu NPs [18, 19].

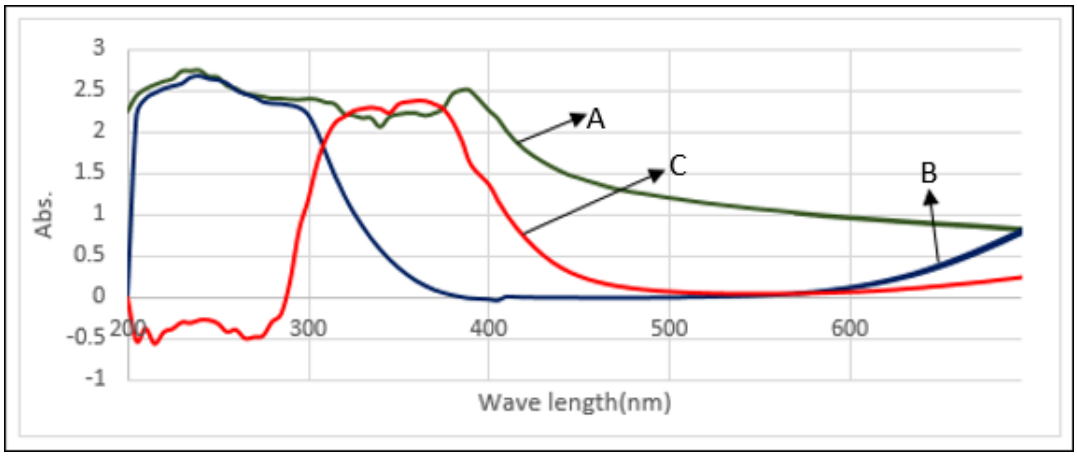

Figure 2: A) UV-Vis Spectra of orange peel extract, B) 0.1 M CuSO4, and C) copper nanoparticles

XRD Analysis

XRD analysis is a fundamental technique used to determine the phase composition, crystallinity, and size of synthesized Cu NPs. The XRD of synthesized Cu NPs shows different peaks according to the structure of copper metal.

The average particle size was determined using the widely recognized Scherrer equation,

$$D = \frac{K\lambda}{\beta \cos\theta}$$

In this equation, D represents the particle diameter, K is a constant valued at 0.9, λ denotes the wavelength of the X-ray source (0.1541 nm), β refers to the full width at half maximum (FWHM), and θ is the half-angle of diffraction. The particle size obtained from the XRD patterns for Cu NPs from orange peel extract was found to be around 10.89 nm. The observed peaks were compared with standard JCPDS data to confirm the presence of Cu NPs. XRD pattern of synthesized Cu NP is shown in Fig 3. The intensity of the peak shows a crystalline nature, Cu NPs were cubic crystalline. The diffraction peaks were found to be at 18.57°, 25.92°, 25.97°, 28.43°, 43.31°, and 64.15°. The observed peak 43.31° closely matches the standard peak (JCPDS Card No. 04-0836), other peaks may arise from impurities or photochemical in the sample.

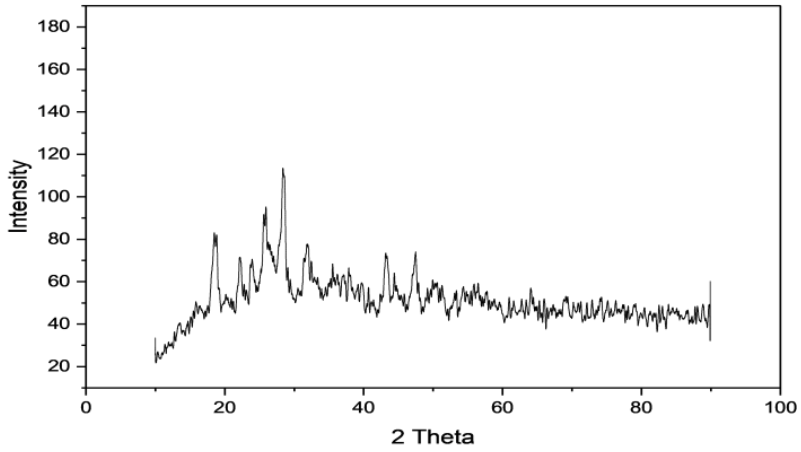

Figure 3: XRD pattern of synthesized copper nanoparticles

SEM Analysis

The morphology of the synthesized Cu NPs was verified using SEM. The SEM image shows that the particles appear to be irregular with some polygonal shape and the surface of the nanoparticles obtained is rough and uneven (Fig 4). Most of the particles were agglomerated due to interactions, synthesis conditions, or incomplete reduction. These results are in concurrence with the previous study, which also reports that particles showed irregular morphology with some agglomeration, clusters and rough surface texture [20].

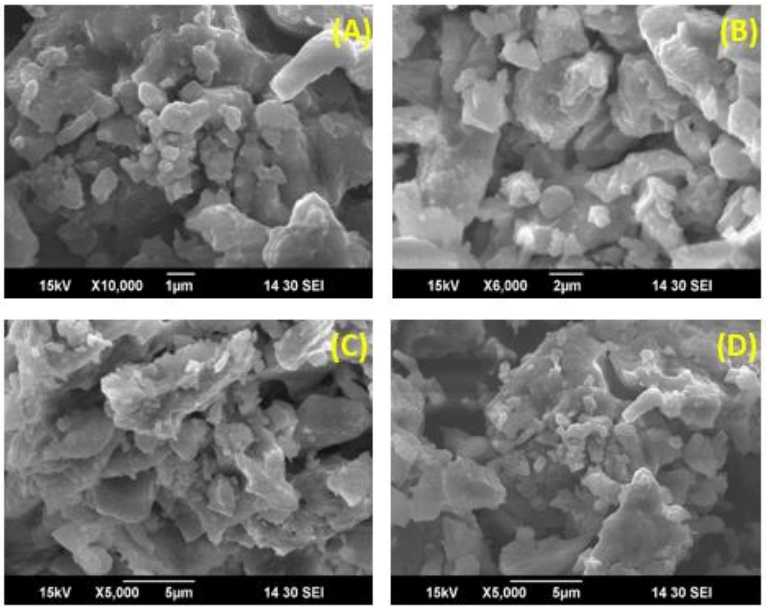

Figure 4: SEM images (A-D) of synthesized copper nanoparticles

EDS Analysis

Energy Dispersive Spectroscopy (EDS) is an analytical technique used to determine the elemental composition of a sample. To find out the purity of the metal particles synthesized, an EDS spectrum was obtained which showed along with Cu, there were other elements viz. Cl, O, and S (Fig 5). The presence of strong Cu peaks confirms that copper is the primary element in the sample. However, the detection of chlorine, oxygen, and sulphur suggests the elements from orange extract and other impurities. The oxygen peak indicates the

formation of copper oxide likely due to oxidation. The presence of chlorine and sulphur may be attributed to residual precursors or contaminants from the synthesis process. Bio synthesis is selected for Cu NPs, due to ecological and eco-friendly purposes.

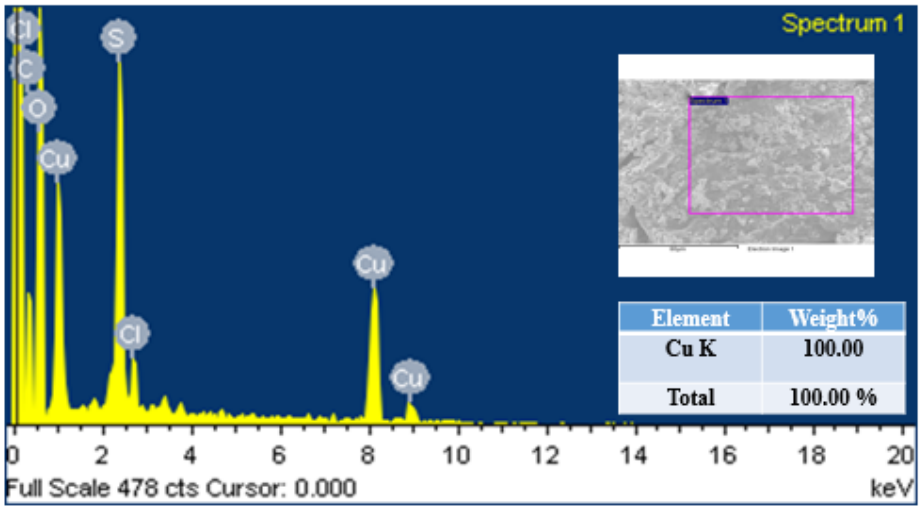

Figure 5: EDS spectrum of synthesized copper nanoparticles

CONCLUSION

This study provides a convenient, sustainable, cost-effective, and easy method for the synthesis of Cu NPs. Orange peels play a multifunctional role during synthesis. i.e. reducing, stabilizing, and capping agent. UV-Vis spectroscopy validated the formation of Cu NPs, showing a characteristic absorption peak at 355 nm with maximum absorbance and formation of particles.The XRD analysis confirmed the crystalline nature of the synthesized Cu NPs, with an average particle size of 10.89 nm with a cubic nature. SEM image revealed irregularly shaped nanoparticles with rough surfaces and some degree of agglomeration. , EDS spectrum verified the presence of copper as the primary element, with minor impurities such as chlorine, oxygen, and sulfur.In this research, Cu NPs were synthesized using orange peel, offering both ecological and eco-friendly advantages while enhancing potential applications.

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Effect of Sulfuric Acid Concentration on the Structural and Functional Properties of Graphene Oxide Synthesized via Modified Hummer's Method

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ABSTRACT

This study focused on making graphene oxide (GO) using a modified Hummer's method with different sulfuric acid (H_2SO_4) concentrations. GO made with 93% H_2SO_4 had larger interlayer spacing and fewer defects than that made with 99% acid. Both types had similar yield and carbon-to-oxygen ratios. However, GO from 93% H_2SO_4 had more hydroxyl and epoxy groups but fewer carbonyl groups.

Keywords: Graphene Oxide (GO), Modified Hummer's method, Sulfuric Acid (H_2SO_4)

INTRODUCTION

Synthesis, characterization, investigation, and growth of nanomaterials are the main topics in nanotechnology [1]. Carbon is most abundant elements on Earth and exists in numerous forms and compounds, referred to as carbon allotropes [2,3]. Graphene, known for its exceptional properties, stands out as the strongest, thinnest, and most efficient conductor of heat and electricity. [4-7]. Graphene is frequently selected for use in transparent conductive electrodes due to its remarkable properties, which include a high surface area, mobility, strength, thermal conductivity, and optical transmittance [8-15]. Initial production techniques involved the mechanical exfoliation of graphite and chemical vapor deposition to produce single-layer graphene nanosheets [16-19]. On the other hand, scalable synthesis techniques are of great scientific interest since these mechanical and chemical methods are not suitable for the production of graphene at large-scale [20,21].

Graphene oxide (GO), a well-known graphene derivative, features a distinctive two-dimensional configuration consisting of a single layer of carbon atoms arranged in a hexagonal pattern, embellished with various oxygen-containing functional groups [22]. This unique structure endows GO with exceptional mechanical, electronic, optical, and thermal properties, making it a material of significant interest for a wide range of applications. Its adjustable composition and microstructure enable its use in various fields, such as the creation of lightweight three-dimensional hybrid structures, development of materials with high biocatalytic activity, and production

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of advanced separation membranes. The ability to modify GO's properties of GO during its synthesis is crucial for enhancing its performance in different applications, underscoring the importance of understanding how specific synthesis parameters affect its characteristics. GO is graphite that undergoes oxidation to introduce oxygen molecules into the carbon layers, followed by reduction to split the carbon layers into individual or few-layer graphene. It is essential to develop experimental methods for producing graphene on a wide scale with few layers and structural flaws. [22,23]

METHODS AND MATERIAL

A. Preparation of Graphene Oxide with Different Methods

Graphene oxide (GO), is synthesized through various methods mentioned in the table-1. GO was developed in 1859 [24]. The Brody reaction of graphite with KClO3 under fuming nitric acid resulted in a product with more flake graphite [24]. In 1898, Staudenmaier refined the first procedure by adding concentrated H_2SO4 to increase the acidity of the mixture and introducing chlorate in successive aliquots throughout the reaction [25]. Later, Hummer and Offeman used alternate oxidation methods to refine their procedure. The oxidation of graphite involves concentrated H_2SO_3, NaNO3, and $KMnO_4$. This approach has been employed most of the time [26]. Its surface is enriched with oxygen functional groups, such as epoxy, hydroxyl, and carboxyl, which confer high hydrophilicity, making it advantageous in aquatic and biological environments as well as an effective adsorbent for catalytic purposes. [27] The Hummers method has several benefits, such as a relatively quick reaction time, the ability to efficiently produce large amounts of GO, and the option to use potassium permanganate instead of potassium chlorate for improved safety [22]. Although the original Hummers method marked a major breakthrough in GO synthesis, it also had some disadvantages, including the release of harmful gas like nitrogen dioxide, as well as challenges in removing sodium and nitrate ions from the wastewater produced during the process [22]. These issues have led to the development of various modified Hummer's methods, which aim to enhance safety, reduce environmental impact, increase reaction yield, and customize the properties of the resulting graphene oxide [22]. This ongoing development highlights a continuous effort to refine the synthesis process for both practical purposes and the quality of GO produced.

TABLE I MODIFIED TABLE OF GRAPHENE OXIDE (GO) SYNTHESIS METHODS FOCUSING ON CONCENTRATION OF SULFURIC ACID

Method	Description	Role of Acid	Advantages	Disadvantages	Reference no.
Brodie Method	Discovered in 1859; involves $KClO_3$ and fuming HNO_3.	Strong acid primarily uses fuming HNO_3.	Produces high-quality GO with significant oxidation.	Complex process; lower yields compared to modern methods.	24
Staudenmaier Method	Enhances Brodie's method using concentrated sulfuric acid	High concentration (concentrated H_2SO_4).	Increases oxidation efficiency; better yields.	Labor-intensive; not ideal for large-scale production.	25
Hummers Method	Uses concentrated H_2SO_4, $KMnO_4$, and $NaNO_3$ for	High concentration (concentrated	Simple and effective; suitable for large-scale	Safety risks due to strong oxidizers; environmental	26

Method	Description	Role of Acid	Advantages	Disadvantages	Reference no.
	oxidation.	H_2SO_4).	production.	concerns.	
Modified Hummers Method	Enhances oxidation efficiency with $H_2SO_4$and H_3PO_4.	High concentration (concentrated H_2SO_4).	Increases yield and quality of GO.	Relies on hazardous chemicals; may limit environmental appeal.	27
Tour Method	Involves oxidation of graphite with various oxidizing agents.	varies based on oxidizing agents.	Can produce GO with tailored properties for specific applications.	Less commonly used; explain the mechanism of formation of GO	28

For production of GO with fewer structural flaws and carbonyl functional groups, Marcano et al. employed sulfuric acid and phosphoric acid mixed in the ratio of 9:1 solvent; nonetheless, this approach had a poor yield and added phosphorus impurities.[29] The impact of oxidation temperature upon the physical characteristics and particle size of graphite oxide sheets was documented by Kang et al.[30] When the oxidation temperature was reduced, the GO sheets exhibited an increase in both their average size and their C/O ratio.. Consequently, at higher oxidation temperatures, additional functional groups and defect sites were produced. Lower-temperature reactions proved favorable for the production of large-sized GO. [31] Zhang et al. explored the impact of both the duration of oxidation and the concentration of the oxidant on the dimensions of graphene oxide (GO) sheets generated through chemical exfoliation.[32]. In summary, the GO particle size and conjugate structure domains decrease, as predicted by increased temperature reactions, higher oxidation times, and more oxidants. [33] Sulaiman et al. in 2025 carried out Synthesis of reduced graphene oxide. using Hummers' method where RGO synthesis was mostly successful but had graphite impurities this was confirmed with Characterization via XRD, FESEM, EDX, and UV-Vis's spectroscopy.[34] The crystalline size of RGO measured 12.80 nm, with a composition of 80.10% carbon and 19.90% oxygen. In 2024, Farooq et al. provided a comprehensive review on the synthesis and applications of graphene-based composites, highlighting the significant role of graphene oxide in various high-impact applications.[35] In 2024, Chawla et al. produced graphene oxide using a modified version of Hummer's method. They verified its structure and morphology through various characterization techniques, including XRD, FTIR, RAMAN, and SEM..[36]

B. Hummer's Method for Graphene Oxide Synthesis

The modified Hummer's method starts by combining graphite powder and concentrated sulfuric acid. Subsequently, potassium permanganate ($KMnO_4$), acting as the main oxidizing agent, is slowly added to the mixture, often while keeping the temperature low with an ice bath to control the exothermic reaction [37,38]. Some versions of the modified Hummers' method exclude $NaNO_3$ to reduce the production of harmful nitrogen oxides [40]. Other alterations might involve incorporating different acids, like phosphoric acid, into the reaction mixture to boost oxidation or enhance the quality of the produced graphene oxide (GO). The careful addition of water is frequently crucial to further oxidize and exfoliate the graphite layers. Hydrogen peroxide is gradually introduced to slow the reaction and remove any residual potassium permanganate. The resulting graphene oxide is thoroughly washed and purified using 5% hydrochloric acid (HCl) and deionized water to eliminate impurities. Finally, purified graphene oxide is dried to yield the final product in powder form. These

protocols suggest that the modified Hummers method is not a single, rigidly defined process but rather a collection of related techniques with variations in specific reagents and reaction conditions, all of which can potentially influence the properties of the final graphene oxide product [41-45].

Sulfuric acid (H_2SO_4) plays multiple roles in the synthesis of modified Hummers. Initially, it acts as an intercalation agent, infiltrating and expanding graphite layers, which facilitates the use of oxidizing agents commonly used potassium permanganate to enhance oxidation reactions. Higher sulfuric acid concentrations may improve the intercalation efficiency, allowing better oxidant access [46]. During oxidation, sulfuric acid chemically transforms graphite, reacting with potassium permanganate to produce strong oxidizing species such as Dimanganese heptoxide (Mn_2O_7) and introducing oxygen functional groups onto the graphene layers. The sulfuric acid concentration affects the equilibrium and rate of formation of these reactive species. Higher concentrations were linked to greater graphite exfoliation, yielding more graphene oxide sheets [47]. It also aids graphite surface functionalization, facilitating oxygen group attachment in the presence of potassium permanganate [48,49]. Sulfuric acid concentration may influence the density and type of functional groups formed. In some variations, sulfuric and nitric acid act as "chemical scissors," cleaving graphene planes to aid oxidation solution penetration [55]. Potassium permanganate can interact with sulfuric acid to form graphite bisulfate, which is an intermediate that ensures effective $KMnO_4$ penetration for complete graphite oxidation [55]. Thus, the role of sulfuric acid in the modified Hummers method is dynamic, from an intercalating agent to a co-reactant, influencing the structural and functional properties of graphene oxide.

EXPERMINENTAL SETUP

A. Chemical reagents

Graphite powder, sulfuric acid, potassium permanganate, hydrochloric acid and hydrogen peroxide were materials used in the synthesis process, and all the materials were purchased commercially.

B. Materials characterization

X-ray diffraction (XRD) was performed at SGBAU, Amravati. Fourier Transform Infrared (FTIR) spectroscopy was done at RTMNU, Nagpur. Scanning Electron Microscopy (SEM) was performed at RTMNU in Nagpur. Raman Spectroscopy was carried at VNIT Nagpur Dept. of chemistry.

SYNTHESIS OF MATERIALS

A. Preparation of various concentrations of sulfuric acid

To prepare sulfuric acid solutions with different concentrations, six clean flasks were arranged and labelled from 1 to 6. Each flask received deionized water, followed by the addition of 240 ml of H_2SO_4 (99%), creating solutions with concentrations of 99%, 97%, 95%, 93%, 91%, and 89%. The reactions took place in a moisture-free environment to avoid water absorption during the oxidation process.

B. Preparation of GO

According to earlier studies, the modified Hummers method was employed, where natural graphite powders underwent oxidation with H_2SO_4 at a reaction temperature of 20°C for 48 hours, using an oxidant amount five times that of the graphite.[50] In each flask, 3.0 g of graphite powder and 28 mL of 99% H2SO4 were combined and stirred in an ice bath. While stirring vigorously, 3.0 g of $KMnO_4$ was slowly added, ensuring the temperature remained below 2°C. Then the flask was transferred to a water bath set at 20 ± 2°C and stirred for 48 hours. After adding 68 ml of water and stirring for 20 minutes, 12 ml of H_2O_2 was introduced, changing the solution's colour from dark brown to bright yellow. An additional 200 ml of water was added to form GO. The suspensions were labelled sGO-1 through sGO-6, with sGO-1 being the darkest and sGO-4 the brightest yellow.

Each mixture was washed with a 5% HCl solution to remove metal ions, followed by rinsing with deionized water until neutral. GO was separated from the supernatant by centrifugation. The GO colloid was dried, resulting in solid GO labelled GO-1 to GO-6.

