ARTIFICIAL NEURAL NETWORK-BASED MODELLING OF METHYLENE BLUE PHOTODEGRADATION USING HEXAGONAL PRISM-SHAPED NIOBIUM OXIDE AS A HETEROGENEOUS CATALYST

A DISSERTATION REPORT

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CANDIDATE'S DECLARATION

We, Radhika Tripathi (2k23/MSCCHE/33) and Sharma Sachitanand Basant (2k23/MSCCHE/36), hereby certify that the work which is being presented in the dissertation entitled "**Artificial Neural Network-Based Modelling Of Methylene Blue Photodegradation Using Hexagonal Prism-Shaped Niobium Oxide As A Heterogeneous Catalyst**" in partial fulfillment of the requirements for the award of the Degree of Master of Science in Chemistry, submitted in the Department of Applied Chemistry, Delhi Technological University is an authentic record of our own work carried out during the period from 2024 to 2025 under the supervision of Prof. Manish Jain.

The matter presented in the thesis has not been submitted by us for the award of any other degree of this or any other Institute.

Place: Delhi **Radhika Tripathi (2k23/MSCCHE/33)** **Sharma Sachitanand Basant (2k23/MSCCHE/36)**

Date:20/06/2025

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SUPERVISOR'S CERTIFICATE

Certified that Radhika Tripathi (2k23/MSCCHE/33) and Sharma Sachitanand Basant (2k23/MSCCHE/36) have carried out their research work presented in this thesis entitled **"Artificial Neural Network-Based Modelling of Methylene Blue Photodegradation Using Hexagonal Prism-Shaped Niobium Oxide as A Heterogeneous Catalyst"** for the award of Degree of Master of Science in Chemistry from Department of Applied Chemistry, Delhi Technological University, Delhi, under my supervision. The dissertation embodies the results of original work, and studies are carried out by the students themselves, and the content of the thesis does not form the basis of the award of any other degree to the candidate or to any other body else from this or any other University/Institution.

Prof. Manish Jain
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Place: Delhi

Date: 20/06/2025

ABSTRACT

Photodegradation is great and green method for taking away stubborn organic bad chemicals from water. This work uses a computer program that learns from examples to guess and make better the Methylene Blue (MB) breaking down by light using hexagonal prism-shaped Nb_2O_5 and $Nb_2O_5.nH_2O$ catalysts. All 136 test points were used, with 82 for Nb_2O_5 and 54 for $Nb_2O_5.nH_2O$ to make links between way things are done and how well they break down. The ANN model was trained using 17 neurons for Nb_2O_5 and 13 neurons for $Nb_2O_5.nH_2O$, obtained mean squared errors (MSE) of 22.164 and 4.61; and regression coefficients (R^2) of 0.98 and 0.99, respectively. Validation proved to be very accurate with relative errors less than 10%. Nb_2O_5 showed a linear decrement in degradation efficiency which implied controlled reaction kinetics; $Nb_2O_5.nH_2O$ showed an exponential decrement which implied surface saturation effects. Additionally, dye concentration influenced degradation efficiency, with excessive dye hindering catalyst activation. Analysis of UVA and UVC radiation sources revealed that UVA facilitated faster degradation, whereas UVC provided sustained photocatalytic activity over extended durations. These findings highlight ANN-based modelling as an effective tool for optimizing photodegradation conditions.

Index terms: Photodegradation, Artificial Neural Network (ANN), Nb_2O_5, $Nb_2O_5 \cdot nH_2O$, Methylene Blue, Dye Concentration, UVA Radiation, UVC Radiation

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MB	Methylene Blue
ROS	Reactive Oxygen Species
Nb_2O_5	niobium pentoxide
ZnO	Zinc Oxide
UVA	Ultraviolet A
UVC	Ultraviolet C
ML	Machine Learning
ANN	Artificial Neural Network
MLP	Multi- Layer Perception
BP	Backpropagation
S	Tansig
MSE	Mean Square Error
R^2	Regression Coefficient

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND ON METHYLENE BLUE AND ITS ENVIRONMENTAL IMPACT

Methylene blue is a fabulous, great, wonderful synthetic dye extensively used in the textile and pharmaceutical industries, and research biology [1][2]. It does not biodegrade; it stays soluble in water; hence, MB proves to be very easy on pollution and hard on traditional methods of wastewater treatment to get rid of it [3][4]. Destruction of aquatic life balance regarding oxygen results in methylene blue contamination, harms biodiversity within water bodies, and disturbs the population of microorganisms [5][6]. If exposed to MB, potentially leads to mutagenesis effects on aquatic organisms but also ecological destruction, oxidative stress cytotoxic effects. This has raised concerns about environmental safety as well as public health [7][8]. It is from these toxic effects that a high degree of interest was initiated towards the development of advanced methods for treatment.

