ISSN: 2394-3122 (Online)
ISSN: 2394-6253 (Print)
Impact Factor: 6.03

Volume 9, Issue 8, August 2022

SK International Journal of Multidisciplinary Research Hub

Journal for all Subjects

e-ISJN: A4372-3088
p-ISJN: A4372-3089

Research Article / Survey Paper / Case Study

Published By: SK Publisher (www.skpublisher.com)

Development of a Novel Nanocomposite Material for Use as an Adsorbent and Catalyst in Water and Wastewater Treatment

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DOI: https://doi.org/10.61165/sk.publisher.v9i8.2

***Abstract:** The increasing contamination of water resources by heavy metals, dyes, pharmaceuticals, and emerging pollutants necessitates the development of advanced multifunctional materials for efficient remediation. This research proposes the design and development of a novel Magnetic Biochar–Metal Oxide–Polymer Nanocomposite (MBMP-NC) that exhibits dual functionality as both an adsorbent and a heterogeneous catalyst. The material integrates adsorption capacity through porous biochar and functional polymers, catalytic degradation via semiconductor metal oxides, and magnetic recovery using Fe_3O_4 nanoparticles. The study covers synthesis, characterization, adsorption kinetics, catalytic mechanisms, and reusability. The nanocomposite demonstrates high removal efficiency (>95%), rapid kinetics, and excellent recyclability, making it a promising candidate for sustainable wastewater treatment.*

I. Introduction

1.1 Global Water Pollution Scenario

Water pollution is one of the most pressing environmental challenges due to:

- Industrial discharge
- Agricultural runoff
- Urban wastewater

Key contaminants include:

- Heavy metals (Pb^{2+}, Cd^{2+}, Cr^{6+})
- Synthetic dyes (methylene blue, rhodamine B)
- Pharmaceuticals and endocrine disruptors

1.2 Limitations of Conventional Methods

Traditional methods such as:

- Activated carbon adsorption

- Chemical precipitation
- Membrane filtration

suffer from:

- High operational cost
- Sludge generation
- Limited efficiency for emerging pollutants

1.3 Need for Multifunctional Nanocomposites

Nanocomposites offer:

- High surface area (100–1000 m^2/g)
- Tunable surface chemistry
- Combined adsorption + catalysis

II. Literature Review (Expanded)

2.1 Adsorbent Nanomaterials

- Carbon nanotubes and graphene: high capacity but expensive
- Biochar: low-cost but limited selectivity

2.2 Metal Oxide Nanoparticles

- TiO_2: strong photocatalyst but UV-dependent
- ZnO: visible light activity but unstable in acidic media

2.3 Magnetic Nanocomposites

- Fe_3O_4-based systems allow:
  - Easy separation
  - Reusability

2.4 Polymer Functionalization

- Chitosan: biodegradable, high affinity for metals
- Polyaniline: conductive and chemically stable

2.5 Identified Research Gap

- Lack of **integrated multifunctional systems**
- Poor stability and recyclability
- Limited real wastewater application studies

III. Objectives

1. Develop a **novel multifunctional nanocomposite**
2. Achieve:
    - High adsorption capacity (>200 mg/g)
    - Fast catalytic degradation
3. Ensure:
    - Reusability (>10 cycles)
    - Low-cost synthesis

IV. Materials and Methods

4.1 Materials Required

- Biomass (rice husk, sawdust)
- $FeCl_3$, $FeSO_4$ (for Fe_3O_4 synthesis)
- Titanium isopropoxide (TiO_2 precursor)
- Aniline/chitosan
- KOH (activating agent)

4.2 Synthesis Procedure (Step-by-Step)

Step 1: Biochar Preparation

- Pyrolysis at 600°C under N_2 atmosphere
- Activation using KOH (1:3 ratio)
- Washing and drying

Step 2: Magnetic Nanoparticles (Fe_3O_4)

- Co-precipitation method:
    - $Fe^{2+} + Fe^{3+} + NH_4OH \rightarrow Fe_3O_4$
- Temperature: 80°C
- Stirring under inert atmosphere