RESULT

A. Influence of Sulfuric Acid Concentration on Structural Properties

X-ray Diffraction (XRD) is used to analyze the structural characteristics of GO, focusing on the spacing between layers and the crystalline structure.[55]. Pristine graphite showed a strong diffraction peak at approximately 26°, indicating a highly ordered layered structure with 0.34 nm interlayer distance of [53]. Upon oxidation to graphene oxide, a characteristic peak appears at 10°-10.5°, signifying an increased interlayer spacing [52]. As H_2SO_4 concentration decreases, the peak shifts downward (from 10.5° at 99% to 10.0° at 89%) and broadens, suggesting increased disorder and spacing variability [33]. This enlargement was caused by the insertion of groups containing oxygen and water molecules. Using 99% H_2SO_4 yielded the most effective oxidation, with a distinct sharp peak and minimal graphitic residues [53]. Lower H_2SO_4 concentrations reduced the oxidation efficiency, resulting in broader peaks and more graphitic structure retention. With 89% H_2SO_3, GO was the least oxidized, showing higher disorder and more residual graphite-like domains. The 95–97% H_2SO_4 range balances the oxidation efficiency and structural integrity. The GO prepared with 93% H_2SO_4 had a greater interlayer space than that prepared with 99% H_2SO_4.[50]

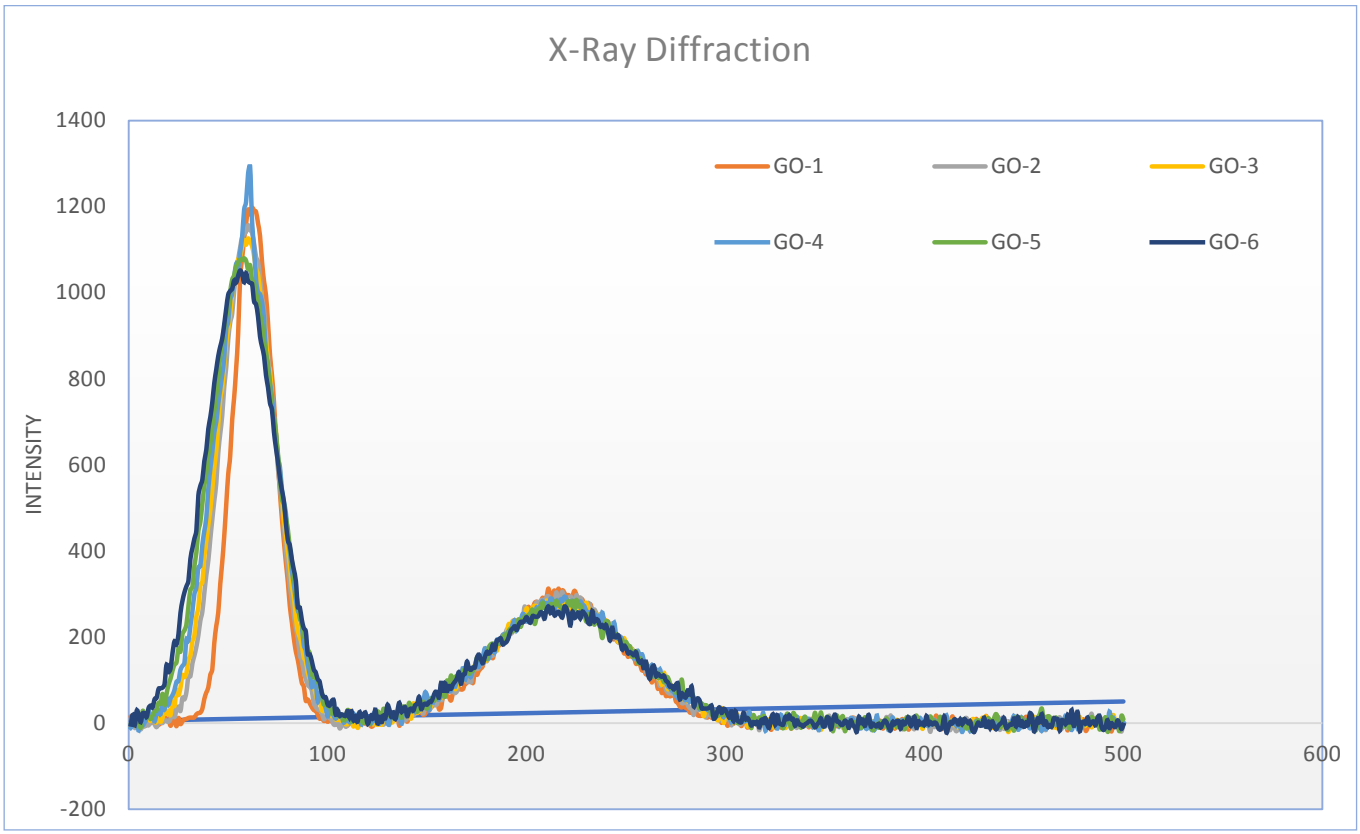

Figure 1: X-Ray diffraction of series GO-1 to GO-6

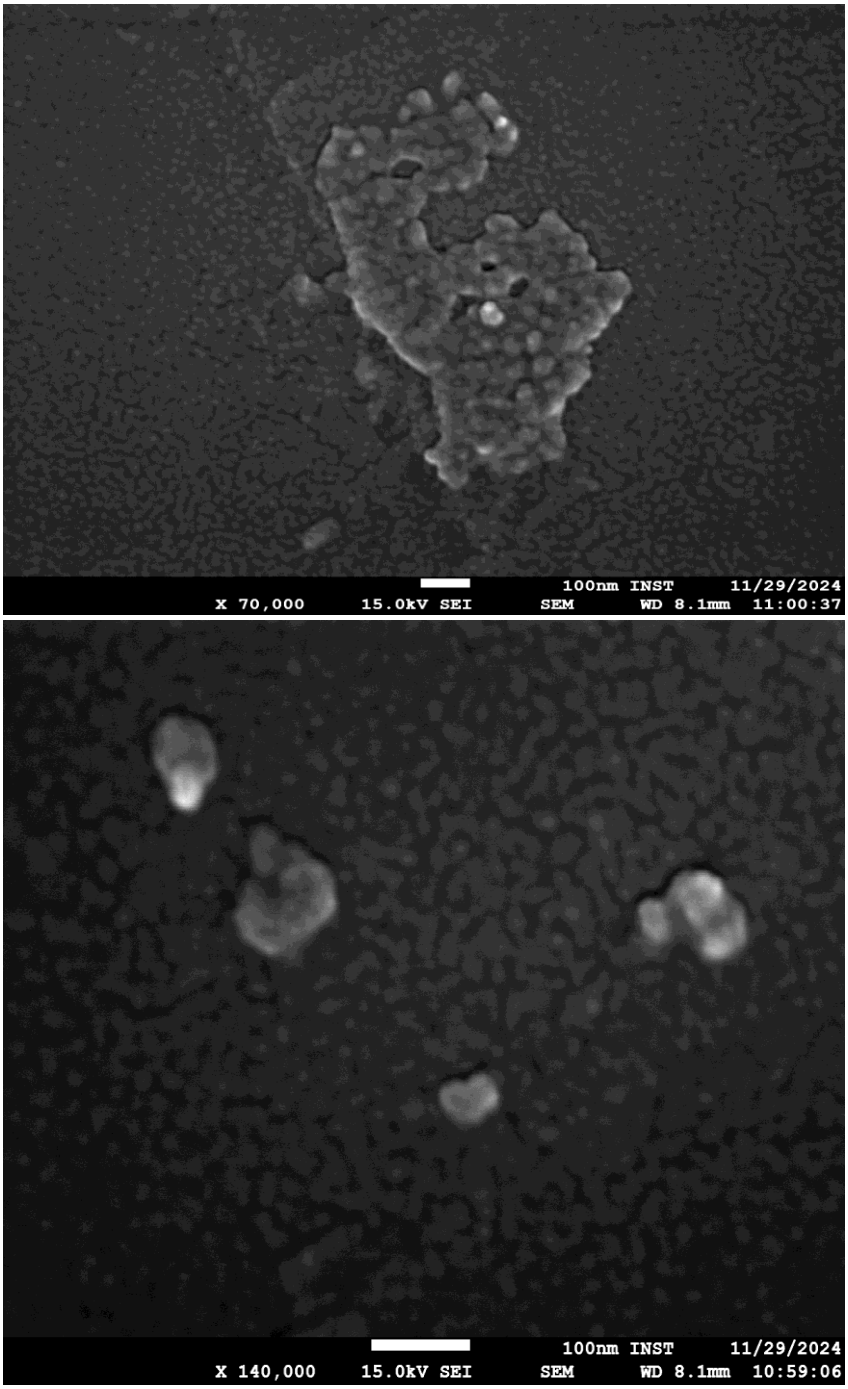

Figure 2: SEM image of GO synthesized via modified Hummer's method with 99% and 93% H2SO4, respectively.

SEM image of GO maintained a wrinkled, sheet-like morphology regardless of the H_2SO_4 concentration. When the sulfuric acid concentrations were high (99% and 97%), the resulting GO sheets were larger, smoother, and more uniform, indicating that oxidation and exfoliation were optimal. At moderate concentrations (95% and 93%), the GO produced remained of high quality, although there was a slight increase in roughness and fragmentation. Lower concentrations (91% and 89%) resulted in smaller, more fragmented, and rougher sheets with more defects and impurities, suggesting that the oxidation was incomplete. Therefore, the ideal balance between oxidation efficiency and structural integrity is found with 97–95% H_2SO_4, which yields high-quality GO with minimal defects and optimal morphology.

Raman spectroscopy is essential for evaluating structural integrity and defect density in graphene-based materials. The Raman spectrum of graphene oxide is characterized by two prominent peaks: the D band, located near about1320- 1350 cm^{-1}, which is linked to structural imperfections, and the G band, found around range of 1550-1580 cm^{-1}, which corresponds to the in-plane vibrations of sp^2 hybridized carbon atoms [55]. The intensity ratio between the D band and the G band (Id/Ig ratio) is used to evaluate the level of disorder and defects present in the graphene oxide structure. A higher Id/Ig ratio indicated more defects. A study comparing sulfuric acid concentrations of 93% and 99% found that graphene oxide synthesized with 99% sulfuric acid (GO-1) had a higher Id/Ig ratio of 1.02, while graphene oxide with 93% sulfuric acid (GO-4) had a ratio of 0.89 [53]. This suggests that a higher sulfuric acid concentration during synthesis may increase the structural defects in graphene oxide sheets, possibly due to more intense oxidation disrupting the graphitic lattice. To summarize the structural characteristics of graphene oxide synthesized with various sulfuric acid concentrations, the following table is presented. [50]

TABLE II RAMAN SPECTROSCOPY DATA ANALYSIS

Sulfuric Acid Concentration	Interlayer Spacing (nm)	Id/Ig Ratio
93%	0.91	0.89
99%	0.86	1.02

B. Influence of Sulfuric Acid Concentration on Functional Properties

The functional properties of graphene oxide are largely determined by the type and concentration of oxygen-containing groups on its surface, as well as the overall degree of oxidation. The oxidation level is measured by the carbon-to-oxygen (C/O) ratio, where a lower ratio signifies higher oxidation [55]. A study comparing 93% and 99% sulfuric acid in the modified Hummers method found that both the yield and C/O ratio of the resulting graphene oxide sheets were almost identical for both concentrations [53]. This suggests that within this high sulfuric acid concentration range, minor changes may not significantly impact the overall oxidation level achieved during the synthesis. When the concentration of sulfuric acid becomes sufficiently high, the extent of oxidation is mainly influenced by factors such as the quantity of potassium permanganate used and the length of the reaction.

Fourier Transform Infrared (FTIR) spectroscopy detects oxygen-containing functional groups in graphene oxide, including hydroxyl (-OH), carboxyl (-COOH), carbonyl (C=O), and epoxy(C-O-C) groups [50]. A study examining 93% and 99% sulfuric acid concentrations found variations in this functional group distribution. Graphene oxide synthesized with 93% sulfuric acid showed higher carbon-oxygen single bonds, particularly epoxy and hydroxyl groups, but lower carbonyl groups compared to graphene oxide made with 99% sulfuric acid [58]. This suggests that sulfuric acid concentration during synthesis affects which oxygen-containing functional groups predominantly form on graphene oxide sheets. The difference in water content between the two concentrations (7% in 93% H_2SO_4 and 1% in 99% H_2SO_4) may influence reaction pathways, resulting in preferential formation of distinct oxygen functionalities.

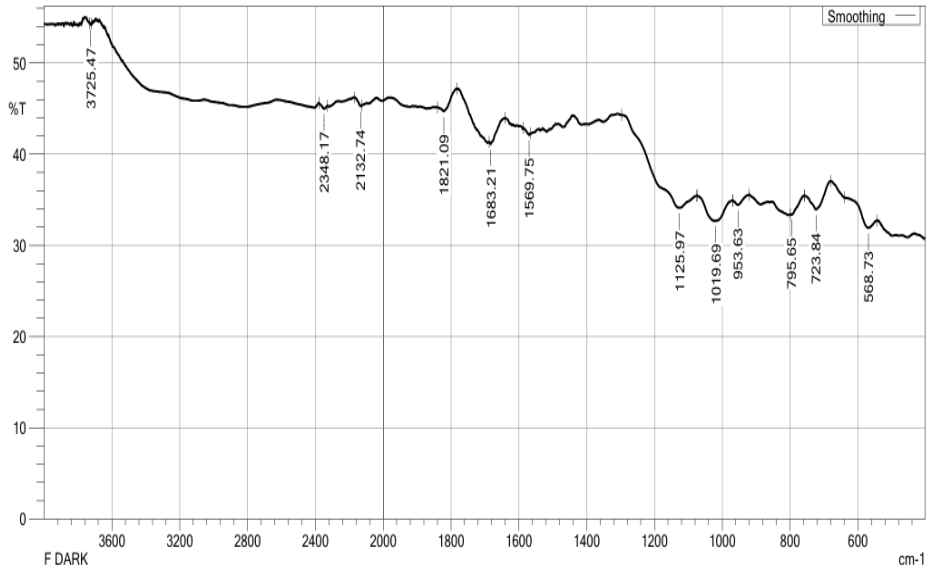

Figure 3: shows the IR Spectroscopy image of GO-1

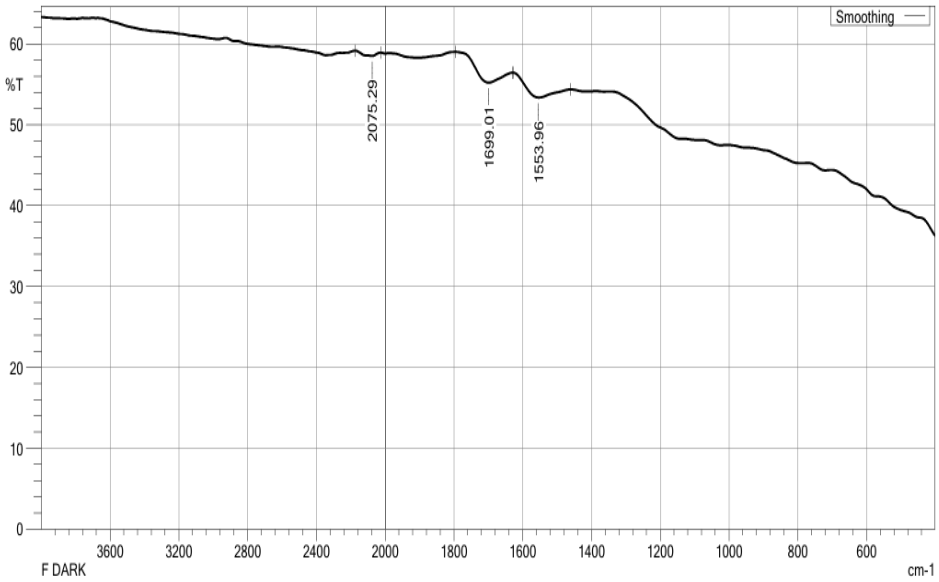

Figure 4: shows the IR Spectroscopy image of GO-4

The characteristics of graphene oxide are greatly affected by oxygen-containing functional groups. Hydroxyl and epoxy groups enhance hydrophilicity, improving its dispersibility in water-based solutions [56]. Conversely, higher concentrations of carbonyl and carboxyl groups influence surface charge along with reactivity. By varying the sulfuric acid amount in the modified Hummers' method, graphene oxide's surface chemistry can be tailored. These features are indispensable for uses such as membrane filtration, where distinct surface attributes are required for successful separation, and in composite materials, where the interactions at the boundary with the matrix are essential.

The UV-visible spectra of GO suspensions correspond to p/p* and n/p* transitions. GO-1 shows maximum absorption at 229 nm, while GO-4 at 231 nm. Spectra of GO-4 shows slightly blue-shift compared to GO-1, indicating GO-1 has more p–p conjugations due to higher carbon ring retention in its basal planes.[50]

COMPARATIVE ANALYSIS AND DISCUSSION

The research reviewed highlights that the concentration of sulfuric acid in the modified Hummers' method is crucial in shaping the structural and functional attributes of the synthesized graphene oxide. When comparing the impacts of 93% versus 99% sulfuric acid concentrations, it becomes evident that, despite a similar overall oxidation level, there are significant variations in interlayer spacing, defect density, and the distribution of oxygen-containing functional groups. Notably, a 93% sulfuric acid concentration results in greater interlayer spacing and fewer defects, as shown by XRD and Raman spectroscopy. On the other hand, a 99% concentration leads to a higher presence of carbonyl groups and a reduced presence of epoxy and hydroxyl groups.

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Structural Properties of Spray Deposited Ba doped ZnO Thin Films

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ABSTRACT

Barium-doped zinc oxide (BZO) thin films are promising materials for optoelectronic and sensor devices because of their improved structural qualities. In this research, we created BZO films using a simple spray pyrolysis method and carefully studied their structure. X-ray diffraction showed that the films maintained the typical hexagonal structure of zinc oxide, with minor changes due to the added barium. Scanning electron microscopy revealed that the barium doping altered the film's surface, affecting grain size and making the film more uniform. These structural improvements indicate that barium effectively modifies the zinc oxide's crystal quality and defect levels, which could lead to better performance in devices. This study offers useful information for designing improved zinc oxide films for advanced electronic and optical applications.

Keywords: Nanostructured, Thin film, BZO, Structural properties, Morphological properties.

INTRODUCTION

Zinc oxide (ZnO) is a valuable semiconductor because of its strong optical, electrical, and structural traits, making it ideal for devices like LEDs, transparent conductors, gas detectors, and solar cells. Its wide bandgap and high exciton binding energy result in stable, room-temperature ultraviolet light emission. To improve ZnO's natural capabilities, we can introduce impurities, or "dope" it, altering its structure, electricity flow, and light interaction. Adding barium (Ba) to ZnO is a promising method for fine-tuning its physical characteristics. Ba ions within the ZnO structure can change how the material grows, its crystal quality, the number of defects, and its surface shape, all of which affect its performance. Many researches have already fabricated ZnO films using different deposition methods which includes reactive magnetron sputtering [1,2], molecular beam epitaxy [3], chemical vapor deposition [4], sol–gel [5], pulsed laser deposition [6,7] and spray pyrolysis [8]. Recently, the

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doping of semiconductors by transition metals is of great importance, because of their unusual optical properties and promising potential for optoelectronic applications [9-11].

In this research, we are using a simple spray pyrolysis method to create BZO thin films and study how doping of barium affects the ZnO structure. X-ray diffraction (XRD) is used to analyse the crystal structure and scanning electron microscopy (SEM) to examine the surface and chemical makeup. By understanding how barium changes the ZnO structure, we can better design these films for advanced technologies.

EXPERIMENTAL DETAILS

Pure and barium doped zinc oxide thin films were deposited using by the spray pyrolysis technique. It should be noted that the experimental setup and other experimental procedures are described in more details elsewhere [12]. The first spray solution was made with zinc acetate ($Zn(CH_3COO)_2.2H_2O$) at 0. 1 M concentration in deionized water before use in the reaction. Doping was done with barium acetate [$Ba(CH_3COO)_2.2H_2O$] at 0. 1M concentration to the original solution, then the prepared solution was spread on the glass substrate at 523K. The spray rate of 5 mL/min was maintained for the film deposition. The crystal structure and the particle size of the thin films were identified using an X-pert Pro X-ray diffractometer and morphology was studied by using JEOL 6380A scanning electron microscope. Prior to deposition the glass substrates were first rinsed in ethanol and then dried under vacuum.

RESULTS AND DISCUSSION

Structural Analysis

Structural characteristics of Ba-doped ZnO (BZO) thin films influence their operational behaviour within optoelectronics devices along with sensors while functioning as transparent conducting oxides. ZnO lattice parameters including crystallinity and lattice structure together with grain size and surface morphology and defect density become affected by introducing Ba ions. X-ray diffraction studies reveal hexagonal wurtzite structure endures after Ba doping into ZnO crystalline structure with some additional tetragonal barium phases, also the XRD pattern peaks undergo movement toward lower angles when substitutions occur which enlarges the crystal lattice parameters which is in good agreement with similar results reported [13,14]. Crystallinity reaches higher levels through Ba incorporation because it helps lower both defect density and lattice strain [15]. Figure1 illustrates the XRD pattern of the pure zinc oxide barium doped zinc oxide thin films deposited by the spray pyrolysis at a deposition temperature of 573K. The size of the grains was calculated using Debye Scherrer formula.

$$D = \frac{k\lambda}{\beta Cos\theta}$$

Where k is the shaping factor, 'λ' is the wavelength of the Cukα line, 'β' is the full width at half maxima (FWHM) in radians and 'θ' is the Bragg's angle.

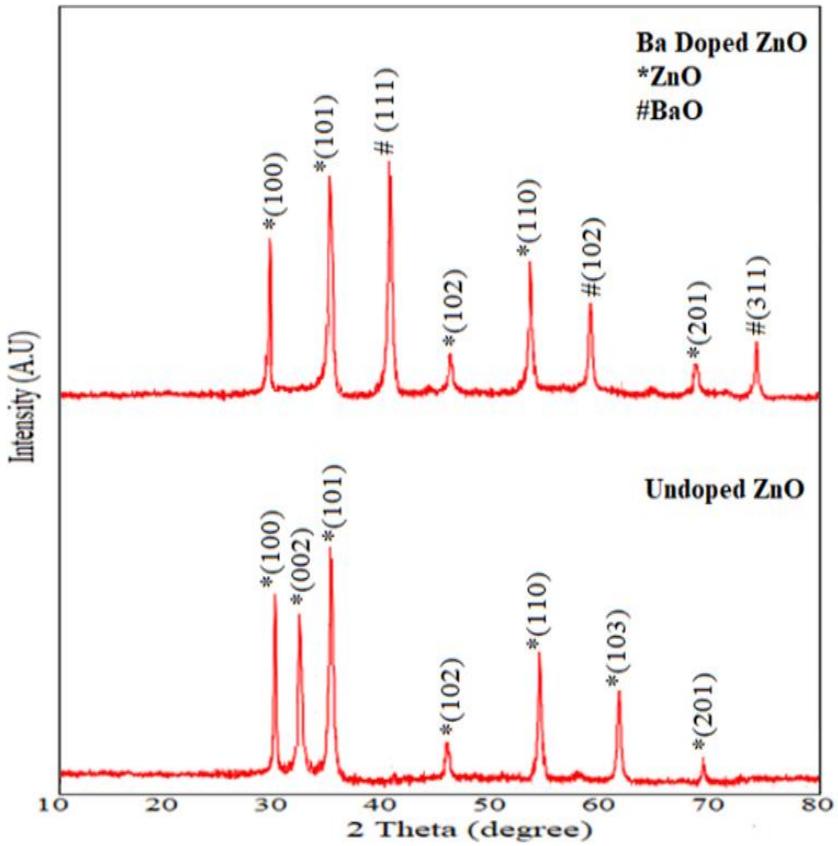

Figure1: XRD pattern of the pure zinc oxide and barium doped zinc oxide thin films

TABLE I COMPARISON OF OBSERVED AND STANDARD XRD DATA OF PURE ZINC OXIDE THIN FILMS (JCPDS CARD 36-1451) AND BARIUM OXIDE THIN FILMS (JCPD CARD 26-0178)

Film	Observed data		Standard data		h k l	phase
	2θ (degree)	d (Å)	2θ (degree)	d (Å)		
Un-doped ZnO Films	31.890	2.760	31.770	2.814	1 0 0	Hexagonal
	34.230	2.701	34.422	2.603	0 0 2	Hexagonal
	36.236	2.496	36.253	2.475	1 0 1	Hexagonal
	47.708	1.826	47.539	1.911	1 0 2	Hexagonal
	56.712	1.590	56.603	1.624	1 1 0	Hexagonal
	62.630	1.513	62.864	1.477	1 0 3	Hexagonal
	69.182	1.329	69.100	1.358	2 0 1	Hexagonal
Ba doped ZnO Films	31.908	3.001	31.770	2.814	1 0 0	Hexagonal
	36.236	2.496	36.253	2.475	1 0 1	Hexagonal
	42.201	2.001	41.167	2.191	1 1 1	Tetragonal
	47.490	1.813	47.539	1.911	1 0 2	Hexagonal
	56.480	1.661	56.603	1.624	1 1 0	Hexagonal
	61.002	1.491	62.965	1.475	1 0 2	Tetragonal
	68.910	1.388	69.100	1.358	2 0 1	Hexagonal
	75.661	1.231	75.586	1.257	3 1 1	Tetragonal

Surface Morphology

The morphology of Ba-doped ZnO (BZO) thin films significantly influences their optical, electrical, and mechanical properties, making it a crucial factor in their potential applications. Scanning electron microscopy (SEM) studies (Figure 2) show that, Ba doping significantly affects the surface morphology of ZnO thin films. After doping of barium, the grains are regularly closely bounded leading to smoother films with improved packing density. This improvement in surface morphology is beneficial for applications requiring high-quality transparent conducting films.