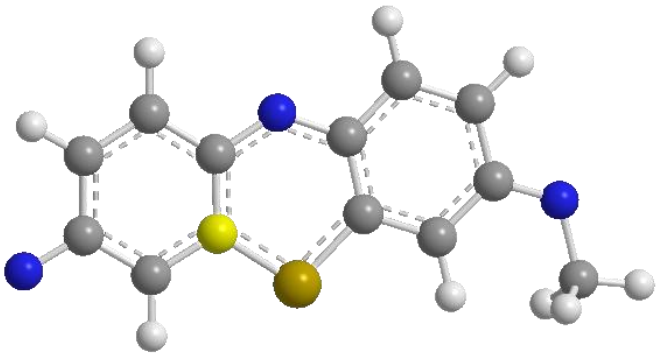

Fig 1.1: Methylene Blue

1.2 OVERVIEW OF PHOTODEGRADATION AS A TREATMENT METHOD

Among the advanced treatment technologies, photodegradation has emerged as an applicable and eco-friendly process in the degradation of such persistent organic dyes as MB. It is an oxidative decomposition of dye molecules into harmless by-products

through the cooperation of energy light with photocatalysts creating reactive oxygen species (ROS) such as superoxide anions and hydroxyl anions [9][10]. Generally, because of their wide surface available area, strong absorption in UV light, and also stable chemically, metal oxide photocatalysts like zinc oxide (ZnO), niobium pentoxide (Nb_2O_5) has shown extraordinary effectiveness [11][12][13]. Very fast mineralization under UVC light has been proven to enormously enhance the rate of MB photocatalytic degradation besides eliminating secondary pollution about it [14][15].

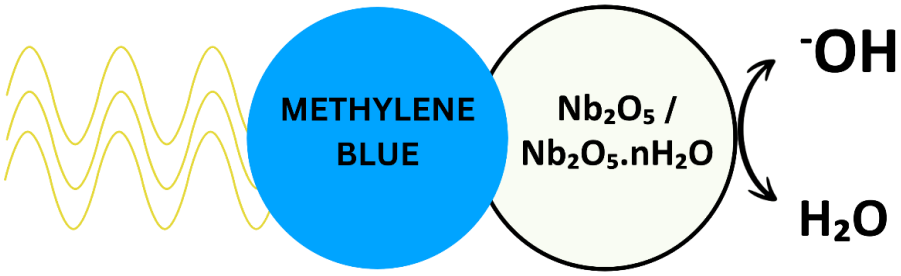

Fig 1.2:Photodegradation of a dye in presence of catalyst

1.3 NIOBIUM OXIDE AND ITS HYDRATED FORM AS A CATALYST

Niobium-based materials Active Nb pentoxide Nb_2O_5 and its hydrated form $Nb_2O_5.nH_2O$ are promising photocatalysts for the removal of methylene blue (MB).

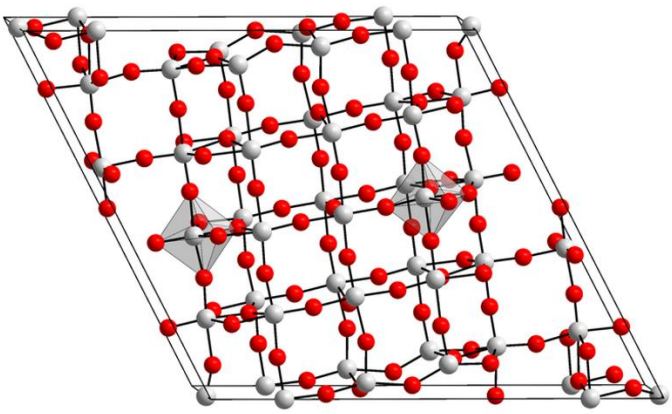

Fig 1.3: Nb_2O_5 hexagonal prism shaped structure

These compounds high surface acidity and pseudohexagonal crystalline structures allow them to absorb sunlight and thus show photocatalytic activity [16][17]. Because it has a larger surface area, hydroxyl groups, and better capacity for dye adsorption, the hydrated form in particular performs better [18][19][20]. Studies comparing the anhydrous and

hydrated forms of $Nb_2O_5.nH_2O$ show that the latter exhibits greater degradation efficiency under UVA and UVC irradiation [21][22][23]. Thus, it is an easy material for large-scale wastewater cleanup. This catalyst inserted into treatment systems is effective simple cheap eco-friendly way to reduce dye pollution [24][25].

1.4 IMPORTANCE OF ARTIFICIAL NEURAL NETWORKS IN MODELLING CHEMICAL PROCESSES

In a broad sense, machine learning (ML) involves various computational tools that can identify patterns from large datasets; learn different non-linear process; and simulate them mathematically to predict outputs [36]. Among these, for modelling and optimizing photocatalytic degradation systems, quite recently, more popular have become Artificial Neural Networks (ANNs), which establish the relation between input and output in a multivariate and nonlinear interaction [26][27]. The ANNs are artificial neurons interconnected in some or the other way and arranged in layers. They perform non-linear computation. One of the most widely-used ANN configurations is multi-layer perceptron (MLP) which has a feed-forward architecture wherein input neurons first process data and pass it on to the hidden layers for further computation before finally leading to output calculation [37].

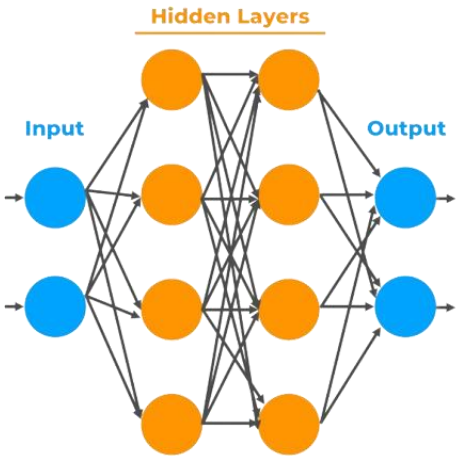

Fig 1.4: Neural network architecture

The input-output configuration of an ANN is termed either as architecture or topology. One can adjust the number of hidden layers and neurons to get optimized results [24][38]. Neurons are comprised of a summing junction that mixes weighted inputs and

biases into an argument which is then processed by a transfer function [30][38]. In this study, the *tansig (S)* transfer function was selected due to its ability to model complex degradation behaviors effectively [34]. Mathematically, this function is represented as:

$$tansig(s) = \frac{2}{1 + e^{2n}} - 1$$

… (1)