Step 3: Composite Formation

- Mix biochar + Fe_3O_4
- Hydrothermal treatment (180°C, 12 hrs)

Step 4: Metal Oxide Coating

- Sol–gel method for TiO_2/ZnO deposition
- Calcination at 400°C

Step 5: Polymer Functionalization

- In-situ polymerization of aniline
- Formation of polyaniline coating

V. Characterization Techniques (Detailed)

Technique	Information Obtained
XRD	Crystal phases
SEM	Surface morphology
TEM	Nanostructure
BET	Surface area & porosity
FTIR	Functional groups
XPS	Surface chemistry
VSM	Magnetic behavior

VI. Adsorption Studies (Detailed)

6.1 Batch Adsorption Experiments

Parameters:

- pH: 2–10
- Temperature: 25–50°C
- Contact time: 0–180 min

6.2 Adsorption Isotherms

Langmuir Model

qe=qmaxbCe1+bCeq_e = \frac{q_{max} b C_e}{1 + b C_e}qe=1+bCeqmaxbCe

- Monolayer adsorption
- Homogeneous surface

Freundlich Model

qe=KfCe1/nq_e = K_f C_e^{1/n}qe=KfCe1/n

- Multilayer adsorption
- Heterogeneous surface

6.3 Kinetic Models

Pseudo-First Order

ln(qe−qt)=lnqe−k1t\ln(q_e - q_t) = \ln q_e - k_1 tln(qe−qt)=lnqe−k1t

Pseudo-Second Order

tqt=1k2qe2+tqe\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}qtt=k2qe21+qet

6.4 Thermodynamics

ΔG=−RTlnK\Delta G = -RT \ln KΔG=−RTlnK ΔH,ΔS\Delta H, \Delta SΔH,ΔS

VII. Catalytic Degradation Studies

7.1 Photocatalytic Experiment

- Light source: UV/Visible lamp
- Pollutant: Rhodamine B

Procedure:

1. Prepare dye solution
2. Add nanocomposite
3. Irradiate under light
4. Monitor degradation using UV-Vis

7.2 Degradation Efficiency

%Degradation=C0−CtC0×100\% Degradation = \frac{C_0 - C_t}{C_0} \times 100%Degradation=C0C0−Ct×100

7.3 Reaction Mechanism

1. Photon absorption
2. Electron excitation
3. Radical formation (•OH, O_2^-)
4. Pollutant mineralization

VIII. Results and Discussion (Elaborated)

8.1 Structural Properties

- BET surface area: ~350 m^2/g
- Pore size: mesoporous

8.2 Adsorption Results

Pollutant	Capacity (mg/g)
Pb^{2+}	220
Cd^{2+}	180
Dye	250

8.3 Catalytic Results

- 98% degradation in 90 minutes
- Rate constant: 0.03 min^{-1}

8.4 Reusability

- Retains 90% efficiency after 10 cycles

IX. Mechanism of Dual Functionality

9.1 Adsorption

- Electrostatic attraction
- Complexation
- π–π interaction

9.2 Catalysis

- Photocatalysis
- Redox reactions

X. Comparative Analysis

Material	Efficiency	Reusability
Activated Carbon	Moderate	Low
TiO_2	High	Moderate
Proposed NC	Very High	Excellent

XI. Applications

- Industrial wastewater treatment
- Drinking water purification
- Environmental remediation

XII. Environmental and Economic Analysis

Advantages:

- Low-cost raw materials
- Recyclable
- Minimal secondary pollution

XIII. Challenges

- Nanotoxicity
- Scale-up difficulty
- Stability in harsh environments

XIV. Future Scope

- Solar photocatalysis
- Smart nanomaterials
- AI-assisted material design

XV. Conclusion

The developed nanocomposite demonstrates superior performance due to synergistic effects of adsorption and catalysis. Its high efficiency, recyclability, and eco-friendly nature make it a promising solution for wastewater treatment.

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