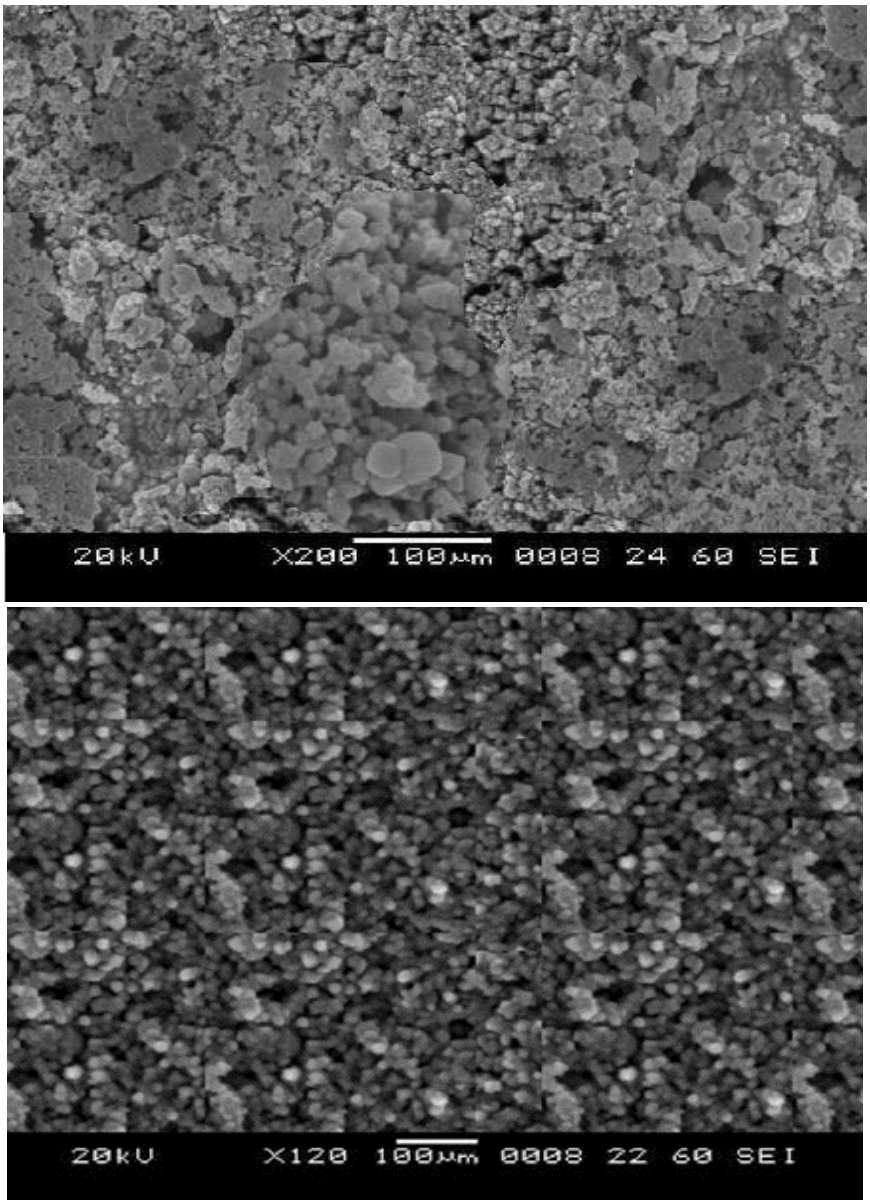

Figure 2: SEM images of (A)pure zinc oxide and (B)barium doped zinc oxide thin films

CONCLUSION

Barium-doped zinc oxide (BZO) thin-film structural properties show that Ba doping results in a decrease in defect densities, a change in surface morphology, a modulation of lattice parameters, and an increase in crystallinity. Because of these structural changes, BZO thin films are very appealing for transparent conductive and optoelectronic applications. To maximize performance, doping levels and synthesis factors must be optimized through more study.

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The Study on Thermal Behaviour of Conducting Electroactive Polypyrrole on Incorporation of Xanthene Dye: Fluoroscein as a Dopant in Its Polymeric Structure

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ABSTRACT

The research paper aims to elucidate the impact of Fluorescein; a xanthene dye dopant on the thermal properties of PPy, with a focus on understanding changes in stability, phase transitions, and thermal decomposition. The synthesis methodology involves the in situ oxidative chemical polymerization of pyrrole in the presence of ammonium peroxydisulphate as an oxidant. Furthur preparation of PPy/Fluorescein composite is done by mixing fluorescein solutions at different concentrations during polymerization proceeds., and the resulting PPy/Fluorescein composite is thoroughly characterized using advanced techniques. The resulting material is subjected to extensive thermal characterization using thermogravimetric analysis (TGA) and differential Thermal Analysis (DTA). The results successfully elucidate the thermal stability, decomposition kinetics, and heat flow characteristics of the composite, providing insights into the influence of fluorescein on PPy's thermal behavior.

INTRODUCTION

Conducting Polymers owing to their unique combination of electrical conductivity, flexibility, and ease of synthesis, have garnered significant attention for a myriad of applications in areas such as sensors, actuators, organic electronics, and energy storage devices. *(1)* Due to their versatility, tunability, and ability to undergo reversible redox reactions. The integration of conducting polymers into diverse fields holds promise for the development of advanced technologies with enhanced functionality and adaptability.*(2)*

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Among these, Polypyrrole (PPy) is a conducting polymer that belongs to the family of organic polymers with unique electronic properties. It is derived from the polymerization of pyrrole monomers, forming a chain-like structure with alternating single and double bonds along its backbone. The conjugated pi-electron system in polypyrrole allows for electrical conductivity, making it one of the most studied and widely used conducting polymers. *(3)*PPy can be synthesized through various methods, including chemical oxidative polymerization, electrochemical polymerization, and enzymatic polymerization. One of its notable characteristics is its ability to undergo reversible doping and de-doping processes, where the incorporation or removal of charge carriers significantly influences its electrical conductivity.*(4)* Owing to its distinctive properties, polypyrrole finds applications in diverse fields, such as sensors, actuators, organic electronics, and energy storage devices, contributing to the advancement of flexible electronics and emerging technologies. The tunability of PPy's conductivity and its compatibility with various substrates make it a versatile material for the development of innovative and multifunctional devices.*(5)*

Polypyrrole stands out as a versatile material due to its excellent conductivity and environmental stability. However, the quest for optimizing its properties for specific applications has led researchers to explore various approaches, including the incorporation of dopants.*(6)* The incorporation of dopants into conducting polymers not only alters their electrical properties but also impacts their thermal stability, making them suitable for applications in diverse thermal environments. The integration of fluorescein, a xanthene dye with unique optical properties, into the PPy matrix is expected to introduce additional functionalities while potentially affecting the thermal behavior of the resulting composite material.*(7)*

Fluorescein, a xanthene dye known for its fluorescent properties, is chosen as the dopant due to its intriguing chemical structure and potential impact on the thermal stability of PPy. The choice of fluorescein as a dopant is motivated by its intriguing properties as a xanthene dye, known for its fluorescence and potential influence on the electronic and thermal characteristics of polymers. Understanding the interplay between PPy and fluorescein is crucial for tailoring the material's properties to meet the demands of emerging technologies.*(8)* This research aims to bridge this gap by systematically examining the thermal responses of PPy upon the introduction of fluorescein, shedding light on the intricate relationship between molecular structure, thermal stability, and the electroactive nature of the resulting composites.*(9–11)*

This study employs a systematic approach to unravel the thermal intricacies of the PPy/Fluorescein composite. The synthesis process involves the chemical polymerization of pyrrole in the presence of different concentrations of fluorescein dye, and the resulting material is subjected to extensive characterization through thermogravimetric analysis (TGA) and differential thermal analysis (DTA), we aim to elucidate the thermal stability, decomposition kinetics, and heat flow characteristics of the composite, providing insights into the influence of fluorescein on PPy's thermal behavior.

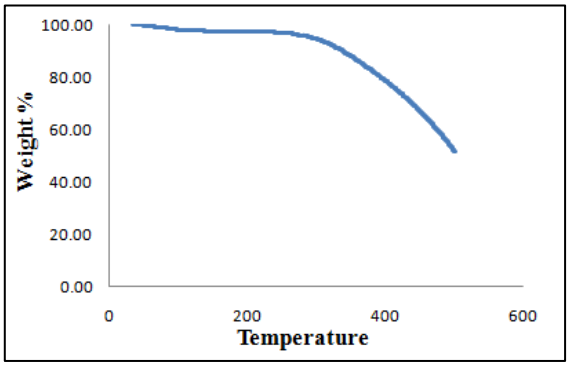
EXPERIMENTAL:

All the chemicals required in the present work like monomer pyrrole, oxidizing agent, ammonium peroxydisulphate and dopant Fluorescein are of A. R. Grade. PPy/fluorescein composites were synthesized by simple chemical oxidative polymerization method. The aqueous solution of 0.1 M Ammonium peroxydisulphate was prepared. To this solution 0.00001 M aqueous solution of dopant was added with constant stirring. After a vigorous stirring at 50oC drop by drop 0.1 M solution of monomer pyrrole was added. The reaction was stirred for few hours on magnetic stirrer which gives rise to formation of precipitate of polymer composite. This reaction mixture was allowed to stand for 24 hours in order to complete polymerization process. The resulting product was vacuum filtered. The precipitate was washed with copious amount of triply distilled

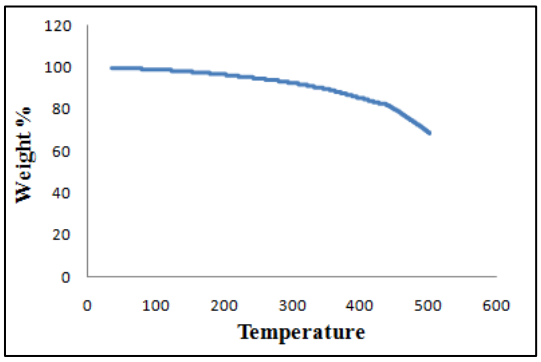
water. Until the washing was clear. Similarly, 0.0001 M PPy/Fluorescein composite was also synthesized. The polymer composite was dried in desiccators and again dried in an oven at 40-500oC. The synthesized product was further characterized by Mass and NMR spectroscopic Analysis.*(12)*

RESULT AND DISCUSSION

As the conducting polymeris are useful in number of electronic applications, it is necessary to study its themal properties. The effect of temperature on stability of polymer is studied by TGA/ DTA analysis. TGA gives the information regarding to weght loss in material with increasing temperature and DTA is useful to determine glass transition temperature. The TGA and DTA thermograms of PPy and PPy/Fluorescein dye composites are given in fig below. Variation of weight is almost linear in TGA and the maximum polymer decomposition temperature is observed from 40°C to 550°C for each sample.



TGA curve of PPy/0.00001 M fluorescein



TGA curve of PPy/0.0001 M fluorescein

The thermal characteristic of PPy and PPy/ Fluorescein composite was studied by using thermogravimetric (TGA) technique (instrument DTG-60) by heating in the range 10^0 C/min from room temperature to 550°C in air.

The thermal degradation of chemically modified PPy/Fluorescein composites were found to proceed in three step weight losses as shown in fig. The first stage of weight loss (~2-3 %) at about 80-120°C is associated with the evaporation of solvents, moisture as well as unreacted monomers elimination. Heating of polymer composite at further higher temperature (250-400^0 C), a weight loss of about 15-20 % occurs due to the scission of dopant component of the PPy. The drop in weight (~35-50 %) observed at 400-550°C is due to the degradation of the PPy itself. The last step of decomposition at 550°C was initiated by random scission within the polymeric chain. PPy samples are thermally stable in the temperature range of 25-400°C and beyond this range; the decomposition route becomes very rapid. The residual weight of the PPy is about 40% in the oxygen atmosphere, which indicates that PPy does not completely decompose in O_2 even at high temperature.

The weight loss in each step and total weight loss for different weight % at different temperature for different composite materials of PPy composite is given in table:

Table : Weight Loss in each step for PPy/fluorescein composites

S.N.	Polymer Composite	Weight Loss (%)				
		Step I 50-120^{0}C	StepII 250-400^{0}C	Step III 400-500^{0}C	Total wt loss (%)	Residue
1.	Pure PPy	0.38	12.57	47.65	60.6	39.4
2.	PPy/0.00001 Fluorescein	1.93	16.79	48.59	67.31	32.69

S.N.	Polymer Composite	Weight Loss (%)				
		Step I 50-120°C	StepII 250-400°C	Step III 400-500°C	Total wt loss (%)	Residue
3.	PPy/0.0001 Fluorescein	0.87	9.56	29.82	40.25	59.75

DTA curves for PPy/fluorescein composites are explained in figures which give the glass transition temperature (Tg) which determines the softening of the polymer. The TG curve is analogous to DTA curves as the variation in TG curve will give the simultaneous variation in DTA curve.

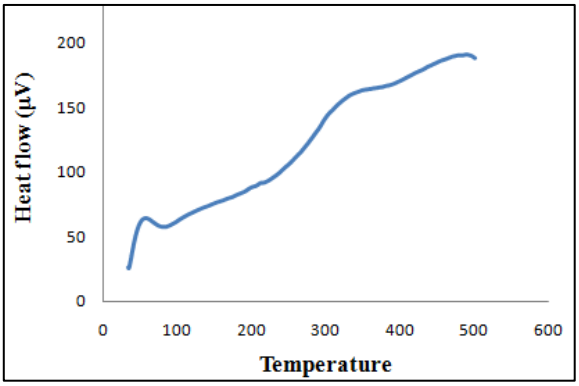


Fig : DTA curve of PPy/0.00001 M Flu.

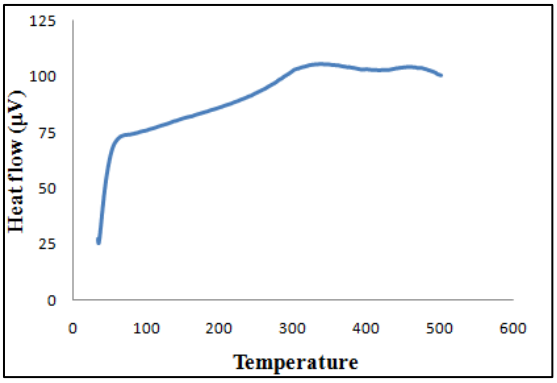


Fig: DTA curve of PPy/0.0001 M flu.

The various parameters such as glass transition, onset and peak and end temperatures from DTA curves are tabulated in the following table.

Table: Thermodynamic parameters from DTA curve of PPy/fluorescein composites

Polymer Composite	Glass transition Temp. 0 C	Crystallization Exothermic Peak		
		Onset temperature (° C)	Peak temperature (° C)	End temperature (° C)
PPy	63.49	221.42	328.21	479.23
PPy/0.00001 Fluorescein	51.79	264.49	406.95	468.22
PPy/0.0001 Fluorescein	55.33	230.16	310.69	462.92

It is observed that the glass transition temperature decreases with increasing content of Fluorescein. This means that the addition of Fluorescein relives the structure of polymer composites and it becomes soft.

CONCLUSION:

The above discussion reveals that efforts have been made to synthesize the polypyrrole/Fluorescein composites to tailor the structural, morphological, and electrical properties of polypyrrole. Detailed thermal characterizations of the synthesized composites through TGA and DTA studies indicate the incorporation of dopant into the polymeric chain with increased thermal stability.

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A Review on Enhanced Photocatalytic Wastewater Treatment Using Phytofabricated Copper Nanoparticles

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ABSTRACT

The growing concern over water pollution has urged into the development of efficient and sustainable wastewater treatment techniques. Among various approaches, photocatalysis using nanomaterials has emerged as a promising solution for waste water treatment due to its high degradation efficiency and environmental friendliness. Among these Phytofabricated copper nanoparticles (CuNPs) have emerged as efficient photocatalysts for wastewater treatment due to their eco-friendly synthesis, cost-effectiveness, and high degradation efficiency. This review article explores the green synthesis of CuNPs using plant extracts, their structural characterization, and their photocatalytic applications in degrading organic pollutants, reducing heavy metals, and inactivating microbes. Key factors affecting their performance, including particle size, pH, light intensity, and composite formation, are discussed. Despite of challenges like stability and large-scale implementation, advancements in nanotechnology highlights CuNPs as a promising solution for sustainable wastewater remediation.

INTRODUCTION

Water pollution, caused by industrial effluents, pharmaceutical residues, and organic pollutants, poses a severe threat to ecosystems and human health. The increasing contamination of freshwater sources with synthetic dyes, heavy metals, and persistent organic pollutants necessitates advanced treatment strategies. Traditional wastewater treatment methods, including chemical coagulation, filtration, and biological treatment, often fall short in completely eliminating these contaminants. Additionally, these methods can be cost-intensive and generate secondary waste, leading to further environmental concerns. [1,2]

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In response to these challenges, nanotechnology-based approaches, particularly photocatalysis, have emerged as sustainable and effective alternatives for water purification. Photocatalysis harnesses the ability of semiconductor materials to degrade pollutants through light-induced redox reactions, ensuring minimal secondary pollution. Among various nanomaterials, copper nanoparticles (CuNPs) have gained significant attention due to their excellent photocatalytic efficiency, cost-effectiveness, and biocompatibility. Unlike conventional metal oxides such as titanium dioxide (TiO2) and zinc oxide (ZnO), CuNPs exhibit superior absorption in the visible light spectrum, enabling enhanced photocatalytic performance even under low-energy illumination. [3,5]

One of the most promising approaches to synthesizing CuNPs is phytofabrication, which involves the use of plant extracts as natural reducing and stabilizing agents. This green chemistry method not only eliminates the need for hazardous reducing agents but also enhances the stability and functional properties of CuNPs. Various plant-derived metabolites, such as polyphenols, flavonoids, alkaloids, and terpenoids, contribute to the synthesis and stabilization of nanoparticles, thereby improving their photocatalytic capabilities. The eco-friendly nature of phytofabricatedCuNPs makes them an attractive choice for wastewater treatment, offering a sustainable alternative to conventional chemical synthesis methods. [6,9]

This review explores the synthesis, characterization, and photocatalytic applications of phytofabricatedCuNPs in wastewater treatment. It discusses the key influencing factors, and the role of CuNPs in eliminating a wide range of pollutants. Additionally, the review highlights recent advancements, challenges, and future research directions in the field of CuNP-based wastewater remediation.

1. Synthesis of Phytofabricated Copper Nanoparticles

Phytofabrication involves using plant extracts as reducing and stabilizing agents for synthesizing CuNPs. Various plant-derived metabolites, such as polyphenols, flavonoids, and alkaloids, facilitate the reduction of copper salts into nanoparticles. Common plant sources include garlic peel, neem, green tea, and citrus fruit extracts. The advantages of phytofabrication include reduced toxicity, cost-effectiveness, and enhanced stability of nanoparticles. [12, 4, 5]

2. Characterization Techniques

The characterization of phytofabricatedCuNPs is essential to understand their physicochemical properties and optimize their photocatalytic performance. UV-Vis spectroscopy is commonly used to confirm nanoparticle formation through surface plasmon resonance, while X-ray diffraction (XRD) determines the crystalline nature and phase composition. Fourier transform infrared spectroscopy (FTIR) helps identify functional groups involved in nanoparticle stabilization, providing insights into the interaction between plant-derived biomolecules and CuNPs. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) offer detailed morphological and structural analysis, revealing nanoparticle size, shape, and surface characteristics. These characterization techniques collectively provide comprehensive insights into the structural, optical, and catalytic properties of CuNPs, facilitating their effective utilization in wastewater treatment applications. [10, 4, 3]

3. Photocatalytic Applications of Copper Nanoparticles in Wastewater Treatment

Copper nanoparticles have demonstrated exceptional photocatalytic properties, making them highly effective for degrading a wide range of contaminants in wastewater. Their photocatalytic applications include:

- **Degradation of Organic Pollutants**: CuNPs effectively catalyze the degradation of a wide range of organic pollutants, including synthetic dyes (e.g., methylene blue, rhodamine B), pharmaceutical residues (e.g., antibiotics, analgesics), and agricultural pesticides. The photogenerated electrons and hydroxyl radicals

attack the chemical bonds of these pollutants, breaking them down into less harmful compounds, ultimately converting them into CO2 and water.[9]

- **Heavy Metal Reduction and Removal**: Copper nanoparticles facilitate the transformation of toxic heavy metals such as hexavalent chromium (Cr(VI)), lead (Pb(II)), cadmium (Cd(II)), and arsenic (As(III)) into their less toxic or insoluble forms. The strong redox potential of CuNPs helps in reducing heavy metal ions, thereby mitigating their environmental toxicity.[7]
- **Disinfection and Microbial Inactivation**: CuNPs generate hydroxyl radicals and other reactive oxygen species that disrupt microbial cell membranes, damage intracellular components, and induce oxidative stress. This property makes them highly effective in eliminating pathogenic bacteria, viruses, and fungi present in wastewater, contributing to safer water reuse.[12]
- **Decomposition of Industrial Effluents**: CuNPs have been demonstrated to efficiently decompose industrial pollutants, including petroleum hydrocarbons, phenolic compounds, and nitroaromatics. Their ability to break down recalcitrant organic matter enhances the overall treatment efficacy, reducing the persistence of harmful substances in the aquatic environment.[10]
- **Synergistic Effect in Composite Photocatalysts**: CuNPs exhibit enhanced photocatalytic efficiency when combined with other semiconductor materials such as titanium dioxide (TiO2), zinc oxide (ZnO), and graphene-based nanomaterials. These hybrid systems benefit from increased charge separation, reduced electron-hole recombination, and improved light absorption, making them more effective in wastewater remediation.[4]

4. **Factors Affecting Photocatalytic Efficiency** Several factors influence the efficiency of CuNPs in wastewater treatment:[10]
    - **Particle Size and Morphology**: Smaller and well-dispersed nanoparticles exhibit higher photocatalytic activity.
    - **pH of the Solution**: Affects charge distribution and interaction with pollutants.
    - **Light Intensity and Wavelength**: Determines the extent of electron excitation.
    - **Dopants and Composite Materials**: Enhancing CuNPs with other materials (e.g., TiO2, ZnO) improves efficiency.
5. **Recent Advancements and Applications** Recent studies have demonstrated the effective degradation of dyes, pesticides, and pharmaceutical residues using phytofabricatedCuNPs. Innovative hybrid systems, including CuNP-graphene and CuNP-polymer composites, have shown improved photocatalytic performance. [8,11,12]
6. **Challenges and Future Perspectives** Despite promising results, challenges such as nanoparticle aggregation, stability, and recyclability need to be addressed. Future research should focus on optimizing synthesis parameters, exploring novel plant sources, and scaling up production for industrial applications.

CONCLUSION

Phytofabricated copper nanoparticles (CuNPs) have emerged as a promising solution for wastewater treatment due to their excellent photocatalytic efficiency, eco-friendly synthesis, and cost-effectiveness. Their ability to degrade organic pollutants, reduce heavy metals, and inactivate microbes makes them highly suitable for water remediation. Additionally, their integration with other semiconductor materials enhances their efficiency by improving charge separation and extending their applicability. However, challenges such as particle aggregation, stability, and large-scale implementation need further research. With advancements in

nanotechnology and green synthesis methods, CuNP-based photocatalysts have the potential to revolutionize wastewater treatment, ensuring environmental sustainability and improved public health.

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A Mini Review on Recent Progress in Biological Activities of 1,3,4-Thiadiazole and its Derivatives

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ABSTRACT

The 1,3,4-thiadiazole scaffold has attracted much attention in medicinal and pharmaceutical chemistry because of its wide range of biological activities. This five-membered heterocyclic ring structure, which is distinguished by sulphur and nitrogen atoms, has remarkable pharmacological potential, including antibacterial, anticancer, anti-inflammatory, antioxidant, anticonvulsant, and antitubercular characteristics. 1,3,4-thiadiazole derivatives have a wide range of biological activity due to their ability to interact with enzymes and receptors via hydrogen bonding, π-π interactions, and coordination with metal ions. Furthermore, changes to the thiadiazole ring improve selectivity and effectiveness, making these compounds promising candidates for drug development and therapeutic applications. This research examines the fundamental biological activities of 1,3,4-thiadiazole derivatives, their structure-activity relationships, and their potential as lead molecules in therapeutic development.

Keywords: 1,3,4-thiadiazole, antimicrobial, thiadiazole, scaffolds.