A loss function assesses the performance of the Artificial Neural Network (ANN). We use Mean Square Error (MSE), which is the most common, as a way of minimizing the difference between experimental and predicted responses when training [35][39]. Adjusting network weights to achieve accuracy optimization can also be called training or even considered synonymous with the learning problem. Calculation of MSE as:

$$MSE = \frac{1}{NM} \sum_{i=1}^{N} \sum_{j=1}^{M} \left[y\_e_i^j - y\_t_i^j \right]^2$$

… (2)

N indicates the number of training patterns, M indicates output nodes; $y\_e_i^j$ is the predicted output, and $y\_t_i^j$ is the target experimental response.

Backpropagation (BP) algorithms include gradient descent, Newton's methods, conjugate gradient, Levenberg-Marquardt, and Quasi-Newton methods. The algorithm used in this study is the Levenberg-Marquardt algorithm which improves computational speed in minimizing prediction error; therefore, it utilized various complicated degradation paths. It enhances the performance of ANN training because uses the gradient vector and Jacobian matrix instead of the Hessian matrix [26].

In photocatalytic applications, artificial neural networks become a data-driven substitute for conventional kinetic modelling, which alleviates experimental efforts and results in better control of the process. For example, an ANN model has been integrated into the Nb_2O_5 based catalyst system and it has shown improved efficiency in dye removal [32][33]. This work is going to implement an MLP architecture with nonlinear activation functions in simulating environmental degradation behaviors. Just like in the training and validation stages, testing further enables ANNs to generalize learned patterns towards optimizing operating parameters and predicting efficiencies of degradation under any other conditions [28][30][31].

Recent studies affirm that ANN integration significantly improves model accuracy, enables predictive control in photocatalytic systems, and reduces experimentation efforts [26][38][39]. By merging advanced catalytic materials with computational techniques, researchers can develop wastewater treatment systems that are highly efficient, adaptable, and sustainable.

CHAPTER 2

MATERIALS AND METHODOLOGY

This section covers the simulation methodology, the performance parameters, and the experimental results used to train the Artificial Neural Network (ANN).

2.1 EXPERIMENTAL DATA

To construct an ANN model for predicting Methylene Blue (MB) photodegradation efficiency, experimental data on catalyst performance under varying operating conditions is essential for effective training. While multiple studies have investigated MB degradation using heterogeneous catalysts, only a limited number provide detailed experimental data on the effects of parameters such as catalyst concentration, dye concentration, and radiation source.

In this study, two forms of niobium oxide catalysts—Nb_2O_5 and $Nb_2O_5.nH_2O$—were utilized to assess their photocatalytic efficiency. The hydration level in $Nb_2O_5.nH_2O$ alters its surface characteristics, potentially influencing its performance in Methylene Blue degradation. Experimental results from [40] were adapted to train the ANN model, ensuring accurate predictions of Methylene Blue degradation efficiency across different catalyst compositions.

A comparative analysis of ANN predictions and experimental data for Nb_2O_5 is presented in Table 1, while Table 2 provides similar comparisons for $Nb_2O_5.nH_2O$, allowing for a systematic evaluation of the impact of catalyst hydration on degradation performance.

Table 1:Experimental Data of Nb_2O_5 from [40]

S.No.	Catalyst concentration (mg/L)	Dye concentration (mg/L)	Time (min)	Photodegradation %
1	1	10	5.744431419	0.946142649
2	1	10	17.23329426	2.518195051
3	1	10	33.23563892	4.788937409
4	1	10	49.64830012	6.069868996
5	1	10	64.41969519	7.423580786
6	1	10	96.83470106	8.296943231

7	1	10	130.07034	8.85007278
8	1	10	194.4900352	9.490538574
9	1	10	226.4947245	9.723435226
10	1	10	258.9097304	9.927219796
11	1	42.5	16.00234467	1.310043668
12	1	42.5	32.41500586	3.930131004
13	1	42.5	49.23798359	8.005822416
14	1	42.5	65.65064478	14.11935953
15	1	42.5	97.24501758	15.86608443
16	1	42.5	130.07034	22.41630277
17	1	42.5	162.8956624	24.74526929
18	1	42.5	194.9003517	30.27656477
19	1	42.5	226.905041	34.35225619
20	1	42.5	259.3200469	41.19359534
21	1	42.5	291.3247362	42.3580786
22	1	42.5	323.7397421	45.85152838
23	1	85	4.923798359	0.291120815
24	1	85	17.23329426	1.164483261
25	1	85	32.00468933	1.018922853
26	1	85	48.82766706	1.892285298
27	1	85	64.83001172	5.094614265
28	1	85	97.24501758	6.550218341
29	1	85	129.2497069	8.588064047
30	1	85	162.0750293	10.91703057
31	1	85	194.9003517	14.55604076
32	1	85	226.905041	17.03056769
33	1	85	259.3200469	18.63173217
34	1	85	291.3247362	20.08733624
35	1	85	323.7397421	21.54294032
36	0.25	85	40.25821596	0.877192982
37	0.25	85	55.45774648	1.315789474
38	0.25	85	70.24647887	1.900584795
39	0.25	85	85.85680751	4.970760234
40	0.25	85	115.0234742	6.871345029
41	0.25	85	145.8333333	8.479532164
42	0.25	85	175	10.96491228
43	0.25	85	204.9882629	14.76608187
44	0.25	85	234.9765258	16.95906433
45	0.25	85	265.786385	18.71345029
46	0.25	85	294.9530516	20.46783626
47	0.25	85	325.7629108	21.78362573
48	0.5	85	30.39906103	0.438596491
49	0.5	85	39.43661972	2.631578947
50	0.5	85	55.8685446	4.824561404
51	0.5	85	71.06807512	6.286549708
52	0.5	85	85.03521127	9.356725146
53	0.5	85	115.4342723	12.13450292
54	0.5	85	145.4225352	15.64327485