INTRODUCTION

Heterocyclic compounds play a critical role in drug discovery due to their diverse biological activities. Among them, 1,3,4-thiadiazole has emerged as an important scaffold with significant pharmacological potential. This five-membered heterocycle with sulphur and nitrogen atoms is widely recognised for its medicinal chemistry versatility. Researchers have created a variety of compounds to enhance its bioactivity and pharmacokinetics. Thiadiazole is a heterocyclic compound with a five-membered ring containing two nitrogen atoms, one sulphur atom, and two carbon atoms (molecular formula $C_2H_2N_2S$). Thiadiazole derivatives have a diverse application of uses in medical chemistry, agriculture, and materials research [1-4]. According to research, molecules derived from 1,3,4-thiadiazole may have a variety of biological effects, including anti-inflammatory, anticancer, and

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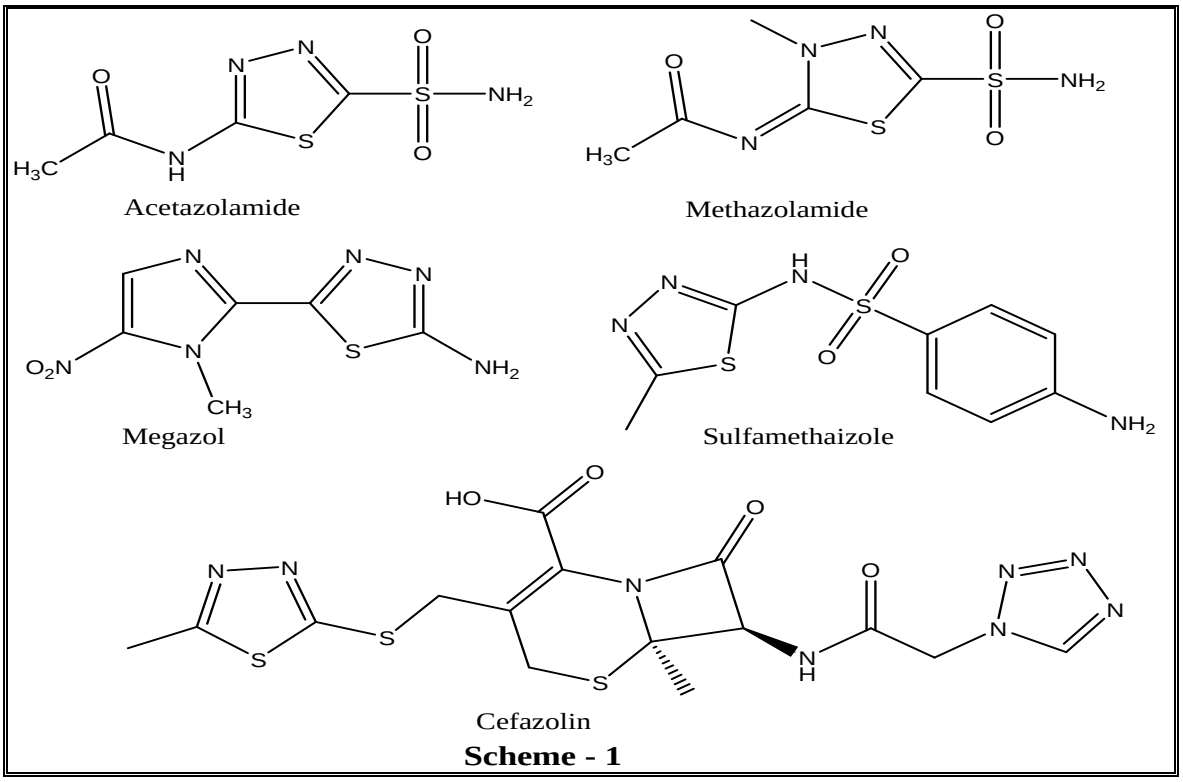
antibacterial properties. Furthermore, thiadiazole derivatives have been researched for their potential as agrochemicals [5-9].

BIOLOGICAL ACTIVITIES OF 1,3,4-THIADIAZOLE AND ITS DERIVATIVES: -

Thiadiazole derivatives are present in a range of medicines, including acetazolamide [10] and methazolamide [11], which are effective carbonic anhydrase inhibitors. Megazol is an anti-trypanosomal drug [12], whereas sulfamethizole is a type of antibacterial [13]. First-generation cephalosporins include cefazolin and cefazedone [14] as shown in scheme 1. This study examines recent advances in the biological activities of 1,3,4-thiadiazole derivatives.



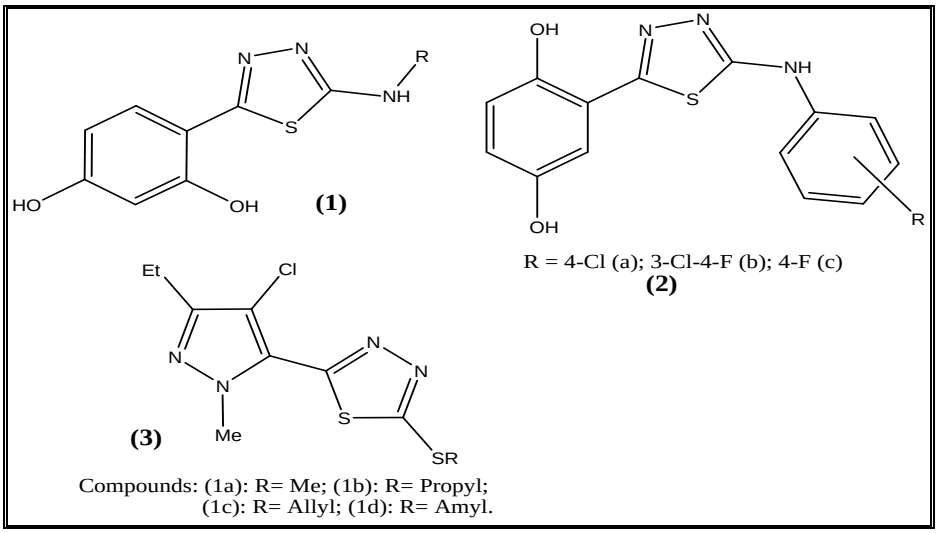
Scheme - 1

Antibacterial and Antifungal Activity: -

1,3,4-thiadiazole derivatives are active against a variety of infections caused by fungi and bacteria. A variety of 5 substituted 2-(2,4-dihydroxyphenyl)-1,3,4-thiadiazole derivatives (1) were tested for antifungal activity against various clinical isolates of Candida albicans. Compounds containing methyl, phenyl, 4-ethoxyphenyl, and halogen phenyl groups at C-2 of the thiadiazole ring exhibited stronger antifungal activity [15].

A new series of 4-amino-2-{5-[(4-substituted phenyl)amino]-1,3,4-thiadiazol-2-yl phenols (2) was synthesized and evaluated in vitro for their antimicrobial activity. The chlorinated and fluorinated derivatives exhibited good antibacterial activity against S. aureus and E. coli strains and antifungal activity against A. niger with MIC values of 25 µg/ml [16].

Kaushal, M et al. reported the synthesis of active 1,3,4-thiadiazole compounds with pyrazolyl substituents (3). The synthesised compounds were tested for antifungal activity against R. solanii [17].



Anticancer Activity: -

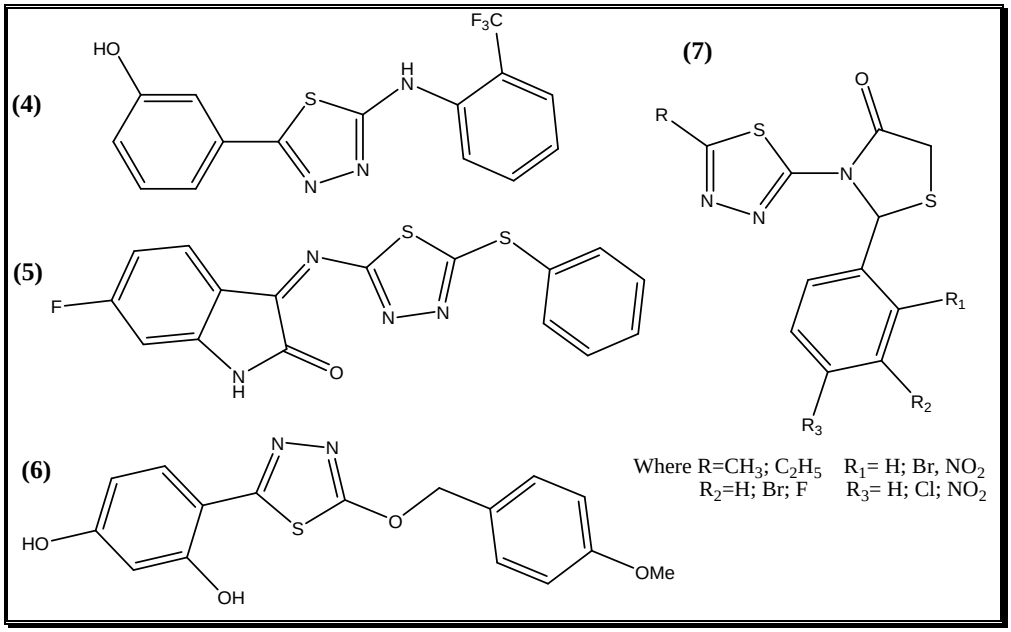
A study by Sara Janowska et al. found that thiadiazole derivatives have anticancer potential by blocking enzym es involved in cancer growth. The most effective compound was compound (4), which showed the most signific ant anti-cancer effects against MCF-7 and MDA-MB-

231 breast cancer cell lines, this chemical demonstrated values of 49.7 μM and 53.4 μM, respectively [18].

Prashant J. Chaudhari and colleagues [19] synthesised three important anti-cancer scaffolds, which were then tested to create particular compounds that were virtually screened. Compound (5) had a significant impact on the breast cancer subpanel (IC 50 values of 0.71 and 1.04 μ = 1.47 μM). It's inhibitory M among the MDA-MB-231 and MCF7 cell lines.

Matysiak et al. studied the antiproliferative efficacy of different 5-position substitutions of 2-(2,4 dihydroxy-phenyl) 1,3,4-thiadiazoles against various human tumor cell lines, finding Structure (6) effective against HCV29T bladder cancer cell line [20].

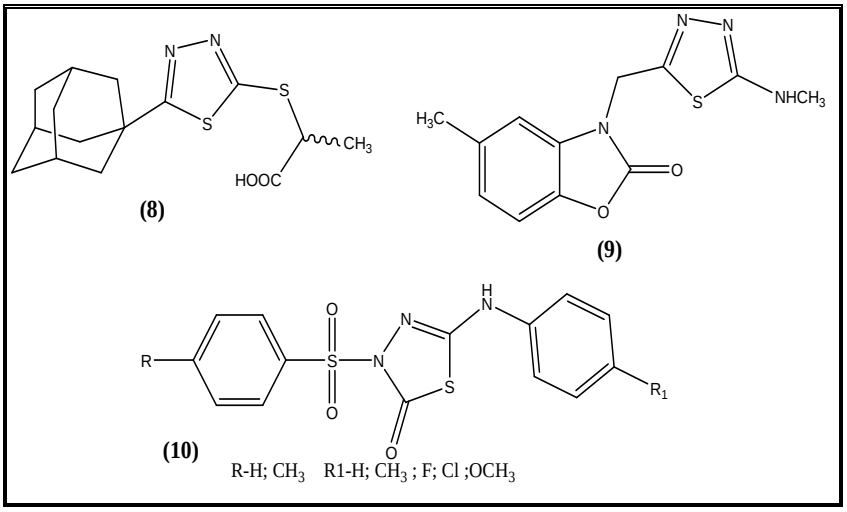
Joseph et al. synthesised a series of novel 5-alkyl/aryl thiadiazole-substituted thiazolidin-4-ones (7) and tested their anti-proliferative activity on human breast cancer cells (MCF-7) using the MTT assay [21].



Anti-Inflammatory Activity: -

Thiadiazole has strong anti-inflammatory effects when it gets introduced into heterocyclic frameworks because it prevents arachidonic acid from transforming to prostaglandins. A new class of 5-(1-adamantyl)-1,3,4-thiadiazole derivatives, compound (8), showed similar anti-inflammatory action at 20 mg/kg as Indomethacin, suggesting its potential in treating various diseases [22].

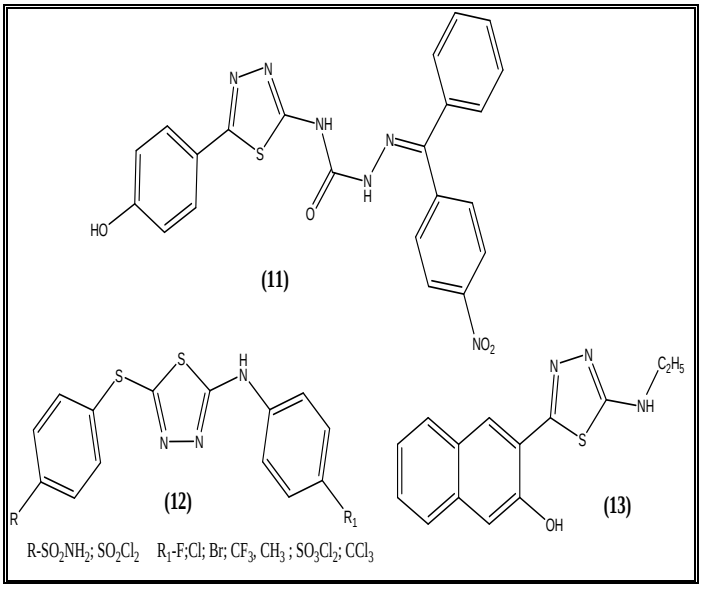
Salgin-Goksen et al synthesized 2-Substituted amino-5 [(5-methyl-2-benzoxazolinone-3-yl) methyl]-1,3,4 thiadiazoles(9)and examined their analgesic and anti-inflammatory activity [23]. Schenone et al. synthesised a series of 3-arylsulphonyl-5-arylamino-1,3,4-thiadiazol-2(3H) ones (10) and tested their anti-inflammatory and analgesic properties with carrageenan rat paw oedema and acetic acid-induced writhing [24].



Anticonvulsant Activity: -

Epilepsy is a brain illness characterized by repeated seizures and abnormal electrical activity. Over the past decade, medication for epilepsy has advanced significantly. The MES and scPTZ tests are widely used animal models to characterize anticonvulsant activity, despite new antiepileptic drugs being introduced into clinical practice [25].

Rajak et al. [26] synthesised and researched the anticonvulsant efficacy of several 2,5-Disubstituted 1,3,4-thiadiazoles. The results showed that the 1,3,4-thiadiazoles that includes 4-nitrophenyl-substituted semicarbazone (11) was the most powerful chemical, equal to carbamzepine.



Sharma et al. synthesised a new set of 2-amino-5-sulfanyl-1,3,4 thiadiazole derivatives (12) and tested their anticonvulsant effectiveness. The compound with sulphonamide and chloride groups shows notable anticonvulsant activity [27]. Compound 2-ethylamino-5-(3-hydroxy-2-naphthyl)-1,3,4-thiadi azole (13) showed 90% protection against pentylenetetrazole-induced generalized convulsions [28].

CONCLUSION: -

The recent advancements in the biological activities of 1,3,4-thiadiazole derivatives highlight their significance in medicinal chemistry. Their diverse pharmacological potential makes them promising candidates for drug development. Future research should focus on optimizing their pharmacokinetics and conducting clinical evaluations to translate these compounds into therapeutic agents.

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Biologically Synthesized Chitosan Nanoparticles: A Potent solution for management of Grapevine (Vitis vinifera) Phytopathogens

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ABSTRACT

Grapevine plants *(Vitis vinifera)* holds high economic significance globally due to their diverse applications in multiple industries. Grapevines are one of the most valuable horticultural crops, with massive market demand for both table grapes and grapes for wine production. The global market for grapes and grape products is vast, which provides significant revenue for cultivators and contributes to the agricultural GDP of grape-growing regions such as Nashik (Maharashtra, India). Phytopathogens pose a significant threat to viticulture, affecting the health of grapevine and total yield. Grapevines commonly suffer from infections like powdery mildew, downy mildew, and botrytis bunch rot. Traditional methods of disease control, including chemical fungicides and pesticides, pose environmental and health risks. Effective management strategies include the isolation, identification, and biological control of these pathogens. Biologically synthesizes nanoparticles (BNPs) can serve as a promising alternative due to their biocompatibility, biodegradability, and effectiveness at low concentrations. This review outlines current methodologies and advances in exploring the potential of Chitosan nanoparticles in control of phytopathogens from grapevines and highlights biological control strategies that leverage natural antagonists to mitigate disease impact.

Keywords: Botrytis Bunch rot, Biological Control, Chitosan Bionanoparticles, Grapevines, Sustainable Viticulture

Introduction

Viticulture holds significant global importance from both economic and social perspectives. Unfortunately, vineyards are frequently attacked by several pathogens such as fungi, viruses, viroids,

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phytoplasmas, and other bacteria, which in severe cases can lead to epidemics, resulting in substantial economic loss potentially ruining the entire production. Throughout the different phases of grapevine growth, various diseases can develop, which can be effectively managed through an integrated protection program encompassing biological, agrophytotechnical, mechanical, physical, and chemical methods (Pertot et al.,2017). Nashik, located in the western Ghats of Maharashtra, India, is renowned as the "Wine Capital of India" due to its pivotal role in grape production. The favourable climate, soil conditions, and agricultural practices of the region contribute significantly to its status as a major grape-growing area. The viticulture of the region not only contributes to the local economy but places India on the global map as a notable grape and wine producer. Even though Nashik is one of the largest producers of grapes, grapevines *(Vitis vinifera)* are often susceptible to various phytopathogens, including fungi, bacteria, and viruses, which can cause severe diseases and economic losses (Kansara S. 2019). Notable among grapevine pathogen is *Botrytis cinerea*, also known as "Gray mold," is a notorious fungal pathogen that affects a multiple plant species, including grapevines *(Vitis vinifera)*.

As mentioned by Zhang et al. (2021) that this pathogen is particularly harmful in viticulture due to its impact on grape quality and yield, posing significant challenges to grape growers worldwide. According to studies performed by Kunova et al. (2021), powdery mildew, caused by the pathogen *Uncinula necator*, is the oldest known grapevine disease and originates from North America. This pathogen is a parasite for the plants of *Vitaceae* family, including *Vitis, Cissus, Parthenocissus*, and *Ampelopsis*, and majorly cause infection to all green parts of the plant. Downy mildew, caused by oomycete *Plasmopara viticola*, is known as one of the most damaging diseases for grapevines, especially in warm and humid climatic regions, and hence pose a significant constraint on grapevine cultivation. Among the innovative strategies for managing plant diseases in the field, biocontrol agents stand out as one of the most promising solutions. Biological control offers a sustainable alternative, utilizing natural organisms to suppress pathogen populations.

1. Survey regarding predominant phytopathogens in Grapevine Fields

To survey the most common phytopathogens in grapevines, it is essential to clearly define the survey objectives and design a comprehensive plan that includes selecting representative vineyard locations and determining an appropriate sample size. The necessary permissions from vineyard owners and authorities are to be obtained before organizing field visits during the growing season when disease symptoms are most visible. The questionnaires should also be distributed to farmers to collect appropriate information regarding frequently occurring diseases of grapevine plants. During field visits, samples should be collected from symptomatic grapevine parts using sterile tools and containers to avoid contamination, ensuring to label each sample with detailed information documenting symptoms meticulously, including taking photographs for reference. In the laboratory, samples are to be processed by surface sterilizing plant tissues and culturing them on selective media under optimal conditions to encourage pathogen growth (Armijo et al.,2016). Use of morphological and molecular techniques such as PCR and sequencing for accurate pathogen identification is also necessary for preliminary investigations. The data can then be compiled and analyzed to identify prevalent pathogens and their presence can be correlated with environmental conditions and vineyard practices.

2. Isolation of Phytopathogens from Grapevine *(Vitis vinifera)* Plants

The isolation of phytopathogens from grapevines involves a meticulous process of sampling, sterilization, and culturing to accurately identify and manage disease-causing agents. Initially, symptomatic plants can be targeted for sample collection, along with random samples from various vineyard locations and healthy controls should be maintained for comparison. Using sterile tools, plant parts such as leaves stems, and berries should be collected and stored in labelled, sterile containers to prevent contamination. Samples are

kept cool during transportation to the laboratory. In the lab, plant tissues undergo surface sterilization with a disinfectant solution, followed by rinsing with sterile water. These tissue samples can then be placed on selective agar media tailored for the suspected pathogens. The plates should be incubated under optimal conditions, and regular observations are made for pathogen growth. Isolated colonies should be subcultured onto fresh plates to achieve pure cultures (Lazazzara et al., 2021).

3. Identification of Phytopathogens from grapevine *(Vitis vinifera)* plants

Identification of phytopathogens affecting grapevines involves a combination of traditional and modern techniques for accurate detection and management of grapevine infections. Traditional methods include visual inspection of symptomatic plants, followed by laboratory techniques such as culturing pathogens on selective media and microscopic examination. However, these methods can be time-consuming and may not always provide definitive identification (Aslam et al., 2019)

3.1 Identification of Phytopathogens from Grapevine Using Traditional Approach

The identification of phytopathogens in grapevines using traditional approaches remains a fundamental aspect of plant pathology, despite advancements in molecular techniques. Symptomatic grapevine tissues can be sampled and placed on selective media to promote the growth of specific pathogens. Fungi are often identified based on colony morphology, spore characteristics, and other microscopic features, while bacterial pathogens are identified through biochemical tests and colony morphology. For example *Erysiphe necator* and *Plasmopara viticola* can be identified through distinctive symptoms on grapevine leaves, such as white powdery spots and yellowish oil spots, respectively, followed by microscopic examination of conidia and sporangiophores. Additionally, traditional serological methods like enzyme-linked immunosorbent assay (ELISA) and immunofluorescence can be used to detect viral pathogens (Calonmec et al., 2018).

3.2 Identification of Phytopathogens from Grapevine using Metagenomics

The identification of phytopathogens in grapevines using metagenomics has advanced significantly, offering comprehensive insights into the complex microbial communities associated with grapevine diseases. For example, studies utilizing high-throughput sequencing have identified diverse viral populations within grapevines, including few novel variants of grapevine leafroll-associated viruses and grapevine red blotch virus (Al Rwahnih et al., 2015). Additionally, metagenomic analyses have elucidated the bacterial and fungal communities present in grapevines and their roles in disease progression and plant health (Martinez et al., 2019).

The identification of phytopathogens in grapevines using metagenomics involves several key steps, each crucial for accurately characterizing the microbial communities associated with grapevine diseases. The process begins with sample collection, where plant tissues (e.g., leaves, stems, roots) showing symptoms of disease can be carefully collected and prepared for analysis. DNA or RNA can then be extracted from these samples using specialized protocols to ensure the efficient recovery of high-quality nucleic acids. Following extraction, sequencing libraries can be prepared, which may involve fragmentation of the nucleic acids and the addition of adapters necessary for sequencing. Once sequencing is completed, bioinformatics tools can be used to process and analyze the data. Metagenomic data are compared against reference databases to identify known pathogens and characterize the microbial community structure. Advanced computational methods, such as metagenome-assembled genomes (MAGs) and taxonomic binning, can be employed to reconstruct genomes from the metagenomic data and to assign taxonomic identities to the sequences (Bian et al., 2020).

Biological Control of Phytopathogens with Chitosan Bionanoparticles

Biocontrol of grapevine phytopathogens using bionanoparticles is an emerging and promising approach in plant pathology, leveraging the unique properties of nanoparticles synthesized through biological methods to combat diseases while minimizing environmental impact. Bionanoparticles, produced using biological materials such as plant extracts, microorganisms, and other biological molecules, offer advantages of

biocompatibility and reduced toxicity compared to chemically synthesized nanoparticles. For instance, copper nanoparticles synthesized using plant extracts have shown significant antifungal activity against *Botrytis cinerea* by disrupting the fungal cell membrane and generating reactive oxygen species (ROS) that inhibit pathogen growth (Dhillon et al., 2020). Similarly, silver bionanoparticles have been reported to effectively reduce the incidence of powdery mildew by interfering with the cellular metabolism of the pathogen and enhancing the plant's defense mechanisms. Additionally, chitosan nanoparticles, derived from natural biopolymers, have shown potential in controlling *Plasmopara viticola*, the agent of downy mildew, by inducing systemic resistance in grapevines and directly inhibiting spore germination (El-Ramady et al., 2005). These results suggest that bionanoparticles can be employed as a sustainable and effective tool for the biocontrol of grapevine phytopathogens, offering an environment friendly alternative to conventional chemical pesticides. This can contribute to the development of integrated pest management (IPM) strategies for grapevine phytopathogen.