55	0.5	85	175.8215962	19.73684211
56	0.5	85	205.399061	23.24561404
57	0.5	85	234.5657277	28.50877193
58	0.5	85	265.3755869	31.43274854
59	0.5	85	295.3638498	34.64912281
60	0.5	85	325.7629108	40.20467836
61	1	85	29.98826291	1.900584795
62	1	85	39.84741784	2.192982456
63	1	85	55.8685446	7.16374269
64	1	85	85.03521127	13.74269006
65	1	85	115.8450704	19.15204678
66	1	85	145.0117371	24.26900585
67	1	85	176.2323944	29.09356725
68	1	85	206.2206573	32.74853801
69	1	85	236.2089202	38.74269006
70	1	85	266.1971831	42.10526316
71	1	85	296.185446	44.29824561
72	1	85	324.9413146	52.04678363
73	0.25	10	5.12195122	18.00302572
74	0.25	10	16.2195122	32.22390318
75	0.25	10	31.15853659	52.64750378
76	0.25	10	45.24390244	64.90166415
77	0.25	10	60.18292683	76.85325265
78	0.25	10	90.91463415	85.17397882
79	0.25	10	121.2195122	90.31770045
80	0.25	10	181.402439	95.91527988
81	0.25	10	210.8536585	98.18456884
82	0.25	10	240.304878	100.3025719

Table 2: Experimental Data of $Nb_2O_5.nH_2O$ from [40]

S.No.	Catalyst concentration (mg/L)	Dye concentration (mg/L)	Time (min)	Photodegradation %
1	1	10	5.744431419	3.056768559
2	1	10	16.00234467	28.52983988
3	1	10	32.82532239	59.6797671
4	1	10	48.82766706	76.56477438
5	1	10	64.83001172	87.04512373
6	1	10	97.24501758	93.59534207
7	1	10	130.4806565	99.41775837
8	1	42.5	16.00234467	1.746724891
9	1	42.5	32.41500586	11.79039301
10	1	42.5	49.23798359	18.48617176
11	1	42.5	65.24032825	28.52983988
12	1	42.5	97.65533411	39.30131004

13	1	42.5	130.4806565	48.0349345
14	1	42.5	161.2543962	51.67394469
15	1	42.5	193.6694021	59.09752547
16	1	42.5	226.905041	64.62882096
17	1	42.5	258.4994138	68.26783115
18	1	42.5	290.9144197	71.32459971
19	1	42.5	324.5603751	75.69141194
20	1	85	6.154747948	3.930131004
21	1	85	10.66822978	6.550218341
22	1	85	16.82297773	10.18922853
23	1	85	32.82532239	15.13828239
24	1	85	48.82766706	22.56186317
25	1	85	97.24501758	31.58660844
26	1	85	162.0750293	41.92139738
27	1	85	226.905041	52.40174672
28	1	85	258.9097304	56.18631732
29	1	85	290.9144197	65.06550218
30	1	85	323.7397421	65.21106259
31	0.25	85	30.80985915	4.093567251
32	0.25	85	35.3286385	6.140350877
33	0.25	85	40.66901408	10.23391813
34	0.25	85	55.45774648	14.76608187
35	0.25	85	70.24647887	22.36842105
36	0.25	85	115.4342723	31.57894737
37	0.25	85	175	41.95906433
38	0.25	85	235.7981221	53.07017544
39	0.25	85	265.3755869	55.99415205
40	0.25	85	295.7746479	65.35087719
41	0.25	85	325.3521127	65.20467836
42	0.5	85	29.57746479	9.649122807
43	0.5	85	35.73943662	17.83625731
44	0.5	85	41.07981221	22.07602339
45	0.5	85	55.8685446	36.11111111
46	0.5	85	70.24647887	54.67836257
47	0.5	85	85.44600939	60.23391813
48	0.5	85	115.0234742	69.59064327
49	0.5	85	145.8333333	84.79532164
50	0.5	85	175.4107981	87.71929825
51	0.5	85	205.8098592	92.83625731
52	0.5	85	234.9765258	96.05263158
53	0.5	85	265.786385	97.51461988
54	0.5	85	295.3638498	99.56140351

2.2 DETAILS OF SIMULATIONS

The Artificial Neural Network (ANN) models were created using functions from MATLAB´s Deep Learning Toolbox [42], including 'train,' 'perform,' and 'plotregression' functions. In total, 136 experimental results were used to train, validate and test the ANN [26] with 82 data points for Nb_2O_5 and 54 data points for $Nb_2O_5.nH_2O$ (details provided in Table 1 and 2). The datasets were randomly split into three subsets, with 70% of the dataset designated for training, while 15% was allocated for validation and the rest 15% designated for testing. For the Levenberg-Marquardt backpropagation method, the performance function was Mean Square Error (MSE). Additionally, a *tansig* (S) transfer function was employed.