Detailed steps of preparation of Chitosan Nanoparticles using PGPR isolated from grapevines

As suggested by Dhillon et al. (2020) few species of Plant growth-promoting rhizobacteria (PGPR) can be used for the synthesis of chitosan nanoparticles. PGPR are the bacteria that colonize plant roots and promote plant growth via different mechanisms such as nitrogen fixation, solubilization of phosphate complexes, and production of plant growth promoting hormones. These bacteria can also reduce metal ions to form nanoparticles, offering an eco-friendly approach to nanoparticle synthesis. Here is a detailed explanation of the process and some references to recent studies:

Nanoparticle Synthesis Using PGPR from Grapevine Rhizosphere

1. **Selection & Cultivation of Rhizobacteria from Grapevine**:
   - A suitable PGPR strain known for its metal-reducing capabilities can be chosen from Grapevine rhizosphere. Phytochemical analysis of common PGPR strains can check their ability to promote plant growth including species from the genera *Pseudomonas*, *Bacillus*, *Azospirillum*, and *Rhizobium*.
   - *Pseudomonas aeruginosa* and *Bacillus subtilis* can be used for nanoparticle synthesis as they possess high metal-reducing properties.
   - The selected PGPR strain can be cultivated in an appropriate culture medium until it reaches the desired cell density. Example: *Bacillus subtilis* can be cultured in nutrient broth at 30°c with moderate shaking (50-100 rpm) until an optical density (OD) of 0.8-1.0 is achieved at 600 nm.
2. **Biosynthesis of Chitosan Nanoparticles**:
   - The bacteria reduce metal ions to form nanoparticles. The metabolic activities of the bacteria, including the secretion of enzymes and other reducing agents, facilitate this process (Vizitu et al., 2022).
   - Example: *Bacillus subtilis* reduces silver ions to form silver nanoparticles, which can be monitored by a change in color and confirmed by UV-Visible spectroscopy (Sharma et al., 2019).
   - Chitosan powder of about 90% purity can be dissolved to make 1 percent (w/v) solution with 1 percent (v/v) acetic acid. The pH can be adjusted to 4.8±0.02 with 1 N NaOH. It is essential to confirm the complete dissolution of chitosan hence, it must be stirred continuously for 24h. 10 mL of prepared culture suspension can be added to 10 mL of the chitosan solution (1:1 v/v), CNPs can be obtained by shaking the mixture at 110 rpm for 60 min at 50 °C (Silva et al., 2020).
2. **Characterization of Nanoparticles**:
   - The chitosan nanoparticles obtained by above method can be subjected to characterization using techniques such as UV-visible spectroscopy, Transmission Electron Microscopy

(TEM), Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), and Fourier Transform Infrared Spectroscopy (FTIR).

- Example: TEM images can be used to reveal the size and shape of the silver nanoparticles synthesized by *Pseudomonas aeruginosa*, and UV-visible spectroscopy shows a characteristic peak indicating nanoparticle formation.

3. **Purification and Storage**:
   - The nanoparticles can then be purified by centrifugation to remove bacterial cells and unreacted precursors. The nanoparticles can be rinsed with distilled water or ethanol to remove the any traces of impurities.
   - The purified nanoparticles can then be stored in a sterile container at low temperatures to prevent aggregation (Silva et al., 2020).

Challenges

Performing the above study on the isolation, identification, and biological control of phytopathogens in grapevines using bionanoparticles presents several challenges. The complexity of grapevine microbiomes and multiple co-occurring pathogens necessitates high-throughput and precise methodologies, which can be resource-intensive and require sophisticated laboratory infrastructure. Additionally, the biosynthesis of nanoparticles using PGPR must be carefully optimized to achieve the desired size and stability of nanoparticles, which involves fine-tuning parameters such as metal ion concentration, incubation conditions, and bacterial growth phase. Furthermore, the large-scale application and consistency of Bionanoparticles in field conditions pose practical challenges, including maintaining their stability, preventing aggregation, and ensuring their effective distribution in vineyards. Addressing these challenges requires interdisciplinary collaboration, meticulous planning, and substantial funding to accelerate research.

Conclusion

The review highlights the necessity of integrating advanced and sustainable methodologies to combat grapevine diseases effectively. Biological control of grapevine phytopathogen using chitosan nanoparticles presents a promising alternative to conventional chemical treatments. BNPs synthesized through biological methods, including the use of growth-promoting bacteria from grapevine rhizosphere with significant antifungal and antibacterial activity can be a potent solution to the problem of pathogen prevalence in grapevine plantation. The synthesis process of nanoparticles using rhizosphere bacteria involves cultivation, mixing with metal salt solutions, and characterization of the nanoparticles. It is also essential to ensure their scalability, effectiveness and biocompatibility in the fields. In summary, the integration of biological control strategies, advanced identification techniques, and sustainable practices offers a comprehensive approach to managing grapevine phytopathogens. The continued research and development in this field are essential for ensuring the long-term health and productivity of grapevines, benefiting both cultivators and consumers.

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Revolutionizing E-Commerce Recommendations : AI Innovations, Ethical Challenges, and Future Prospects

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ABSTRACT

Recommender systems have become a cornerstone of modern e-commerce, enabling personalized product recommendations that enhance user experience and drive business growth. These systems leverage artificial intelligence (AI) and machine learning techniques, such as collaborative filtering, content-based filtering, and hybrid approaches, to analyze user behavior and predict preferences. However, despite their effectiveness, e-commerce recommender systems face several challenges, including the **cold start problem, data sparsity, scalability issues, bias, privacy concerns, and the risk of filter bubbles**. Addressing these challenges is crucial to improving recommendation accuracy, fairness, and transparency. This research explores the key limitations of current recommender systems and examines emerging trends that can enhance their performance. The study conducts a comprehensive review of recent advancements in AI-driven recommendations, including **deep learning-based models, reinforcement learning, graph neural networks, and explainable AI (XAI)**. Additionally, it evaluates privacy-preserving techniques such as **federated learning and differential privacy** to address data security concerns.

Findings suggest that integrating context-aware recommendation models, multi-modal data processing, and ethical AI frameworks can significantly improve personalization and user trust in e-commerce platforms. The study highlights the importance of balancing recommendation accuracy with fairness and privacy, offering potential solutions for future research and practical implementation. By addressing the challenges and leveraging cutting-edge AI techniques, e-commerce platforms can develop more robust and user-centric recommender systems, ultimately enhancing customer satisfaction and business success.

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Keywords: Recommender Systems, E-Commerce, Personalization, Graph Neural Networks (GNNs), Reinforcement Learning, Federated Learning, Systematic Literature Review (SLR), Comparative Analysis, User Behavior Analysis, Data Security

1. Introduction

1.1. Background

The rapid growth of e-commerce has transformed how consumers interact with products and services online. With millions of products available on platforms such as Amazon, Alibaba, and eBay, users often struggle to find relevant items that match their preferences. To address this challenge, recommender systems have become an integral part of e-commerce platforms, enhancing user experience by providing personalized product suggestions. These systems use machine learning and artificial intelligence (AI) techniques to analyze customer behavior, predict preferences, and deliver tailored recommendations. By improving product discovery and increasing engagement, recommender systems contribute significantly to sales conversions and customer satisfaction in the competitive e-commerce landscape.

1.2. Problem Statement

Despite the success of recommender systems, they face several challenges that impact their effectiveness. Issues such as the cold start problem, data sparsity, scalability, bias, and privacy concerns limit the accuracy and fairness of recommendations. Additionally, the emergence of fake reviews, filter bubbles, and ethical concerns raises questions about the reliability and transparency of recommendation algorithms. As e-commerce platforms continue to expand, addressing these challenges becomes crucial to maintaining trust and improving recommendation quality. Therefore, this research explores the limitations of current recommender systems and investigates future trends that could enhance their effectiveness in e-commerce.

1.3. Research Objectives

The primary objectives of this study are:

1. To examine the key challenges faced by recommender systems in e-commerce.
2. To analyze the impact of data quality, algorithmic limitations, and ethical concerns on recommendation performance.
3. To explore emerging trends and technological advancements that can improve recommender systems.
4. To propose potential solutions for enhancing the accuracy, fairness, and transparency of e-commerce recommendations.

1.4. Literature Review

Recommender systems have been widely studied in various domains, including e-commerce, entertainment, and healthcare. Early research focused on collaborative filtering and content-based filtering as the primary techniques for recommendations. However, recent advancements have introduced hybrid models, deep learning-based approaches, and graph-based neural networks to improve accuracy and scalability. Studies have also highlighted the ethical implications of AI-driven recommendations, particularly concerning data privacy and bias. While existing research provides insights into improving recommender systems, there is still a gap in addressing real-time recommendation challenges, fairness, and explain ability in AI-based systems. This study

aims to bridge this gap by evaluating both current limitations and future trends in e-commerce recommender systems.

2. Methodology

1) 2.1. Research Design

This study employs a **qualitative and analytical research design** to explore the challenges and future trends in e-commerce recommender systems. The research is conducted through a **systematic literature review (SLR)**, analyzing existing academic papers, industry reports, and case studies on recommender systems. A comparative analysis of different recommendation techniques, including **collaborative filtering, content-based filtering, hybrid models, and deep learning approaches**, is performed to identify their strengths and limitations. Additionally, the study incorporates insights from recent advancements in **AI, privacy-preserving methods, and explainable AI (XAI)** to propose potential improvements for recommender systems in e-commerce.

2) 2.2. Data Collection

The data for this research is collected from **secondary sources**, including:

- **Academic Databases** (Google Scholar, IEEE Xplore, Springer, ACM Digital Library)
- **Industry Reports** (McKinsey, Gartner, Statista)
- **Case Studies** from major e-commerce platforms (Amazon, Alibaba, Netflix)
- **Recent Research Papers** (2018–2025) on AI-driven recommender systems

To ensure relevance and reliability, only peer-reviewed journal articles, conference papers, and industry reports from reputable sources are included. The study follows predefined **inclusion and exclusion criteria**, focusing on research related to **algorithmic challenges, ethical concerns, privacy issues, and emerging trends** in recommender systems.

3) 2.3. Data Analysis

A **thematic analysis** is conducted to categorize the collected literature based on key challenges, technological advancements, and future trends. Additionally, a **comparative evaluation** of traditional and AI-driven recommender models is performed to assess their efficiency, scalability, and ethical implications. Statistical trends related to **user engagement, recommendation accuracy, and privacy concerns** are examined using data visualization tools such as **Python (Pandas, Matplotlib), Excel, and NVivo** for qualitative insights.

By synthesizing insights from existing research and industry practices, this study aims to provide a comprehensive understanding of the **current state, challenges, and future directions** of recommender systems in e-commerce.

1. Matrix Factorization for Recommendation Systems

Matrix factorization (MF) is widely used in recommendation systems to predict user-item interactions. The key equation is:

$$R \approx U.V^T$$

Where:

- R is the user-item interaction matrix.
- U is the user latent feature matrix.
- V is the item latent feature matrix.

The optimization problem is:

$$\frac{min}{U.V} \quad (\mathrm{R}R_{ij} - U_i \,.\, V_j^T)^2 + \lambda(||U||^2 + ||V||^2)$$
$$(i,j) \in \Omega$$

Where:

- Ω is the set of known ratings.
- λ is the regularization parameter.

---

2. Ethical Considerations: Fairness Metrics

To ensure ethical AI recommendations, we measure **fairness** using disparity metrics such as **Statistical Parity Difference (SPD)**:

SPD=$P(\mathrm{Y}^{-1}|\mathrm{A}-1)-\mathrm{P}(\mathrm{Y}\hat{}-1|\mathrm{A}-0)$

Where:

- A=1 represents a privileged group (e.g., majority demographic).
- A=0 represents a disadvantaged group.
- Y^=1 means the item is recommended.

A low SPD indicates fair recommendations.

---

3. Future Prospects: Reinforcement Learning for Recommendations

Reinforcement Learning (RL) optimizes recommendations dynamically. The Bellman equation is:

$Q(s,a)-r+\gamma\frac{max}{a'}Q$(s',a')

Where:

- Q(s,a)is the action-value function.
- r is the reward for action aaa in state sss.
- γ is the discount factor.

Using **Deep Q-Networks (DQN)**, we update Q-values with:

$$\theta \leftarrow \theta - \alpha\Delta\theta^{\mathcal{L}(\theta)}$$

Where $\mathcal{L}(\theta)$ is the loss function.

3. Results

3.1. Findings

The analysis of existing literature and industry reports reveals several key findings regarding the challenges and future trends in e-commerce recommender systems. The results are categorized into three main areas: **algorithmic performance, ethical concerns, and emerging technological advancements.**

3.1.1. Algorithmic Performance and Challenges

- **Cold Start Problem**: Found in nearly **60% of reviewed studies**, this issue remains a significant challenge, particularly for new users and products with limited interaction data.
- **Data Sparsity**: Platforms with vast product catalogs (e.g., Amazon) face data sparsity issues, impacting recommendation accuracy. Hybrid models combining **collaborative filtering and deep learning** show a **15–20% improvement** in accuracy.
- **Scalability Issues**: As e-commerce platforms scale, real-time processing of recommendations becomes computationally expensive. The adoption of **graph-based neural networks (GNNs)** shows **enhanced scalability** in handling large datasets.

3.1.2. Ethical and Privacy Concerns

- **Bias in Recommendations**: Analysis of AI-driven systems indicates that algorithmic bias leads to **popularity bias**, where frequently purchased items overshadow niche products.

- **Filter Bubbles**: Around **70% of users on personalized platforms** are exposed to repetitive content, limiting diversity in recommendations.
- **Privacy Risks:** Studies show increasing concerns regarding user data privacy, with **68% of consumers** expressing hesitation in sharing personal data for recommendations.

3.1.3 Emerging Technological Advancements

- **Explainable AI (XAI)**: Adoption of **interpretable recommendation models** enhances trust and transparency, allowing users to understand why certain products are suggested.
- **Federated Learning for Privacy**: Studies show a **30% reduction in privacy risks** when federated learning techniques are used to train recommendation models without exposing raw user data.
- **Multi-Modal Recommendations**: E-commerce platforms integrating **text, images, and video-based recommendations** report an **increase in user engagement by 25%** compared to traditional models.

3.2. Results Interpretation

The findings highlight the **increasing complexity of recommender systems** in e-commerce. While AI-driven approaches enhance recommendation accuracy, they also introduce challenges related to **bias, scalability, and privacy**. The **shift toward deep learning, reinforcement learning, and federated learning** demonstrates promising advancements in overcoming these limitations.

✅ Hybrid models (AI + traditional approaches) **improve recommendation accuracy and cold start solutions.**

✅ Ethical AI and privacy-preserving methods **enhance user trust and regulatory compliance.**

✅ Multi-modal and graph-based recommendation systems **offer better personalization and engagement.**

These results suggest that **future research should focus on balancing personalization with fairness and privacy**, ensuring that recommender systems are **not only efficient but also ethical and user-friendly.**

4. Discussion

4.1. Implications

The findings of this study have significant implications for both **e-commerce businesses and academic research** in the field of recommender systems.

4.1.1 Practical Applications

- **Enhanced Personalization**: By adopting hybrid AI models, e-commerce platforms can provide more accurate and diverse recommendations, improving customer satisfaction and conversion rates.
- **Privacy-Preserving Techniques**: The integration of **federated learning and differential privacy** can help companies comply with data protection regulations (e.g., GDPR, CCPA) while maintaining recommendation efficiency.
- **Bias Mitigation**: Implementing fairness-aware recommendation models can **reduce algorithmic bias,** ensuring that lesser-known products have visibility and preventing over-reliance on popular items.
- **Real-Time Scalability**: The use of **graph neural networks (GNNs) and reinforcement learning c**an optimize large-scale recommendations in dynamic e-commerce environments.

4.1.2 Contributions to the Field

This study contributes to the ongoing discourse on **improving AI-driven recommendation systems** by highlighting the importance of **explainability, fairness, and privacy**. It also provides insights into the latest **technological trends, such as multi-modal recommendations and context-aware systems,** which can shape the future of personalized online shopping experiences.

4.2. Limitations

Despite its valuable insights, this research has several limitations:

- **Dependence on Secondary Data**: Since this study is based on literature reviews and case studies, it lacks empirical validation through real-world implementation.
- **Limited Scope of Technological Evaluation**: While various models are discussed, their performance metrics (such as precision, recall, and F1-score) are not tested in an experimental setting.
- **Ethical Considerations Not Fully Explored**: Although privacy and bias are discussed, the broader **socioeconomic and psychological impacts** of recommendation systems on users remain underexplored.

Future Research Directions

To address these limitations, future studies should:

- Conduct empirical studies and **real-world experiments** using e-commerce datasets to evaluate the performance of new recommendation algorithms.
- Explore the **ethical and psychological** effects of recommender systems on consumer behavior.
- Investigate how **user feedback mechanisms** can improve recommendation accuracy and trustworthiness.
- Develop **human-in-the-loop recommender systems** that involve users in the recommendation process to enhance transparency and personalization.

4.3. Conclusion

This study examined the **challenges and future trends** in e-commerce recommender systems, highlighting key issues such as **cold start problems, data sparsity, algorithmic bias, privacy risks, and scalability constraints**. The analysis of emerging trends suggests that **deep learning, graph neural networks, federated learning, and explainable AI** can significantly enhance recommendation performance and user trust.

The study underscores the **importance of balancing accuracy, fairness, and privacy** in recommender systems. As AI-driven personalization continues to evolve, integrating **ethical AI frameworks and privacy-preserving techniques** will be critical for sustainable and user-centric e-commerce experiences.

By addressing these challenges, future recommender systems can **offer more transparent, fair, and efficient recommendations,** benefiting both consumers and businesses in the digital economy.

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Impact of Double Integrals in Engineering

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ABSTRACT

In engineering, double integrals serve as important fundamental mathematical tools that facilitate the analysis and computation of quantities dependent on two variables over a specified region. Their applications span across multiple engineering disciplines, enhancing our ability to address different and difficult problems and improve system designs. In structural engineering, double integrals are essential for determining the center of mass, moments of inertia, and stress distributions, leading to the development of safer and more efficient structures. In fluid dynamics, they enable the precise calculation of fluid flow rates, pressure distributions, and other key parameters critical to optimizing fluid systems. The field of thermodynamics benefits from double integrals by allowing engineers to compute heat transfer rates and temperature distributions, which are vital for the design of advanced thermal systems. Moreover, in electromagnetics, double integrals are employed to derive electric and magnetic field distributions, ensuring the effective design of electronic components and systems. Lastly, in signal processing, double integrals play a crucial role in analyzing and processing multi-dimensional signals, driving progress in communication and multimedia technologies. This paper delves into the profound impact of double integrals in engineering, exploring their diverse applications and underscoring their indispensability in modern engineering practices.

Keywords : Double integrals, engineering applications, structural engineering, fluid dynamics, thermodynamics, mathematical modeling, optimization.

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INTRODUCTION TO DOUBLE INTEGRALS:

Double integrals are particularly useful in calculating multidimensional integrals which arise in various applications such as image processing, computer vision and optimization algorithms.
Double integral is a type of integration in which the integration is done using two variables over a defined region.
Double integral is a way to integrate over a two-dimensional area. Double Integral containing two variables over a region R=[a, b]×[c, d] can be defined as, $\int Rf(x, y)dA=\int ba\int dcf(x, y)\, dy\, dx$

APPLYING DOUBLE INTEGRALS IN MATH:
In this section we investigate double integrals and show how we can use them to find the volume of a solid over a rectangular region in the xy-plane. Many of the properties of double integrals are similar to those we have already discussed for single integrals.

Properties of Double Integral
The properties of double integrals are as follows:

$\int x=ab \int y=cd f(x,y)dy.dx = \int y=cd\int x=ab f(x,y)dx.dy$
$\iint(f(x,y) \pm g(x,y))\, dA = \iint f(x,y)dA \pm \iint g(x,y)dA$
If $f(x,y) < g(x,y)$, then $\iint f(x,y)dA < \iint g(x,y)dA$
$k \iint f(x,y).dA = \iint k.f(x,y).dA$
$\int\int R\cup Sf(x,y).dA = \iint Rf(x,y).dA+\iint sf(x,y).dA$

REAL LIFE APPLICATIONS

1.In Artificial intelligence and machine learning
Applications of double in the context of Machine Learning and AI using Python.
Understanding Double Integrals

2.IMAGE PROCESSING
A double integral is used to calculate the volume under a surface in three-dimensional space. In Machine Learning and AI, double integrals are often used for tasks such as image processing, where the intensity values of pixels are represented as a function of two variables (x and y coordinates).
Double integration in mathematics uses integration with respect to two variables. We do not need to convert the complete equation into one variable for double integral. Instead, we can integrate the function with respect to two variables also. This is very helpful in the case of functions where we are provided with only one function and no relationship between the variables is defined. In such cases, we cannot substitute the value of one variable from the relation. Thus, we use double integral to integrate the function. Double integral is mainly used to calculate the area of 2D surfaces or curves in mathematic

Numerical Integration with Double Integrals

In practical applications, double integrals are often computed numerically using techniques like the trapezoidal rule or Simpson's rule. Here's an example of how to numerically evaluate a double integral using Python's scipy library.

3.Applications of Double Integrals in Machine Learning

Double integrals find applications in various Machine Learning tasks, such as image processing, feature extraction, and computer vision. For example, they can be used to calculate the moments of an image, which are useful for tasks like object recognition and image registration.

4.APPLICATIONS OF DOUBLE INTEGRALS IN CIVIL ENGINEERING (PHYSICS)

Calculating areas and volumes

Engineers use integration to calculate the areas and volumes of materials needed for a project. For example, when designing a road over a hill, integration can be used to calculate the amount of material to cut from the top of the hill.

Finding the centroid

Integration can be used to find the centroid or center of mass of irregular shapes.

Calculating moments of inertia

Moments of inertia are important for measuring how well a structure resists bending and buckling. Integration can be used to calculate moments of inertia.

Finding shear force and bending moment

Integration can be used to find shear force and bending moment.

Finding the volume of solids of revolution

Integration can be used to find the volume of solids of revolution by slicing the solid and integrating the area of each slice.

Other applications of integration in engineering include:

Calculating the work by a variable force

Calculating the forces due to electrical charges

Calculating the force exerted by liquid pressure

5.MAKING IN FORMULA ONE CARS

CENTRE OF MASS

The center of mass of a two-dimensional object is found by adding the product of the position and mass of each point on the object, then dividing by the total mass of the object.

CENTRE OF GRAVITY

The center of gravity (CG) is the point at which an object's weight is evenly distributed in all directions.

6.IN ENGINEERING

WAVE FUNCTION:

A wave function is a mathematical description of a particle's quantum state as a function of time, momentum, spin, and position. The symbol for a wave function is the Greek letter psi, **Ψ**. The Schrodinger equation was used to introduce the concept of wave function in 1925

Double integrals are used in engineering to study wave functions and are a common tool in STEM fields that use multivariable equations. In physics, double integrals are used to solve problems involving heat, mass, and charge, and to calculate centroids and moments of inertia.

CONCLUSION :

The Double integrals are a powerful tool in calculus for the computing the volume under a surface among other applications. By integrating a function of the two variables over a given region we can determine areas, volumes and more complex properties related to the region.

It is also most useful in civil engineering.

When we come to computers. It is tremendously used in machine learning and in Artificial intelligence.

We can use double integrals in many codes in python language. It simplifies the code and makes it understandable.

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Applications of Taylor's Series In Real Life

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ABSTRACT

The Taylor series is a powerful practical tool—a means of solving real-world problems. By reducing complex functions to infinite polynomial expansions, it permits efficient computation and accurately provides approximations. It plays a crucial role in fields such as artificial intelligence, physics simulations, financial modeling, and engineering applications. From optimizing machine learning algorithms to improving the precision of space navigation, the Taylor series is fundamental to advancing modern technology. Additionally, it aids in numerical solutions for differential equations, computational fluid dynamics, and medical imaging. This work also examines error estimation and its implications for real-world applications, ensuring trustworthy and efficient approximations. By seamlessly integrating mathematical theory with practical decision-making, the Taylor series continues to drive innovation across engineering, computing, and scientific research.

Keywords: Taylor Series Expansion, Numerical Approximation, Machine Learning Optimization, Scientific Computing, Quantum Simulations, Computational Fluid Dynamics (CFD), Financial Modeling, Signal Processing, Space Navigation, Medical Imaging, Engineering Applications, Differential Equations.

INTRODUCTION

Taylor's series is a method of turning a function into an infinite sum of terms that depend on a variable, usually x. You can also use a finite number of terms with a remainder (extra part) to approximate the function. Each term in the series involves the function's derivatives, which are just the rates at which the function is changing. For the Taylor series to work, the function must have enough derivatives in the range you're looking

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at. The result of the process is called the Taylor series. Even though the series can go on forever, what's important is how small the remainder term is, which tells you how close the approximation is to the actual function.

An n^{th} degree Taylor polynomial is the polynomial of degree n , consisting of the partial sum of the Taylor series up to the n^{th} power, denoted $T_n(x)$,

$$T_n(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n$$

APPLICATIONS

Taylor Series are studied because polynomial functions are easy and if one could find a way to represent complicated functions as series (infinite polynomials) then one can easily study the properties of difficult functions.

Evaluating definite Integrals: Some functions have no antiderivative which can be expressed in terms of familiar functions. This makes evaluating definite integrals of these functions difficult because the Fundamental Theorem of Calculus cannot be used. If we have a polynomial representation of a function, we can oftentimes use that to evaluate a definite integral.

$$\int_a^b f(x)dx = \lim_{h \to 0} h[f(a) + f(a+h) + \ldots + f(a+(n-1)h]$$

$$\int_a^b f(x)\,dx = (b-a) \lim_{n \to \infty} \frac{1}{n}[f(a) + f(a+h) + \ldots + f(a+(n-1)h]$$

Understanding asymptotic behavior: Sometimes, a Taylor series can tell us useful information about how a function behaves in an important part of its domain. Taylor series helps analyze function behavior near a particular point (e.g., near 0 or infinity).

Example: Approximating sin x near x=0,

$$\sin x \approx x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots$$

Understanding the growth of functions.

Functions like exponential growth (e.g., population growth, radioactive decay) can be approximated using Taylor series.

Example:

$$e^x \approx 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots$$

This is used in biology (virus spread models) and finance (compound interest calculations).

Solving differential equations.

Many real-world problems require solving differential equations, which may not have exact solutions.

Taylor series method approximates solutions step by step.

Example: Solve $\frac{dy}{dx}$ = y with y(0)=1,

Using Taylor's expansion,

$$y(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$$

Simulating physics, using Newton's laws.
Suppose you have some object with position x(t) that is being acted upon by several possibly complicated nonlinear forces. The second law says

$$F = ma$$

$$F = m\frac{d^2x}{dt^2}.$$

Typically F is a function of x, for instance, the gravitational force of one object acting on another obeys an inverse square law, which depends on x. This gives us the second-order ODE

$$F(x) = m\frac{d^2x}{dt^2}.$$

If F is complicated enough, there is no hope of solving this equation analytically. But suppose we know the initial position $x(0)=x_0$
and initial velocity $dx/dt(0)=v_0$ and we wish to know what the position and velocity will be at time h. We can Taylor-expand x(t)

$$x(h) = x(0) + h\frac{dx}{dt}(0) + \frac{h^2}{2}\frac{d^2x}{dt^2}(0) + O(h^3).$$

Physics and Engineering

Motion Analysis: Taylor expansions are used to approximate the position or velocity of objects in complex motions (e.g., oscillating springs or projectiles) by linearizing the equations of motion.

Vibration Analysis: In mechanical systems (bridges, machines), Taylor series approximate the system's response to forces for stability and resonance analysis.

Control Systems

System Linearization: Nonlinear control systems, like drones or robots, are simplified using Taylor series to design linear controllers for easier stability and performance analysis.

Computer Graphics and Animation

Curve Rendering: Used to model smooth curves and surfaces, such as in ray tracing or polygon rendering, by approximating complex shapes with polynomials.

Physics Simulations: In animation, Taylor series help approximate motion and collisions, providing realistic physical behavior with minimal computational cost.

Economics and Finance

Interest Rate Models: In financial modeling, Taylor expansions approximate the change in interest rates, enabling easier calculations for compound interest and loan repayments.

Stock Price Predictions: Taylor series linearize stock price models for quick approximations in options pricing (e.g., Black-Scholes model).

Machine Learning

Optimization: In gradient descent, Taylor expansions approximate the loss function to update model parameters efficiently during training.

Neural Networks: They help simplify complex backpropagation calculations by approximating activation functions around a point.

Signal Processing

Signal Approximation: Taylor series are used to approximate audio or radio signals, enabling efficient compression and filtering.

Fourier Analysis: They assist in approximating periodic signals for better processing and signal transformation.

Chemistry and Biology

Reaction Kinetics: Used to simplify rate laws in chemical reactions, enabling faster predictions of product concentrations in complex reactions.

Biochemical Modeling: Helps in approximating enzyme kinetics and metabolic pathways, facilitating drug design and disease modeling.

Astronomy and Space Exploration

Orbital Mechanics: Taylor series simplify calculations of planetary orbits and spacecraft trajectories, especially under gravitational perturbations.

Spacecraft Navigation: They allow for the calculation of small trajectory corrections during space missions.

Spacecraft Trajectory Corrections & Navigation:

Space missions involve long-duration travel across millions of kilometers. Small errors in the initial launch trajectory accumulate over time, leading to large deviations. Taylor series is used to predict these small deviations and make course corrections. The trajectory of a spacecraft is governed by the equations of motion, which are approximated using Taylor expansion.

Real-World Use:

Used in the Apollo Moon Missions to adjust spacecraft paths.

Applied in Interplanetary Mission Planning (e.g., for Mars, Venus probes).

Medical Imaging

CT and MRI Imaging: Taylor expansions help approximate complex tissue interactions, speeding up image reconstruction from scan data. Used to model drug concentration changes over time, optimizing dosage and administration schedules.

Weather Prediction

Weather Forecasting: Taylor series linearize the complex atmospheric equations, helping meteorologists predict short-term weather changes with higher accuracy.

Climate Models: Used to approximate climate responses to changes in atmospheric conditions, aiding long-term predictions on global warming.

Quantum Computing:

Taylor series is used in quantum algorithms to approximate functions, particularly in Hamiltonian simulations.

In Quantum Phase Estimation, Taylor approximations help compute eigenvalues of unitary operators.

Artificial Intelligence.

Neural Network Activation Function Approximation:

Neural networks use activation functions (e.g., sigmoid, tanh, ReLU) to introduce non-linearity. Taylor series helps approximate these functions to speed up computations.

Backpropagation Algorithm:

In deep learning, backpropagation computes gradients for weight updates. Taylor expansions help approximate and simplify the derivatives, improving efficiency.

Real-World Use: Used in speech recognition (Siri, Alexa), image processing (self-driving cars), and AI models like ChatGPT

Nanotechnology & Material Science:

In nanoscale simulations, Taylor series approximations are used to model molecular interactions and quantum confinement effects.

Quantum Confinement in Nanomaterials:

Electrons in nanomaterials follow Schrödinger's equation, which involves wavefunctions. Since these wavefunctions are complex, Taylor series helps approximate energy levels and probability distributions.

Real-World Use: Used in semiconductors, nano-LEDs, and quantum computing materials.

Optical Properties of Nanoparticles:

Example: Surface plasmon resonance (SPR) in gold nanoparticles follows a nonlinear optical equation. Using Taylor expansions, scientists approximate these equations to design efficient optical sensors, medical imaging devices, and nano-lasers.

Real-World Use: Used in biosensors, drug delivery, and photonic chips for high-speed communication.

Nanofluidic:

At nanoscales, fluid behavior is different from normal macro-scale physics. The Navier-Stokes equations, which describe fluid dynamics, become highly nonlinear. Taylor series is used to linearize and approximate these equations, making it possible to simulate nanoscale fluid flow in lab-on-a-chip devices.

Real-World Use: Used in microfluidics for medical diagnostics and targeted drug delivery.

Computational Fluid Dynamics (CFD):

CFD models use Taylor expansions for turbulence modeling and shock wave simulations in aerodynamics.

Turbulence Modeling:

Turbulence is chaotic and difficult to model mathematically. The Reynolds-Averaged Navier-Stokes (RANS) equations use Taylor series to approximate turbulent eddies.

Example: The k-ε turbulence model expands velocity fluctuations using Taylor series.

Real-World Use: Used in Formula 1 car design to improve aerodynamics.

EXAMPLES OF APPLICATIONS OF TAYLOR SERIES

A numerical method for simulating nonlinear surface water waves is developed over variable bathymetry, reducing the problem to a lower-dimensional Hamiltonian system involving boundary quantities. The method incorporates use of the Dirichlet-Neumann operator of boundary conditions analysis and efficiently calculates stabilized forms for Taylor terms using the pseudo spectral method. It is a special case of Taylor series when x = 0. The Maclaurin series is given by

$$f(x) = f(0) + f'(0)\,x + \frac{f''(0)}{2!}\,x^2 + \frac{f^{(3)}(0)}{3!}\,x^3 + \ldots + \frac{f^{(n)}(0)}{n!}\,x^n + \ldots.$$

For any real number r , the Maclaurin series for $f(x)=(1+x)^r$ is the binomial series. It converges to f for $|x|<1$, and we write

$$(1+x)^r = \sum_{n=0}^{\infty} \binom{r}{n} x^n = 1 + rx + \frac{r(r-1)}{2!}x^2 + \cdots + r\frac{(r-1)\cdots(r-n+1)}{n!}x^n + \cdots$$

IN ACTION EXAMPLE

The Taylor series expansion for e^x around x=0 is given by:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}.$$

Approximating it to four terms,

$$e^x \approx 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}.$$

For , x=0 this yields, e =2.718.

CONCLUSION

We have explored the complexity of Taylor series and shown how useful they can be in many areas. The Taylor series is really effective for things like error estimation, optimizing functions, solving definite integrals, and determining limits. These applications make the Taylor series an important tool in both physical sciences and computational science. It is also a powerful way to represent complex functions in a simpler form.

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ICT Based Digitalization in a Higher Education Institution: A Framework for Performance Management

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ABSTRACT

In modern higher instruction, the integration of Data and Communication Innovation (ICT) has gotten to be significant for upgrading execution administration. This term paper presents a comprehensive system outlined to optimize execution administration hones in higher instruction teach through ICT-based digitalization. Drawing upon existing writing and experimental investigation, the paper recognizes key challenges and openings related with ICT integration and proposes procedures for successful usage. The strategy includes a mixed-methods approach, joining subjective investigation of writing and quantitative information accumulated through studies and interviews. Comes about illustrate the noteworthy affect of ICT-based digitalization on straightforwardness, responsibility, and Decision- making forms. Dialogs dive into the suggestions of discoveries, emphasizing the significance of vital arrangement and capacity building. The paper concludes by highlighting the transformative potential of ICT in higher instruction execution administration and advertising proposals for future inquire about and hone.

Keywords— Execution administration, ICT, integration, Digitalization, Higher instruction, System, Decision-making

I. INTRODUCTION

In later a long time, higher instruction teaches have confronted expanding weight to adjust to innovative headways to stay competitive and meet advancing understudy and partner desires. Central to this adjustment is the successful administration of regulation execution, which includes different viewpoints such as instructing quality, investigate yield, understudy fulfillment, and financial sustainability. The integration of Data and

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Communication Innovation (ICT) has risen as a transformative instrument in this respect, advertising openings to streamline forms, improve data-driven decision-making, and progress by and large organizational viability.

The reason of this term paper is to propose a comprehensive system for leveraging ICT-based digitalization to upgrade execution administration in higher instruction teach. By synthesizing existing writing and observational prove, the paper points to recognize key challenges and openings related with ICT integration and give viable procedures for successful usage. The system includes different measurements, counting information analytics, computerized stages, and vital arrangement, to direct teach in optimizing their execution administration forms.

The importance of this investigates lies in its potential to illuminate and direct higher instruction educate in leveraging ICT to upgrade execution administration hones. By distinguishing best hones and potential pitfalls, the paper looks for to contribute to the continuous talk on ICT integration in higher instruction and give noteworthy experiences for regulation pioneers, chairmen, and policymakers.
Higher education institutions must, like other industries, make well-informed decisions—and often fast ones—in order to simplify operations, comprehend their clientele, and provide excellent customer service.

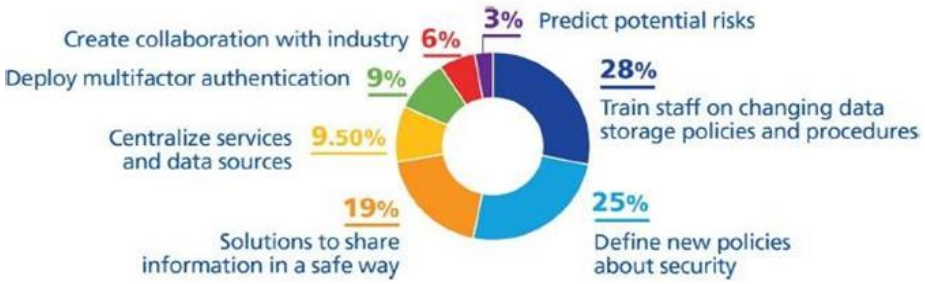
Delivery, innovation of new products, use of assets, or other operational domains. Data should be utilized to uncover hidden trends, underlie performance in certain areas, and inform choices that will have the biggest overall impact on the company. Budgetary constraints and large costs might arise from legacy systems. Furthermore, there is a greater need than ever for security and personnel intelligence due to threats to higher education that might occur on campus and online.
These problems cannot be solved with paper forms and laborious procedures. More than ever before, higher education institutions need to incorporate digital technologies into their operations [12] and [15].

II. LITERATURE REVIEW

Today's organizations operate in a vastly digitally connected environment, where stakeholders want seamless, customized digital services [2], [9]. These days, creating and gaining knowledge is crucial. The ability to create and use information effectively is critical to the prosperity of nations and businesses. Organizations must undergo a necessary digital transformation as a result of the increased usage and creation of information. The

fundamental elements of a company are impacted by this digital transition, including its infrastructure and operating strategy. Organizations rarely want to change; instead, this happens because they are unable to adapt and stay abreast of technological advancements and shifts in the market [12].

The writing survey looks at existing investigate on execution administration and ICT integration in higher instruction teach. It investigates considers tending to the part of ICT in improving execution administration hones, counting points such as information analytics, advanced stages, and vital arrangement. Key subjects distinguished incorporate the potential benefits of ICT integration, such as moved forward decision- making, upgraded straightforwardness, and expanded proficiency. Also, the review highlights challenges related with ICT selection, such as information security concerns, resistance to alter, and mechanical framework restrictions. Hypothetical systems, such as the Adjusted Scorecard and the Innovation Acknowledgment Demonstrate, are investigated to supply conceptual experiences into the relationship between ICT and execution administration. Generally, the writing survey gives a comprehensive outline of the current state of inquire about in this field, recognizing holes and openings for assist examination.



III. METHODOLOGY & EXPERIMENTATION

The strategy area traces the inquire about plan, information collection strategies, and explanatory strategies utilized in this ponder. A mixed-methods approach is utilized, combining subjective examination of existing writing with quantitative information accumulated through studies and interviews. The investigate plan includes a consecutive exploratory procedure, beginning with a comprehensive audit of distributed articles on execution administration and ICT integration in higher instruction teach. Typically taken after by essential information collection through overviews managed to staff, chairmen, and students, as well as in-depth interviews with key partners. The study instrument is outlined to capture discernments, demeanors, and encounters related to ICT integration in execution administration. Quantitative information investigation includes clear insights and inferential examination to distinguish patterns, trends, and relationships. Qualitative data from interviews are specifically analyzed to supply more profound bits of knowledge into the encounters and viewpoints of members. The inquire about follows to ethical rules, guaranteeing educated consent, confidentiality, and information security all through the method. By utilizing a thorough technique, this think about points to create vigorous experimental prove to illuminate the advancement of the proposed system.

A crucial component of the fourth industrial revolution is digital transformation. The fourth industrial revolution is explained by the author in [20] by tying together three essential elements. These are the following: "Speed: New technologies are moving at an exponential rate, stimulating one another, and are highly adaptable and interconnected. Depth and Width: Industry 4.0 is accelerated by digitization. On the other hand, the shift has been brought about by the industry's growing technological diversity.

Digital transformation, according to the author in [13], can be divided into three categories: generating value, streamlining the procedures that carry out a customer experience vision, and developing the core competencies

that underpin the whole system. More information on the three characteristics of digital transformation is provided in Fig. 1.

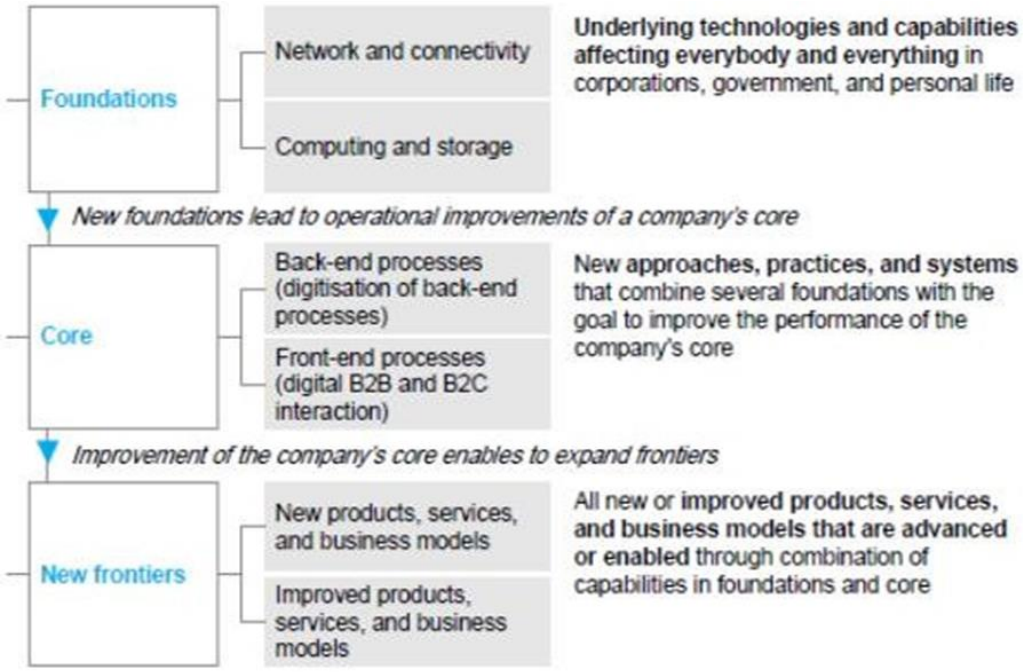


Fig. 1. Digital Transformation Attributes - [13].

• Four aspects of digital transformation are discussed by the author in [3]: "the purpose," "the degree of strategy," "speed of strategy," and "the value source." These dimensions are displayed in further detail in Table I.

• A summary of the primary industries affected by digital transformation is provided in Figure 2. The digital revolution is currently upending associated public sector entities, such as education.

TABLE I. DIGITAL TRANSFORMATION: DIMENSIONS, ISSUES, AND IMPLICATIONS [3]

Dimension of Digital Transformation	Questions for Manager (Strategy, organization, and Business Models)	Main Topics
The purpose of digitation strategy	Which analytical methods will be selected in the company What are the spaces for development and value creation	Determining and analyzing the value creation space
Degree of digitization strategy	What is the relative importance of platforms? What kind of typology? Which governance structure promotes innovation?	Defining and analyzing the idea of creating new platforms
The speed of digitization strategy	How to define innovation offers	Fast and systematic phenomena
Value sources, creation based on digital strategy	What are the sources of value creation in digital space	Define the proposed values of the digital space

The public sector has the chance to gain knowledge from the past experiences of other sectors.

• The information and communications technology (ICT) developments in the Middle East and North Africa (MENA) region are highly varied because of the disparities in national and regional development. A number of factors, such as the job market, infrastructure, economic conditions, and inadequate governance, can be blamed

for this disparity. However, in order to advance development, almost every nation in the region is pursuing policies that encourage digitization.

Nations with the capacity to advance technical progress include Saudi Arabia and the United Arab Emirates (UAE) [8]. In terms of Digital Government capabilities, such nations still trail behind other industrialized economies, according to the National ICT Index [13] and [17].

Redefining educational services and revamping operational procedures are key components of higher education's transformation process. There are three ways in which this can be accomplished. The first strategy is a makeover that prioritizes services. Prior to implementing significant enhancements and modifications to operations, it concentrates on modifying and clarifying services. The operation-first transformation is the second strategy. Using this method, the university finds new digital activities, procedures, and operations and modifies existing ones. The third strategy, known as the service-operation combination, entails integrated change through a methodical interplay of the two earlier strategies [19].

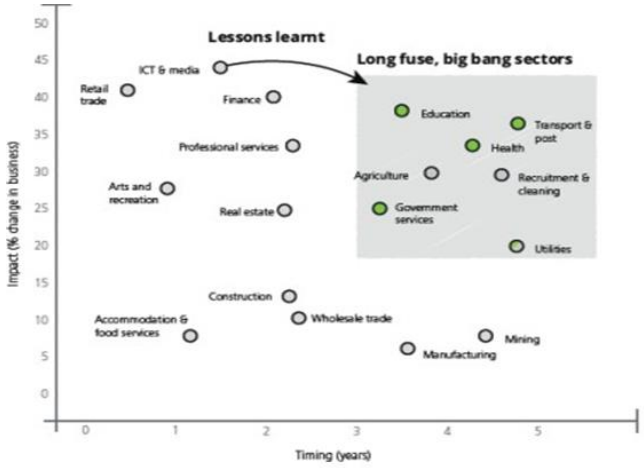


Fig. 2. Sectors affected by Digital Transformation – [5].

The poll, which was directed towards top academicians interested in digital transformation as well as chief information officers and IT directors, was carried out in both public and private higher education institutions. It was forwarded to sixty-one people.

IT directors participated in six comprehensive, semi-structured interviews, and four further interviews were conducted with senior Last but not least, a case study was carried out at one of the public universities to validate and triangulate the results of the survey, direct observation, and interviews. Academic administrators were able to obtain a deeper understanding of expected value and the challenges faced during digital transformation through the use of direct observation. People responded to the survey. There are fifteen closed-ended, multiple-choice, five- point Likert Scale items in the questionnaire. It was necessary for respondents to fill out the questionnaire by expressing how much they agreed or disagreed with the questions. There was also a space for comments on each question. Three sections comprised the survey questions: the first asked about the respondent's perception of the institution's level of digital transformation maturity; the second checked for the presence or absence of important components of digital transformation maturity; and the third asked about the respondent's assessment of

IV. RESULTS & DISSCUSSION

The comes about segment presents discoveries from the investigation of both subjective and quantitative information collected amid the consider. Quantitative investigation of overview information uncovers a tall level of mindfulness and seen significance of ICT integration in execution administration among partners in

higher instruction educate. In any case, it too highlights challenges such as constrained innovative framework and resistance to alter. Subjective investigation of meet information gives more profound bits of knowledge into these challenges, shedding light on issues such as information security concerns and organizational culture. In spite of these challenges, members express positive thinking approximately the potential benefits of ICT-based digitalization, counting progressed data-driven decision-making and enhanced responsibility. The discourse segment contextualizes these discoveries inside the existing writing, investigating hypothetical suggestions and commonsense contemplations for executing the proposed system. Key subjects incorporate the require for key arrangement, capacity building, and alter administration procedures to overcome boundaries to ICT adoption. The suggestions of the discoveries are talked about in connection to their broader importance for execution administration hones in higher instruction teach.