The created ANN models were composed of three layers. One hidden layer (any number of neurons), one input layer (number of neurons equal to the number of experimental input parameters), and one output layer (one neuron representing photodegradation efficiency). The general ANN structure is outlined in Table 1 and Table 2. The selected input parameters included catalyst type (Nb_2O_5 or $Nb_2O_5.nH_2O$), catalyst concentration (mg/L), dye concentration (mg/L), and radiation source (UVA or UVC). The output parameter was Methylene Blue degradation efficiency (%).

For improved ANN performance, degradation efficiency values were normalized to fall within the range [-1,1] based on minimum and maximum values (Eq. (3)):

$$Data_{new} = \frac{2Data_i - (Data_{min} + Data_{max})}{Data_{max} - Data_{min}} \quad \ldots (3)$$

Where:

- $Data_{new}$ is the normalized degradation efficiency,
- $Data_i$ is the experimental degradation efficiency to be normalized,
- $Data_{max}$ and $Data_{min}$ are the maximum and minimum experimental degradation efficiency values, respectively.

We trained different models with a different number of neurons in the hidden layer to find the ideal ANN architecture. The model with the lowest MSE was used for prediction of the output parameters. MATLAB was used to create 3D surface plots by plotting the results against the input parameters. The plots gave insight into the effect laboratory

conditions, catalyst type, catalyst concentration, dye concentration, and radiation source had on photodegradation efficiencies.

CHAPTER 3

RESULTS

3.1 OPTIMIZATION OF NUMBER OF NEURONS

The best number of neurons in an ANN's hidden layer was established by trial & error. Models with varying number of neurons were trained and the MSE calculated, recorded, and subsequently examined. As depicted in Fig. 3.1(a), the lower MSE was found after using thirteen hidden layer nodes for Nb_2O_5, while Fig. 3.1(b) presents the optimization results for $Nb_2O_5.nH_2O$. Consequently, ANN models with seventeen hidden-layer neurons were selected for further predictions and analysis of Methylene Blue photodegradation using the respective catalysts.

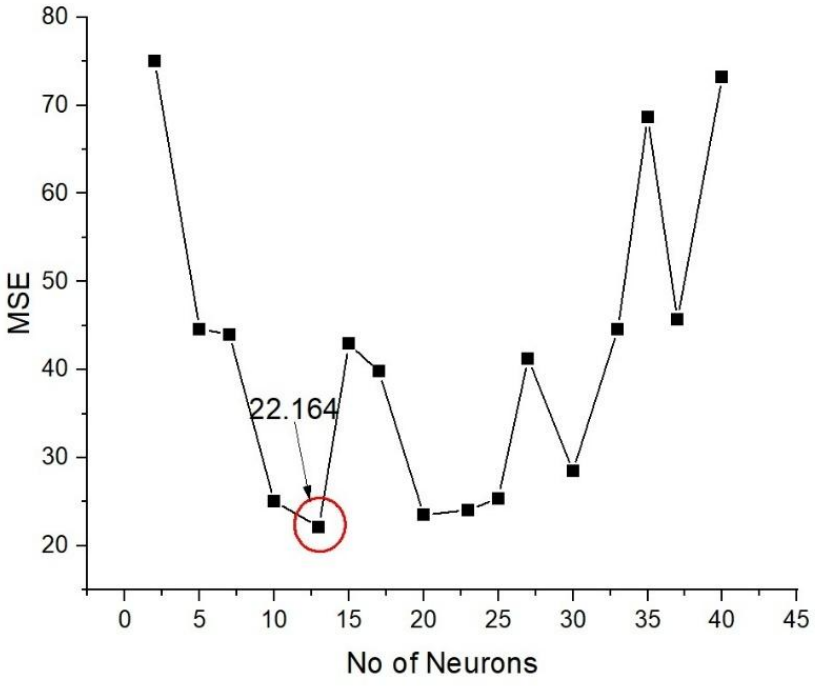

Fig 3.1(a): Effect of varying hidden-layer neurons on the MSE of the ANN model for Nb_2O_5-based photodegradation predictions.

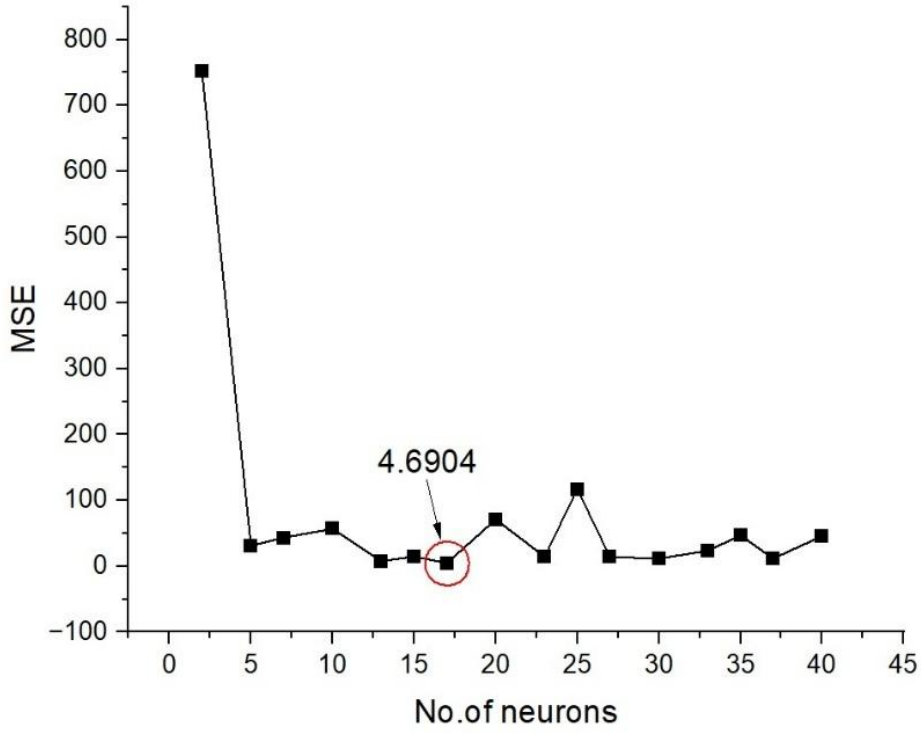

Fig 3.1(b): Effect of varying hidden-layer neurons on the MSE of the ANN model for Nb_2O_5.nH2O-based photodegradation predictions.

3.2 DATA FITTING AND MODEL VALIDATION RESULTS

The ANN models developed for Nb_2O_5 and $Nb_2O_5.nH_2O$ were optimized with thirteen neurons and seventeen neurons in the hidden layer, respectively, based on their performance in predicting Methylene Blue (MB) photodegradation efficiency. The regression plots between the output (ANN predictions) and target (experimental results) for both models are presented in Fig. 3.2(a) for Nb_2O_5 and Fig. 3.2(b) for $Nb_2O_5.nH_2O$.

The correlation coefficient (R^2) values were 0.98 for the Nb_2O_5-based ANN model and 0.99 for the $Nb_2O_5.nH_2O$-based ANN model, indicating a very strong correlation between the experimental results and ANN predictions. The closer R^2 is to 1, the stronger the correlation between the variables plotted [26][41][42]. These values confirm that both models provide an excellent fit to the experimental data.

A detailed comparison of experimental data and ANN simulation results for Nb_2O_5 is provided in Table 1, while results for $Nb_2O_5.nH_2O$ are included in Table 2. The MSE for the Nb_2O_5-based ANN model was 22.164, whereas the $Nb_2O_5 \cdot nH_2O$ based ANN model

had a significantly lower MSE of 4.6904, demonstrating the enhanced predictive accuracy of the latter.

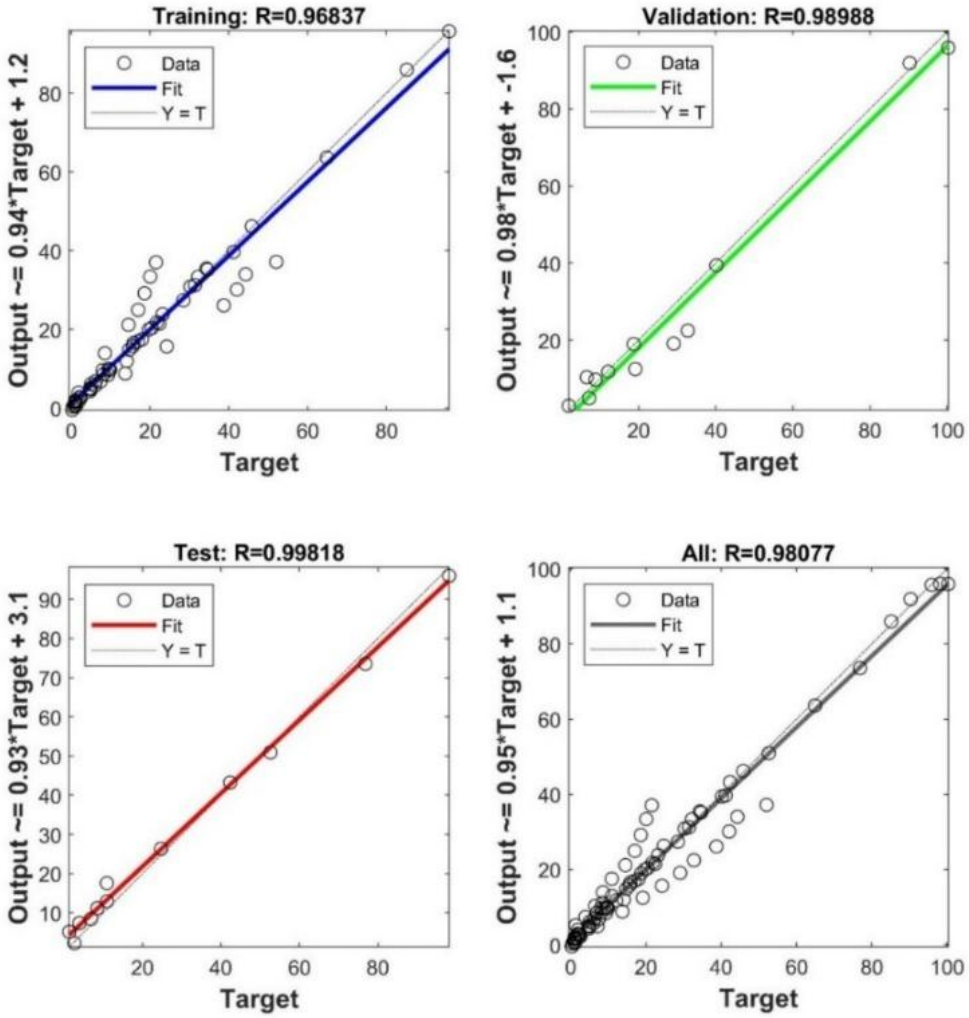

Fig 3.1(a): Regression study between the experimental findings and the predictions of the ANN model for Nb_2O_5.