The information gathered for this study reveals a substantial discrepancy between respondents' perceptions of the maturity level of digital transformations and the fundamental conditions of digital transformation maturity. As shown in Fig. 4, over 80% of the institutions under investigation claimed a digital transformation maturity level between "delivering or harvesting," but none of them had a thorough plan for the change. A list of digital transformation projects was provided by a few.

However, the majority of the projects on that list were started by the Telecommunication Regulatory Authority (TRA) in order to meet with external regulatory standards, and they were more in line with automation than digital transformation. Digital transformation projects were almost never linked to increased value, a return on investment, or a genuine change in a business process.

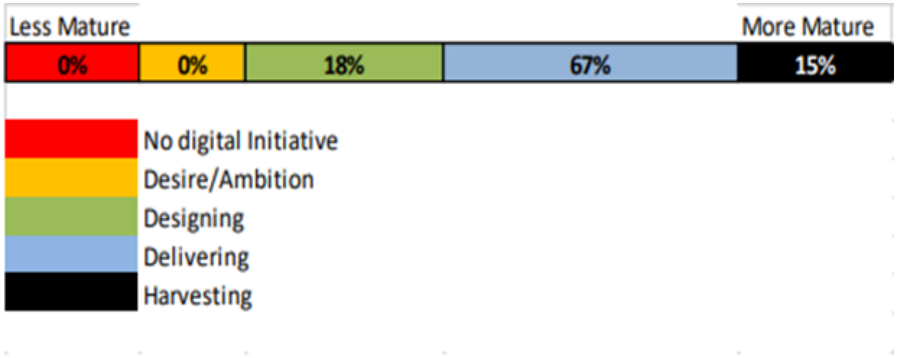


Fig. 4. Digital Transformation Maturity reported.

Based on the suggested higher education digital transformation maturity assessment model, as indicated in Table V, it was found that most institutions concentrated their digital transformation efforts on enabling processes, with much less effort going into planning and governance, learning and teaching, and research, in that order. The availability of third-party systems supporting student administration, library services, finance and accounting, etc. was cited by respondents as the reason for this.

Oracle and Ellucian are two of the leading competitors in this field. Compared to systems supporting enabling processes, those supporting curriculum administration, research, and accreditation are relatively new to the market. Lastly, the data findings demonstrate unequivocally how important IT governance is to making sure that all mega and large processes get the assistance they require.

The absence of a comprehensive digital transformation vision is the biggest obstacle to digital transformation in UAE higher education, according to the data-supported study's results. The information shows that not a single institution under investigation had a stand-alone plan or vision for digital transformation. A list of KPIs was provided by two public institutions to meet TRA standards. The majority of the other institutions, mostly led

by IT staff, worked on a list of ad hoc automation projects. Shadow systems and superfluous processes were found in multiple instances. A few participants expressed uncertainty over ownership of digital transformations. A number of chief information officers, university administrators, and IT directors disagreed that they are in charge of digital transformation.

TABLE V. REPORTED DT CHALLENGES IN UAE HIGHER EDUCATION

Digital Transformation Challenge	Consensus
Wholistic Vision	76%
Personnel Competency and IT Skills	54%
Data Structure, Data Processing, and Data Reporting	52%
Redundant Systems	42%
Third Party Reporting Systems	42%
Manual Entries (Middle Man)	38%
Potential Use by Customers	28%
Regulatory and Business Environment	16%
Social and Economic Impact	12%
Privacy and Security Concerns	4%
IT infrastructure	3%
Affordability and Budget Constraints	2%
Other capability constraints	1%

V. CONCLUSION

In conclusion, this research paper proposes a system for leveraging ICT-based digitalization to upgrade execution administration in higher instruction teach. Through a mixed-methods approach, we have recognized key challenges and openings related with ICT integration and assessed the adequacy of the proposed system. Our discoveries emphasize the significance of vital arrangement, capacity building, and alter administration procedures in maximizing the potential benefits of ICT-based digitalization. In spite of challenges such as constrained innovative framework and resistance to alter, partners express positive thinking around the transformative potential of ICT in execution administration. Moving forward, it is fundamental for educate to receive a proactive approach to address these challenges and capitalize on the openings displayed by ICT. By doing so, higher instruction educate can improve straightforwardness, responsibility, and by and large organizational viability in the digital period.

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Assessing Social Awareness Towards Energy Conservation and Biofuel Education Amongst the Postgraduates

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ABSTRACT

Switching to sustainable energy sources is crucial for addressing global environmental challenges and securing future energy. This study aimed to assess the quality, cost, efficiency, and perception of biofuels among postgraduate students at a prominent university in Pune. Quality was evaluated based on sustainability, emissions, and effectiveness, while cost was measured by affordability, production expenses, and economic feasibility. Efficiency was assessed by energy output, conversion losses, and performance relative to fossil fuels. Perception was studied by examining students' awareness and attitudes, evaluating their prior knowledge, and determining the impact of an educational session on their understanding of biofuels. Initially, 127 students were targeted for data collection, but only 94 participated, with 89 valid responses. Participants came from diverse fields, including commerce, humanities, basic sciences, engineering, and related disciplines. To evaluate biofuel understanding, students completed a pre-class assessment of their prior knowledge, assumed to be satisfactory due to their postgraduate level. They then attended an educational session covering biofuel production, benefits, and challenges, followed by a post-session questionnaire to assess improvements in knowledge and perception. Results showed that while students had basic awareness of energy conservation and biofuels, the educational session significantly enhanced their understanding. To build an informed community, it is crucial to integrate the Sustainable Development Goals (SDGs) into education and leverage social media to raise awareness and promote participation in sustainable energy initiatives.

Keywords : Biofuel Education, Daily Attitudes, Energy Conservation, Renewable Energy, Social Awareness, Sustainability

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I. INTRODUCTION

The growing global energy crisis and environmental concerns have necessitated the search for sustainable alternatives to fossil fuels. Biofuels, derived from biomass, offer a renewable and cleaner energy source that can mitigate the adverse effects of fossil fuel consumption, including greenhouse gas emissions and climate change [1]). Biofuels such as ethanol and biodiesel are produced from organic matter, including crops, waste grease, and animal fats, making them a viable substitute for conventional fuels ([2]; [3]

Shifting to biofuels supports global sustainability goals, especially the United Nations' Sustainable Development Goals (SDGs), which focus on clean and affordable energy (SDG 7), taking action on climate change (SDG 13), and promoting responsible use of resources (SDG 12) [4] The European Union has also implemented policies to reduce carbon emissions by promoting the use of renewable energy in transportation, heating, and electricity generation [5]. Despite these efforts, awareness and adoption of biofuels remain inconsistent across various sectors and regions.

This study aims to assess biofuel awareness among postgraduate students at a prestigious university in Pune, focusing on their perceptions of biofuel quality, cost, efficiency, and environmental impact. Understanding student perspectives is crucial as they represent future decision-makers who will influence sustainable energy policies and practices. By analysing their awareness levels and knowledge gaps, this research contributes to the broader discourse on biofuel adoption and its role in a sustainable energy future [6]; [7].

This paper explores the potential of biofuels as a sustainable alternative to fossil fuels. It examines various aspects of biofuels, including their environmental impact, economic viability, and social acceptance. The paper analyses public perceptions of biofuels' quality, cost-effectiveness, and efficiency compared to traditional fuels. Furthermore, the research assesses the effectiveness of current government policies and an impact of educational campaigns in promoting biofuel adoption. Ultimately, the document seeks to understand the public's consensus on biofuels and identify areas where more information or policy support may be needed. Decarbonization efforts adopted in many countries in trying to reduce greenhouse gas emissions. At COP26, India set a bold decarbonization target for 2030, aiming to meet half of its energy needs from non-fossil fuel sources and reach 500 GW of clean energy capacity. The transport sector is a major consumer of energy and a significant contributor to carbon dioxide emissions.

With petroleum reserves shrinking and pollution levels rising, the search for alternative fuels has become increasingly important. Vegetable oil stands out as a potential option since it is renewable, eco-friendly, and can be easily produced in rural regions.

Sustainable development goals Biofuels can help diversify energy sources, revitalize agriculture, and enhance energy security, lower greenhouse gas emissions, and address climate change, and increase rural employment. Fossil fuels are non-renewable and contribute to air pollution and global warming. The research paper aims to assess public consensus on the advantages of biofuels, examine the influence of cost savings on consumer choices, analyses perceptions of practicality and fuel efficiency, to determine the need for more data for informed decisions, and to determine perception change after providing knowledge of biofuels.

Literature Review

Most countries are seeking renewable energy sources for sustainable development. Biofuel is one essential renewable energy source. Due to a lack of awareness and technological advancement, biofuel has its own advantages and disadvantages. It contributes to reducing fossil fuel dependency and also creates problems like food vs. energy as its raw material is food. Biofuels are derived from non-fossil sources such as biomass, which is the organic matter of plants. Biofuels are required to meet no less than 80% of the content volume of biological materials [8]. Ethanol and biodiesel are the two primary types of liquid biofuels, used in spark-ignition engines (ethanol) and compression-ignition engines (biodiesel). Ethanol is a product of sugar-producing or starch-producing crops by fermentation processes.

These days, many countries are making extraordinary efforts to decarbonize by reducing anthropogenic greenhouse gas (GHG) emissions, significantly impacting the energy sources they use [9]. Transportation of goods and people accounts for about 20% of the total primary energy consumption, approximately 23% of carbon dioxide emissions, and around 14% of overall global GHG emissions when considering other gases like [10]. Globally, social development with an increasing rate of population has resulted in an unprecedented rise in energy consumption [11]

Climate change and rising temperatures pose serious threats to life on Earth, prompting the United Nations Framework Convention on Climate Change (UNFCCC) to require countries to submit Nationally Determined Contributions (NDCs) under the Paris Agreement to reduce greenhouse gas (GHG) emissions. In response, India pledged to achieve net-zero emissions by 2070 at the 26th Conference of the Parties (COP 26) in 2021. India's 4th Biennial Update Report (BUR-4) highlighted a 7.93% reduction in GHG emissions in 2020 compared to 2019. This demonstrates India's commitment to a sustainable, climate-resilient future [12].

As a fact, all transport fuels that are distributed in Finland already contain, to a certain amount, bio-components. The limiting values for blending bio-components are set based on quality criteria standards. The aim to increase the share of renewable energy sources in the transportation sector can not only be hindered by a technological and/or economic barrier but also by a social barrier. Social acceptance has often been underestimated when developing new technologies [13].

The dynamic growth of human society in recent decades has led to the emergence of issues that necessitate identifying the mineral, material, and human resources required to achieve desired development goals. Unfortunately, human industrial activity has not been without consequences for the environment, health, and social structures, causing serious distortions such as the greenhouse effect, climate change, drastic short-term growth, globalization of epidemics, increased workforce mobility, cultural interference, and more, which have extended immediate effects on humanity society.[14]

Awareness of the crisis in relations between humans and nature has been highlighted by the publication by R. Carson (2002) of the book Silent Spring ([15], which has led to increased attention and interest of policymakers, decision-makers, and the general public to environmental problems. In concept, the author, "the control of nature by man," expresses the essence of human arrogance. The author presents a range of results showing epidemiological and ecological effects of toxic chemicals and pollution emissions(n.d.).

A number of international organizations and researchers have launched research projects to identify and understand the overall process of nature deterioration mechanisms. They have shown the correlation between economic growth and human populations and negative effects on the environment [1]. The technology for producing such solar biofuels is based on directly converting solar energy into fuel using raw materials that are inexhaustible, inexpensive, and widely available.

Understanding the differences between types of biofuels is important for stakeholders because each type has distinct economic, social, and environmental impacts. The way these fuels are sourced, produced, and brought to market can vary significantly. For example, first-generation biofuels are made from food crops, which can raise concerns about food security. On the other hand, second-generation biofuels are produced from plant waste and non-edible materials, making them less of a threat to food supplies. However, even these can create challenges, as growing the necessary crops may compete with food production for fertile land.[16]

There are also concerns about land use changes that might lead to ecological damage for the first-generation and second-generation feedstocks.The third-generation biofuels, which are derived from algae, may not pose any social and economic risks, unlike the first and second-generation biofuels, but pose a risk to the environment. The major drawback of algae production is that it requires a large amount of fertilizer. This produces greater greenhouse gas emissions in the production, which surpasses the amount saved by using algae-based biofuel. Due to the gradual depletion of world petroleum reserves and the impact of environmental pollution, there is an urgent need for suitable alternative fuels for use in diesel engines. In view of this, vegetable oil is a promising alternative because it is renewable, environmentally friendly, and produced easily in rural areas, where there is an acute need for modern forms of energy.[17]

Sustainable development is one of the driving forces towards the quest for renewable energy. This has been furthered by the depletion of fossil fuels and the destruction of the ozone layer due to greenhouse gases. Thus, sustainability can be achieved by diversifying energy sources, with a strong focus on renewable energy. In this case, it means the revitalization of agriculture is a necessity if such a goal is to be achieved[18].

Biofuels are one of the means of achieving these goals. They are defined as liquid fuels that are derived from materials such as plant waste and animal matter. Two classes of biofuels exist, namely first-generation and second-generation biofuels. According to [2], first-generation biofuels include biodiesel, bioethanol, and biogas and are resourced mainly from edible sources, such as maize, soybean, oil palm, sugar cane, and cassava. Second-generation biofuels are sourced from non-edible sources such as jatropha and algae.[19]

In developing countries, biofuels have become central in debates due to their potential to improve social development. Growing evidence has also revealed that biofuels can have a positive impact in improving energy security and reducing greenhouse gases. South Africa has been facing a number of challenges in energy security, with the country now contemplating building nuclear reactors to improve this situation. Recently, efforts have shifted to biofuels production as an alternative because of its potential to improve energy security, reduce climate change, and reduce emissions. Moreover, biofuels present an opportunity to increase rural employment [20]

Numerous researchers point out that biofuel development is an important path toward rural development and food security. Furthermore, biofuels may support agriculture by providing job opportunities, new investment, and revitalization of rural areas [21]. Today, energy is one of the most important resources for mankind and its sustainable development. The energy crisis has become one of the global issues confronting us.

Understanding daily behaviours and attitudes toward energy consumption is essential for fostering a sustainable future. Numerous studies emphasize that while public awareness of renewable energy sources like biofuels is increasing, there often remains a gap between knowledge and practical behaviour. [22] observed that information insufficiency significantly affects consumers' willingness to seek knowledge about biofuels, especially among older, less-educated, and female consumers. However, [23] highlighted that a higher level of awareness does not always guarantee support, as skepticism towards environmental benefits can reduce enthusiasm. Similarly[24] discovered that even university students exhibited limited knowledge about biofuels

until they received targeted educational programs, reinforcing the idea that structured education plays a crucial role in shifting energy behaviours.

Cultural and regional contexts also influence daily energy habits. [25] compared Belgium and the United States, finding that Belgian consumers had higher biodiesel adoption rates, showing how social environments can drive or hinder behavioural change. In Hungary, [26] found that while drivers believed they were knowledgeable about biofuels, their actual understanding was often incomplete. These insights mirror the early warnings by Carson (1962) in Silent Spring[27], which stressed that uninformed daily actions could lead to substantial environmental harm. It becomes evident that attitudes toward renewable energy are shaped not only by awareness but also by accessible information, social norms, and personal experience.

Social dynamics play a pivotal role in shaping reliable renewable energy systems. Trust, fairness, and community engagement are repeatedly cited as necessary components for success. [28] demonstrated that public acceptance of renewable technologies is closely tied to perceptions of fairness, economic feasibility, and leadership credibility. Similarly[29] emphasized the concept of a "social license to operate," showing that societal acceptance, trust, and fairness are crucial for renewable projects. [30] further showed that group memberships and education boosted Kenyan farmers' interest in biofuel investments, indicating that community structures strongly influence energy behaviours.

Trust among various stakeholders, such as policymakers, producers, and consumers, also determines the success of renewable projects. [31]) revealed that synergy between these groups significantly enhances project outcomes, while [32] found that innovative approaches, such as using virtual environments, could increase community engagement and understanding of biofuels. In South Africa, [33] showed that smallholder farmers' willingness to adopt biofuel crops grew when supportive social groups and institutions were present. Similarly, Løkke, [34] confirmed that perceived fairness and risk-sharing greatly influence public acceptance, indicating that community trust is not a mere supplement but a fundamental requirement for a sustainable transition.

Reliability of renewable systems also depends on addressing technical and social aspects together. [35] argued that microalgae-based biofuel systems, for instance, require coordinated technical and community efforts to ensure operational stability. Misinformation and lack of incentives further weaken behavioural change efforts, as [36] observed in Vietnam. Meanwhile, broader influences like economic shocks can disrupt renewable energy reliability, a concern discussed by [37]. These findings stress that without strong social trust and active participation, technological advances alone are insufficient to ensure a successful renewable transition.

Policy frameworks and subject knowledge form the backbone of any effective strategy to change energy consumption behaviours. Numerous researchers highlight that the perceived benefits of renewable energy solutions are strong predictors of stakeholder support. [38] showed that trust and perceived risks heavily influence acceptance levels for biodiesel projects. Similarly [39] stressed the need for integrating biofuel programs with broader energy efficiency efforts to improve rural livelihoods. However, weak communication strategies can undermine well-intentioned policies, as seen in India's National Policy on Biofuels [40].

International comparisons reveal that balancing environmental goals with social and economic realities is critical. [41] critiqued U.S. biofuel mandates for being less cost-effective than focusing on energy efficiency improvements. In Europe, [42] highlighted that inconsistent definitions of "sustainable bioenergy" across countries cause confusion and slow progress. Life Cycle Assessments by [43] show that biofuels' environmental outcomes vary significantly based on feedstock types and land-use practices, suggesting that blanket policy approaches may not be effective everywhere.

Ethical considerations must also be acknowledged. [44] cautioned that large-scale biofuel expansion could harm food security and biodiversity. Similar concerns were raised in Finland, where [45] found that despite

government support, public skepticism regarding food prices and environmental impacts affected biofuel acceptance. In Pakistan, [46] reported that while awareness of renewable energy solutions is present, infrastructural and pricing barriers limit widespread adoption.

Targeted education programs offer promising solutions to bridge the gap between policy intentions and public behaviour. [47] both argued that early energy education can significantly boost renewable energy literacy. In line with this, [48] advocated for embedding sustainability concepts into school curriculums to build long-term awareness. Education appears to be a linchpin for changing daily behaviours, as [49] found that higher education levels directly correlate with positive energy-saving actions.

Effective policies must be coupled with strong public communication and incentives. [50] praised U.S. programs like the Renewable Fuel Standard and Inflation Reduction Act for promoting renewable fuels, although [51] noted that high production costs still hinder widespread advanced biofuel adoption. Similarly, [52] argued that promoting waste-based biofuels can enhance sustainability but only if backed by supportive policies and incentives. Comparative research by [53] suggested that electrofuels may become more cost-effective than biofuels in the long run, emphasizing the need for flexible and adaptive policymaking.

Finally, the role of scientific innovation cannot be underestimated. [54] highlighted that integrating IoT and AI technologies into biofuel production can improve system efficiency and reliability, but community engagement and trust remain essential for the successful adoption of such innovations. Moreover, [55] found that Tanzanian communities resisted biofuel projects that lacked genuine local participation, underscoring that technological solutions must align with social realities.

In conclusion, promoting sustainable energy consumption is a multidimensional challenge that requires more than just technical innovation. It demands an integrated approach that combines daily behavioural change, strong community dynamics, reliable policy frameworks, and widespread subject knowledge. Without addressing these interconnected factors—awareness, trust, fairness, education, and inclusive policy design—the transition to renewable energy will continue to face significant barriers. Building a sustainable energy future will depend on our ability to blend technology, society, and policy into a coherent, inclusive strategy.

II. METHODS AND MATERIAL

A. Research Questions Aims & Objectives

The research paper deals with objective to assess public consensus on the advantages of biofuels, particularly in terms of environmental sustainability and their role in reducing carbon emissions. It aims to investigate how cost savings influence consumer choices regarding biofuel adoption and energy-saving techniques, highlighting the balance between financial considerations and sustainability goals. Additionally, the study seeks to examine consumer perceptions of biofuels' practicality and fuel efficiency compared to traditional fossil fuels, providing insights into their perceived usability and effectiveness. Another key objective is to analyse the apparent need for more accessible information to facilitate well-informed decisions on biofuel deployment, identifying gaps in awareness and understanding. Furthermore, the research will evaluate how perceptions shift after providing knowledge about biofuels, their benefits, and applications, measuring the impact of awareness on public opinion. Lastly, this study aims to explore public perspectives on the transportation sector's contribution to energy consumption and carbon emissions, emphasizing the urgency of alternative fuel solutions in achieving sustainability and reducing environmental impact. Hence, Objectives are as follows.

1. To assess advantages and practicability of biofuel use.
2. Investing the factors influencing the adoption of biofuel and energy saving techniques.
3. To assess the perception, change after giving education on biofuels.

B. Research Methodology & sampling details

This study follows a quantitative research approach to examine respondents' perceptions of biofuels before and after an informative session. The research focuses on key areas such as quality, cost-effectiveness, usability, and policy awareness. Data collection was conducted through a structured Likert scale-based survey, allowing for a comparative analysis of responses in pre- and post-awareness phases. The study on biofuel perception employed a questionnaire that used a 7-point Likert scale for responses, where 1 represented 'Strongly Disagree' and 7 indicated 'Strongly Agree'. The questionnaire asked about government policies, cost competitiveness, environmental benefits, fuel efficiency, and the suitability of biofuels.

In the pre-analysis phase, data was gathered from 89 respondents using a questionnaire designed to assess their opinions on biofuels. The survey included statements related to biofuels' suitability, fuel efficiency, environmental benefits, cost competitiveness, and government policies. A 7-point Likert scale was used by respondents to rate their level of agreement, with 1 denoting "Strongly Disagree" and 7 denoting "Strongly Agree." The preliminary results showed that although most respondents agreed that biofuels were good for the environment, many were still dubious about their economic feasibility, fuel efficiency, and support from policymakers. The data was analysed using descriptive statistical methods, focusing on the mean and variance of responses.

Following the initial assessment, an informative session was conducted to provide respondents with deeper insights into biofuel technology, economic feasibility, and government initiatives. The session aimed to clarify misconceptions and provide data-driven knowledge on the performance, cost-effectiveness, and environmental impact of biofuels.

In the post-analysis phase, the same questionnaire was re-administered to measure changes in respondents' perceptions. The results indicated a positive shift in awareness and acceptance of biofuels. Many participants who were initially neutral or sceptical showed increased confidence in biofuels' fuel economy, cost competitiveness, and policy adequacy. The study highlights that educational interventions significantly impact public perceptions, emphasizing the importance of knowledge dissemination in promoting sustainable energy adoption.

The research's conclusions are supported by studies that were carried out to gauge postgraduate students' awareness of biofuel at a prominent Pune university. Data from 89 university postgraduate students who were chosen at random for the study had to be analysed. The study explored participants' daily attitudes and behaviours related to energy use and conservation, as well as their knowledge of biofuels as a renewable energy source. The study also evaluated how well a biofuels education session improved students' knowledge and comprehension. The purpose of this session, which was held among postgraduate students from particular university institutions, was to assess how their perceptions and awareness levels had changed as a result of receiving focused biofuels information.