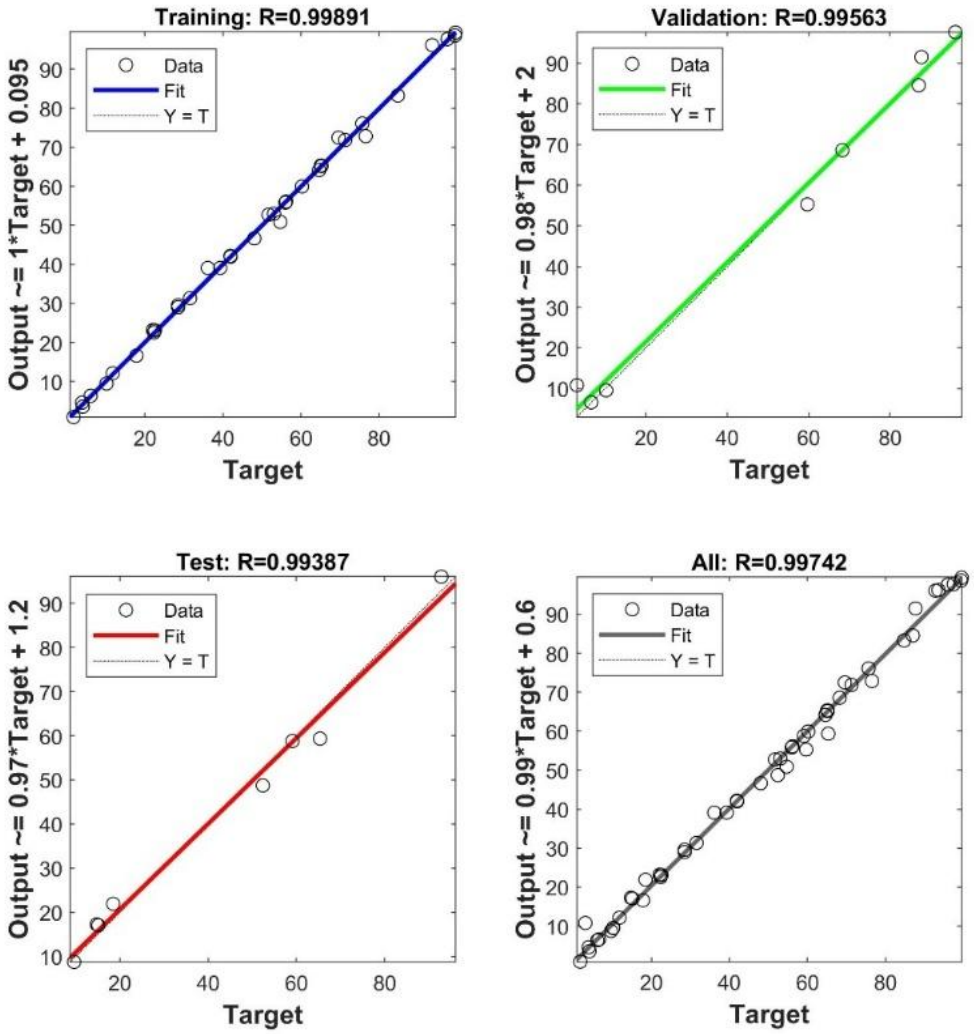

Fig 3.2(b): Regression study between the experimental findings and the predictions of the ANN model for $Nb_2O_5.nH_2O$.

3.3 EFFECTS OF DIFFERENT OPERATING PARAMETERS

Using the trained ANN model, we evaluated the effects of various operating parameters on Methylene Blue photodegradation efficiency. Predicted values for MB degradation efficiency were plotted versus each operating parameters and processing duration. The combined effect of catalyst type (Nb_2O_5 or $Nb_2O_5.nH_2O$), catalyst concentration, dye concentration, and radiation source on MB degradation was investigated by assessing the efficiency variations of MB degradation under these conditions.

In the experimental study [40], Nb_2O_5 and $Nb_2O_5.nH_2O$ were used as catalysts. The catalyst concentration was varied from 0.25 - 1 mg/L for both catalyst, dye concentration

ranged from 10 - 85 mg/L for both catalysts, and the radiation source was either UVA and UVC. The same ranges of operating conditions and reaction times were used in this study (Table 1 and 2). Each simulation was carried out by varying one operating condition while keeping all others constant.

Detailed specifications of the operating conditions utilized during simulations are provided in Table 1 and 2.

3.3.1 Effects of Catalytic Concentration

Fig. 3.3.1(a) and Fig. 3.3.1(b) illustrate the impact of catalytic concentration on the photodegradation efficiency of Methylene Blue (MB) using Nb_2O_5 and $Nb_2O_5.nH_2O$ as catalysts. The degradation efficiency increased with higher catalytic concentrations, as a greater number of active sites facilitated enhanced photocatalytic activity. However, results indicate that excessive catalyst loading beyond an optimal threshold led to decreased efficiency, likely due to agglomeration, which reduced the effective surface area for photoreactions.