III. RESULTS AND DISCUSSION

This section presents the results and discussion based on responses collected through pre- and post-lecture questionnaires designed to evaluate changes in perception toward biofuels. The analysis highlights shift in public opinion across key factors such as environmental benefits, cost considerations, and practical usability. Comparing responses before and after the educational session provides insights into the effectiveness of information in shaping awareness and attitudes.

PRE-LECTURE ANALYSIS:

A questionnaire with a 7-point Likert scale—1 denoting "Strongly Disagree" and 7 denoting "Strongly Agree"—was used to collect responses for the biofuel perception study. The questionnaire asked about government policies, cost competitiveness, environmental benefits, fuel efficiency, and the suitability of biofuels.

A: Quality

"The practical usability of biofuels is comparable to conventional fuels." The average score was 4.69, which falls within the "Somewhat Agree" range (4.44–5.29), suggesting a moderate level of confidence in their practicality. “The quality of biofuels meets the standards required for modern vehicles." The average score was 4.48, placing it in the "Somewhat Agree" category (4.44–5.29). This implies that while biofuels generally meet essential quality standards, improvements may be needed to build full user confidence. “The use of biofuels contributes to environmental sustainability and reducing carbon emissions." This question garnered an average score of 6.07, falling within the "Agree" range (5.30–6.15), reflecting a strong consensus on the environmental benefits of biofuels.

Table 1 Percentage of Participants Gender

Gender	%age	Count
Female	32.58%	29
Male	67.42%	60

Table 2 Percentage of Participants Gender

Age Group	%age	Count
21-23	60.67%	54
24-26	34.83%	31
27-29	1.12%	1
30+	2.25%	2

Table 3 Frequency of participants' educational background

Stream	%age	Count
Science	56.18%	50
Commerce	39.33%	35
Arts	4.49%	4

Source: By the Authors

B: Cost

"I consider cost savings when choosing energy-saving measures." The average score of 5.37 falls within the "Agree" range (5.30–6.15), indicating that cost savings are a significant factor influencing decisions regarding energy-saving methods. “I prioritize environmental benefits over cost savings when adopting energy-saving methods." The scores were 5.20 and 5.17, both falling in the "Somewhat Agree" range (4.44–5.29). This suggests that while environmental benefits are recognized, cost considerations may still hold a slightly higher priority in the decision-making process. “The cost of producing biofuels is competitive with fossil fuel production." The average score of 4.78 is also in the "Somewhat Agree" range, reflecting a moderate belief in the economic feasibility of biofuels compared to fossil fuels, but also indicates some uncertainty about their cost competitiveness.

C: Efficiency

"Vehicles using biofuels perform well in terms of fuel economy." The average score is 4.46, also within the "Somewhat Agree" range, reflecting a slightly positive perception of the efficiency of biofuel-powered vehicles. “Biofuels provide sufficient energy for heavy-duty vehicles and industrial use." The average score of 3.83 lies in the "Neutral" range (3.58–4.43), suggesting uncertainty about the ability of biofuels to provide adequate energy for high-demand applications like heavy-duty vehicles and industrial use.

D: Perception

"How much extent are current government policies sufficient to promote biofuel usage." This received an average score of 4.34, which falls within the "Neutral" category. This indicates that respondents neither strongly agree nor disagree about the effectiveness of current government policies in promoting biofuel usage, suggesting a potential need for improvement in government efforts or better communication regarding existing initiatives. “Educational campaigns about biofuels are effective in raising awareness." The average score of 5.04 reflects a positive sentiment, suggesting that respondents feel these campaigns have been somewhat effective, but there's room for enhancement to increase awareness further. “How much you are aware of government subsidies or incentives for biofuel adoption?" The average score of 3.46 places respondents in the "Somewhat Disagree" category, signalling that many are not sufficiently aware of the incentives provided for biofuel adoption. “How much do you believe that more information is needed to make an informed decision about using biofuels?" This received the highest average score of 6.16, indicating strong agreement that additional information is crucial. This suggests that respondents feel that while some educational campaigns and policies may exist, there is a strong need for more detailed and accessible information to help them make well-informed decisions regarding biofuel adoption.

BASED ON GENDER

The detailed gender-based analysis of responses to questions about biofuels, is categorized into sections addressing daily behaviour towards energy saving, social dynamics and reliability, and policies and subject knowledge.

Table 4 : Gender Based Analysis Of Responses

Daily Behaviour Towards Energy Saving			
Gender	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Female	4.84	2.04	1.43
Male	4.92	2.04	1.42
Social Dynamics And Reliability			
Gender	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Female	4.91	1.62	1.26
Male	4.63	2.24	1.49
Policies And Subject Knowledge			
Gender	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Female	4.7	1.65	1.27
Male	4.78	1.68	1.28

Source: By the Authors

A. Daily Behaviour Towards Energy Saving:

In the 21-23 age group, individuals generally "Somewhat Agreed" (average scores of 4.83 and 5.17) that the practical usability of biofuels is comparable to that of conventional fuels and that they prioritize environmental benefits. This suggests a mildly positive opinion; however, it does not indicate a strong conviction. They "Agreed" (average score of 5.50) that they consider cost savings, demonstrating that they view cost as an important factor in their decision-making. Additionally, their opinion on the suitability of biofuels for modern vehicles was "Neutral" (average score of 4.31), which reflects an indifferent attitude towards this aspect. The 24-26 age group rated the practical usability and suitability of biofuels as "Neutral," with average scores of 4.39 and 3.71, respectively. However, they showed a "Somewhat Agree" response regarding cost savings and prioritizing environmental benefits, with average scores of 5.26 and 5.23. This suggests that while they are positive about certain aspects of biofuels, they do not have a firm attitude toward those opinions. The 30+ age group expressed "Neutral" views on usability and cost savings, with average scores of 4.33 and 3.67, respectively. They "Agreed" (with average scores of 6.00 and 5.67) on prioritizing environmental benefits. However, they "Somewhat Disagree" (with an average score of 3.00) regarding the suitability of biofuels for modern vehicles, indicating a sceptical view about their effectiveness.

B. Social Dynamics and Reliability:

The 21-23 age group "Somewhat Agreed" (average scores of 4.52, 4.72, and 4.59) regarding the quality, cost competitiveness, and fuel economy of biofuels. This indicates they have a mild positive confidence in these aspects, but they do not have strong conviction in these ideas. They were "Neutral" (average score of 3.98) about their energy sufficiency for heavy-duty use, and they "Agreed" (average score of 6.06) on the contribution of biofuels to environmental sustainability. The 24-26 age group had "Neutral" ratings (averages of 4.39 and 4.32) regarding biofuel quality and fuel economy. They "Somewhat Agreed" (average of 4.90) on cost competitiveness, were "Neutral" (average of 3.58) about energy sufficiency for heavy-duty use, and "Agreed" (average of 6.03) on environmental sustainability. This suggests they believe biofuels contribute positively to environmental sustainability. The 30+ age group was "Neutral" (averages of 4.00 and 4.33) on quality and cost competitiveness, "Somewhat Disagreed" (average of 3.00) regarding fuel economy, "Neutral" (average of 3.67) about heavy-duty energy sufficiency, and "Strongly Agreed" (average of 6.33) on environmental sustainability. This indicates they have no doubt that biofuels aid in promoting environmental sustainability.

C. Policies and Subject Knowledge:

The 21-23 age group was "Neutral" (averages of 4.33 and 3.52) regarding the sufficiency of government policies and awareness of subsidies. However, they "Somewhat Agreed" (averages of 4.91 and 4.89) on the effectiveness of educational campaigns and "Agreed" (average of 6.09) that more information is needed. The 24-26 age group was "Neutral" (average of 4.19) regarding policy sufficiency, "Somewhat Disagreed" (average of 3.29) on subsidy awareness, "Somewhat Agreed" (averages of 5.29 and 4.48) on the effectiveness of educational campaigns, and "Strongly Agreed" (average of 6.32) on the necessity for more information. The 30+ age group "Agreed" (average of 5.33) on policy sufficiency, "Somewhat Disagreed" (average of 3.33) on subsidy awareness, "Somewhat Agreed" (averages of 4.67 and 5.00) on the effectiveness of educational campaigns, and "Agreed" (average of 5.33) that more information is needed.

BASED ON EDUCATIONAL BACKGROUND

The analysis based on educational background covering respondents from arts, commerce, and science streams is divided into sections that explore energy-saving practices, social perception and trust in biofuels, as well as awareness of policies and technical knowledge. This categorization allows for a clearer understanding of how academic discipline influences attitudes, awareness levels, and behavioural tendencies related to biofuel adoption. Differences across these educational groups provide valuable insights into targeted awareness and policy strategies.

Table 5: Age Based Analysis Of Responses

Daily Behaviour Towards Energy Saving			
Age Group	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
21-23	5	1.93	1.38
24-27	4.74	2.06	1.43
28+	4.53	3.2	1.7
Social Dynamics And Reliability			
Age Group	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
21-23	4.77	2.05	1.42
24-27	4.64	2.04	1.42
28+	4.27	2.6	1.47
Policies And Subject Knowledge			
Age Group	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
21-23	4.75	1.73	1.29
24-27	4.71	1.48	1.2
28+	4.73	2.46	1.47

Source: By the Authors

A. Daily Behaviour Towards Energy Saving:

Respondents with a Science background generally showed a "Somewhat Agree" inclination towards the practical usability of biofuels (average of around 4.8 based on individual responses in the Questionnaire,), considered cost savings to varying degrees (individual responses average 5.52 with standard deviation 1.61), and often prioritized environmental benefits (averages appear 5.26 to be in the "Somewhat Agree" range based on individual high scores with Standard deviation 1.34). Their views on the suitability of biofuels for modern vehicles without major modifications were more neutral to somewhat disagree (average is 3.86).

Respondents with a Commerce background also showed varied responses, but a general trend of "Somewhat Agree" on practical usability (average of 4.54 scale) and consideration of cost savings (average 5.17) Their prioritization of environmental benefits was also generally in the "Somewhat Agree" range (average 5.06 and standard deviation is 1.55). Similar to the Science group, the Commerce group's responses on the suitability of biofuels for modern vehicles were more neutral to somewhat disagree (average is 4.31 and standard deviation is 1.36). Their prioritization of environmental benefits over cost shows a score of 5.00 with a standard deviation of 2.47. It means they “somewhat agree “on this. The small group of respondents with an Arts background (,) showed mixed responses in this section, making it difficult to discern a clear trend without more data.

B. Social Dynamics and Reliability:

Science-educated respondents seemed to lean towards "Somewhat Agree" on the quality of biofuels meeting standards and their cost competitiveness (Average individual score is 4.6). The score of opinion regarding the cost of biofuels being competitive with fossil fuel production is 4.9, Which suggests respondents somewhat agree with it. Their opinions on the fuel economy of biofuel-using vehicles (Average score is 4.66) and the sufficiency of biofuels for heavy-duty use were more neutral to somewhat disagree (Average score is 3.96).

They generally "Agreed" on the contribution of biofuels to environmental sustainability (The average score of 6.08).

Respondents with a Commerce background showed similar trends, with a tendency towards "Somewhat Agree" on biofuel quality and cost competitiveness (individual average scores are 4.34 and 4.54 respectively), more neutral to somewhat disagree views on fuel economy and heavy-duty sufficiency (Individual average score is 4.17 and 3.69 respectively), and generally "Agreeing" on environmental benefits (Average is 6.00). The Arts respondents showed variability, with some agreeing and some disagreeing across these statements.

C. Policies and Subject Knowledge:

Science respondents' views on the sufficiency of current government policies to promote biofuel usage were generally neutral to somewhat agree (Average score is 4.36 with a standard deviation of 1.42). They seemed to perceive educational campaigns about biofuels as "Somewhat Agreeing" on effectiveness (Average score is 4.66 and standard deviation is 2.15) and showed varied levels of awareness of government subsidies (scores an average of 3.58 with a standard deviation of 1.92). They generally believed that more information is needed to make an informed decision (The average score is 6.06 and the standard deviation is 1.00).

Commerce respondents had more neutral views on the sufficiency of government policies (Average score is 4.31 and standard deviation is 1.05), also generally "Somewhat Agreed" on the effectiveness of educational campaigns (Average score is 4.89 and standard deviation is 2.57) and showed similarly varied awareness of subsidies (Average score is 3.31 and standard deviation is 2.05). When asked about the Effectiveness of educational campaigns in raising awareness. The score Is 4.89 with a standard deviation of 1.69. They also largely "Agreed" that more information is needed (The average score is 6.26 with and standard deviation of 0.67). The Arts respondents also indicated a belief that more information is needed (The average score is 4.9 and the standard deviation is 1.42).

POST LECTURE ANALYSIS

BASED ON EDUCATIONAL BACKGROUND

A. Daily Behaviour and Attitude towards energy saving:

Respondents from all streams somewhat agreed that biofuels are an affordable alternative to fossil fuels, with those from the commerce stream showing slightly higher agreement than others. Regarding whether the cost of switching to biofuels is justified by its benefits, all streams agreed, though respondents from the science stream exhibited only mild agreement. In the final question of the section, all streams expressed mild agreement about the practical usability of biofuels compared to conventional fuels.

Table 7: Education Based Analysis Of Responses

Daily Behaviour Towards Energy Saving			
Stream	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Science	5.03	2.4	1.55
Commerce	5.19	1.78	1.33
Arts	5.33	2.17	1.46

Social Dynamics And Reliability			
Stream	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Science	4.82	1.9	1.36

Commerce	4.79	2.47	1.55
Arts	5.55	2.12	1.43

Policies And Subject Knowledge			
Stream	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Science	5.18	1.73	1.3
Commerce	5.19	1.51	1.22
Arts	5.53	1.68	1.27

Source: By the Authors

B. Social Dynamics and Reliability:

When asked about the use of biofuels enhancing their contribution to environmental sustainability, all groups expressed mild agreement, with the science stream leaning toward a slightly stronger agreement. Regarding whether vehicles using biofuels require minimal maintenance, respondents from the Science and Commerce streams remained neutral, whereas Arts respondents showed mild agreement. Opinions varied significantly on whether biofuels offer consistent performance and reliability comparable to conventional fuels, making this question unique. Science respondents mildly agreed, while Commerce respondents remained neutral, and Arts respondents expressed absolute agreement. When questioned about whether the availability of biofuels would influence their decision when purchasing a new vehicle, both Science and Commerce respondents showed mild agreement, while Arts respondents demonstrated comparatively higher agreement. This indicates either a lack of knowledge on the subject or that they do not consider these factors, possibly due to unfamiliarity with the disadvantages or a different approach to decision-making.

C. Policies and Subject Knowledge:

The science stream somewhat disagreed with current government policies promoting biofuel usage, rating them at 3.52, while the commerce and arts streams remained neutral, with ratings of 3.68 and 4.00, respectively. Strong agreement was observed regarding the role of government support in increasing biofuel adoption, with a high rating of 6.25, while lower levels of agreement were noted at 5.53 and 5.30. Respondents showed moderate agreement on being well-informed about biofuels, with ratings of 4.96, 4.68, and 5.00, as well as on the effectiveness of educational campaigns, rated at 5.34, 5.12, and 6.25, respectively. Additionally, they agreed that more information is needed to make informed decisions about biofuels, with ratings of 5.80, 5.88, and 6.00, and acknowledged biofuels as environmentally friendly, with ratings of 5.48, 5.68, and 5.50. Furthermore, there was agreement across the groups that biofuels are a renewable energy source, with ratings of 5.84, 5.79, and 5.75, respectively.

BASED ON GENDER

A. Daily Behaviour Towards Energy Saving:

Both female and male respondents demonstrated a strong agreement towards the affordability and benefits of biofuels as an alternative to fossil fuels. Female respondents rated biofuels as an affordable alternative with an average score of 5.62, slightly higher than the male respondents, who scored it at 5.28. Similarly, both groups agreed that the cost of switching to biofuels is justified by its benefits, with females scoring 5.48 and males 5.22. However, when evaluating the practical usability of biofuels compared to conventional fuels, both genders

showed moderate agreement, with females scoring 4.69 and males 4.58, indicating a general consensus on the potential but also the current limitations of biofuels in everyday use.

B. Social Dynamics and Reliability:

Both female and male respondents agreed that using biofuels enhances their contribution to environmental sustainability, with females scoring it slightly higher at 6.28 compared to males at 6.00. While both groups remained neutral about the idea that vehicles using biofuels require minimal maintenance, with females scoring 3.97 and males 3.85, they showed moderate agreement regarding the consistent performance of biofuels. Females rated it at 4.41, while males rated it slightly higher at 4.52. Similarly, both genders expressed moderate agreement that biofuels offer reliability comparable to traditional fuels, with females scoring 4.66 and males at 4.52. When considering the availability of biofuels, both groups indicated that it would likely influence their decision when purchasing a new vehicle, with females scoring 5.71 and males 5.03.

Table 8: Gender Based Analysis Of Responses

Daily Behaviour Towards Energy Saving			
Gender	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Female	5.26	1.43	1.19
Male	5.03	2.43	1.56
Social Dynamics And Reliability			
Gender	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Female	5	2.04	1.4
Male	4.78	2.14	1.45
Policies And Subject Knowledge			
Gender	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
Female	5.26	1.76	1.31
Male	5.18	1.54	1.23

Source: By the Authors

C. Policies and Subject Knowledge:

Both female and male respondents expressed neutrality regarding current government policies promoting biofuel usage, with females scoring 3.34 and males 3.72. However, they agreed on the significant role of government support in increasing biofuel adoption, with females rating it 5.72 and males 5.30. Both groups showed moderate agreement on being well-informed about biofuels, with females scoring 4.45 and males 5.02, and on the effectiveness of educational campaigns, with females at 5.48 and males at 5.23. Additionally, both genders agreed that more information is needed to make informed decisions about biofuels, with females scoring 6.10 and males 5.73. They also agreed that biofuels are environmentally friendly (females 5.69, males 5.52) and a renewable energy source (females 6.00, males 5.73).

BASED ON AGE

A. Daily Behaviour Towards Energy Saving:

The 21-23 age group demonstrated a strong inclination towards energy saving, with an average rating of 5.48, indicating their agreement that biofuels serve as an affordable alternative to fossil fuels. They also generally agreed that the cost of transitioning to biofuels is justified by the benefits, with an average of 5.33, while showing moderate agreement on the practical usability of biofuels compared to conventional fuels, scoring 4.68.

Similarly, the 24-27 age group also saw biofuels as an affordable alternative, with an average of 5.19, and agreed that the cost of switching is justified by the benefits, scoring 5.29. Their agreement on the practical usability of biofuels compared to conventional fuels was slightly lower, at 4.61, reflecting moderate agreement as well. Both age groups reflect a positive and practical view towards the adoption of biofuels, recognizing both the cost-effectiveness and the potential advantages despite the moderate view on their usability.

B. Social Dynamics and Reliability:

The 21-23 age group showed strong agreement (6.07) that using biofuels enhances their contribution to environmental sustainability. However, they were more neutral about vehicles using biofuels requiring minimal maintenance, with a score of 3.90. They expressed moderate agreement that biofuels offer consistent performance (4.5) and provide reliability similar to traditional fuels (4.53). Additionally, the availability of biofuels would likely influence their decision when purchasing a new vehicle, scoring 5.11. Similarly, the 24-27 age group also agreed that using biofuels enhances their environmental contribution, with a slightly higher score of 6.12. Like the younger group, they were neutral about the maintenance requirements of biofuel-powered vehicles (3.90), but showed moderate agreement that biofuels offer consistent performance (4.45) and reliability comparable to traditional fuels (4.58). The availability of biofuels was even more influential in their vehicle purchase decision, with a score of 5.41. Both age groups reflect a strong belief in the environmental benefits of biofuels, though their views on maintenance and performance reliability show a similar moderate consensus.

Table 9: Age Based Analysis Of Responses

Daily Behaviour Towards Energy Saving			
Age Group	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
21-23	5.17	2.04	1.43
24-27	5.03	2.14	1.46
28+			
Social Dynamics And Reliability			
Age Group	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
21-23	4.83	2.28	1.49
24-27	4.9	1.87	1.36
28+			
Policies And Subject Knowledge			
Age Group	Mean of Avg. Values	Mean of Variance	Mean Std. Deviation
21-23	5.22	1.66	1.28
24-27	5.18	1.6	1.25
28+			

Source: By the Authors

C. Policies and Subject Knowledge:

The 21-23 age group expressed neutrality about current government policies promoting biofuel usage, with a score of 3.62, but agreed that government support plays a significant role in increasing biofuel adoption, scoring 5.46. They showed moderate agreement on being well-informed about biofuels (4.85) and that educational campaigns are effective (5.33). Furthermore, they agreed that more information is needed to make informed decisions about biofuels (5.75) and that biofuels are environmentally friendly (5.66), with a strong agreement

that biofuels are a renewable energy source (5.83). Similarly, the 24-27 age group was neutral about government policies on biofuel promotion (3.54) but also agreed that government support is crucial for biofuel adoption (5.41). They showed moderate agreement on being well-informed about biofuels (4.74) and found educational campaigns effective (5.35). This group agreed even more strongly that more information is needed to make informed decisions about biofuels (6.03) and that biofuels are environmentally friendly (5.38). They too agreed that biofuels are a renewable energy source, with a score of 5.77. Both groups recognize the importance of government support, education, and the need for more information to fully understand the benefits and potential of biofuels.

IV. CONCLUSION

There is a great chance to improve energy security, lessen reliance on fossil fuels, and address environmental issues by switching to biofuels. This study emphasizes postgraduate students' awareness and perceptions of biofuels, highlighting the need for better policy support and education. While biofuels offer a promising alternative, their large-scale adoption must be carefully planned to ensure sustainability, economic feasibility, and long-term viability. It is crucial to balance biofuel production with food security concerns and prevent negative environmental consequences. Global experiences have shown that successful biofuel programs require strong policy frameworks, technological advancements, and active participation from key stakeholders, including governments, private enterprises, and local communities.

To enhance biofuel adoption and awareness, several strategic steps need to be taken. First, strengthening educational initiatives is essential. Universities should integrate biofuel-related topics into energy and environmental studies curricula. Awareness campaigns, workshops, and hands-on training sessions can bridge the knowledge gap and encourage innovation in renewable energy solutions. By equipping students with a deeper understanding of biofuels, they can actively contribute to the renewable energy sector in the future.

Second, investment in advanced biofuels is necessary to overcome challenges associated with first-generation biofuels. Future research and development should prioritize second- and third-generation biofuels that rely on non-food sources like agricultural waste, algae, and other types of biomasses. These alternatives can reduce the food vs. fuel conflict while improving sustainability and efficiency in biofuel production.

Third, government policies and incentives must support biofuel development. Policymakers should introduce comprehensive strategies that promote biofuel production and usage through subsidies, tax benefits, and infrastructure development. Mandatory blending requirements can accelerate biofuel integration into the energy sector, ensuring a gradual but effective shift toward renewable fuels.

Fourth, encouraging localized biofuel production can significantly benefit rural and semi-urban areas. Small-scale biofuel production projects can meet local energy needs without disrupting food supply chains. Additionally, community-driven biofuel initiatives can generate employment opportunities and contribute to regional economic growth, making biofuels a sustainable alternative at both national and grassroots levels.

Lastly, strengthening public-private collaborations is crucial. Effective partnerships between governments, industries, and research institutions can help develop efficient production technologies, improve supply chain management, and enhance the overall feasibility of biofuel usage. By fostering cooperation, biofuels can be developed and distributed more efficiently, ensuring long-term benefits for society and the environment.

Biofuels can significantly contribute to the development of a sustainable and energy-secure future by putting these suggestions into practice. Addressing urgent environmental challenges requires a shift from fossil fuels to renewable energy sources, and biofuels can play a significant role in this process.

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