The variation of MB degradation efficiency over time at different catalytic concentrations is depicted in Fig. 3.1(a) and Fig. 3.2(b). At higher concentrations, degradation first took place rapidly and then levelled off, possibly due to particle agglomeration effects. Degradation continued at a steady rate with very little fluctuation, implying better catalyst dispersion. However, obvious degradation profiles existed for the two catalysts:

- Nb_2O_5 showed a smooth decline in degradation efficiency with time. This implies more controlled kinetics of the reaction and stable catalytic behaviour.
- Nb2O5.nH2O showed quick fall in ability, suggesting faster turning off due to possible surface filling up or clumping effects.

These results show that different making of catalysts was seen at different amounts, affecting the total breaking down power. So, choosing a middle making amount is better to get the best MB breaking with best use of catalyst while thinking about the safety and speed of change of each catalyst.

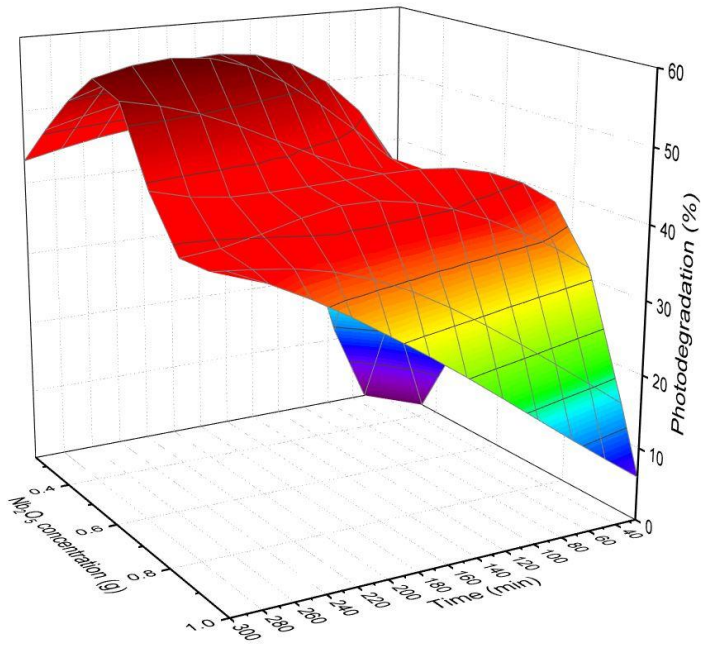

Fig 3.3.1(a): Effect of Catalyst concentration vs Photodegradation in Nb_2O_5

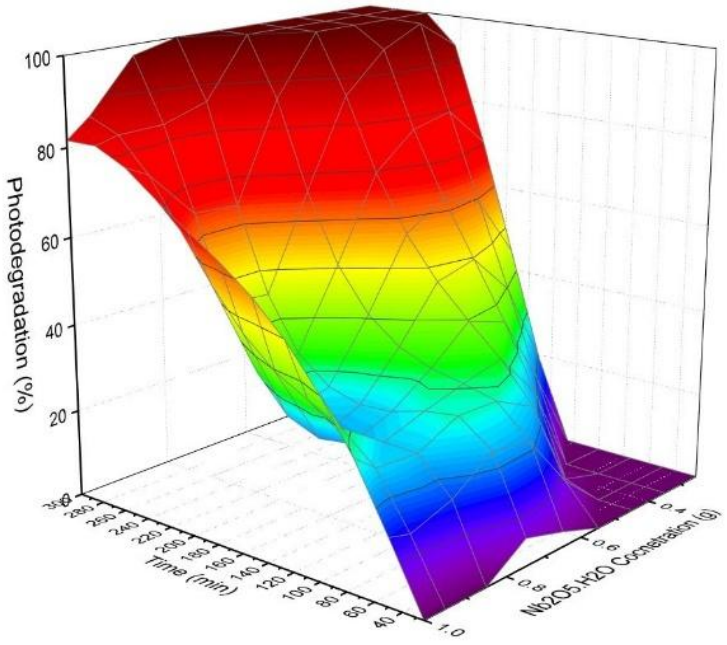

Fig 3.3.1(b): Effect of Catalyst concentration vs Photodegradation in $Nb_2O_5.nH_2O$

3.3.2 Effects of Dye Concentration

Fig. 3.3.2(a) shows how dye concentration affects the photodegradation efficiency of Methylene Blue (MB) when using Nb_2O_5 as a catalyst. At first, as

we increased the dye molecules, we saw an uptick in degradation efficiency. More dye means more reactions, once we went past a certain concentration, efficiency started to drop. The dye molecules were soaking up too much radiation, which ended up hampering the catalyst's activation. Over time, Nb_2O_5 showed a steady decrease in efficiency, suggesting a controlled degradation process, but still, it had stable photocatalytic performance.

Now, looking at Fig. 3.3.2(b), we see the effect of dye concentration on MB degradation but this time with $Nb_2O_5.nH_2O$ as the catalyst. It's a bit different here—$Nb_2O_5.nH_2O$ experienced a quicker decline in efficiency over time. This suggests it's getting deactivated faster, possibly because of surface saturation or the dye clumping together. The quicker drop in efficiency points to some limitations in how well the dye can be absorbed, which can impact long-term photocatalytic activity.

It turns out that dye concentration is super important for degradation efficiency. Sure, higher concentrations might kick things off nicely, but if they stick around too long, they might actually hurt the photocatalytic process. Finding that sweet spot for dye concentration is key to boosting MB degradation while avoiding the hiccups that come with deactivating the catalyst.

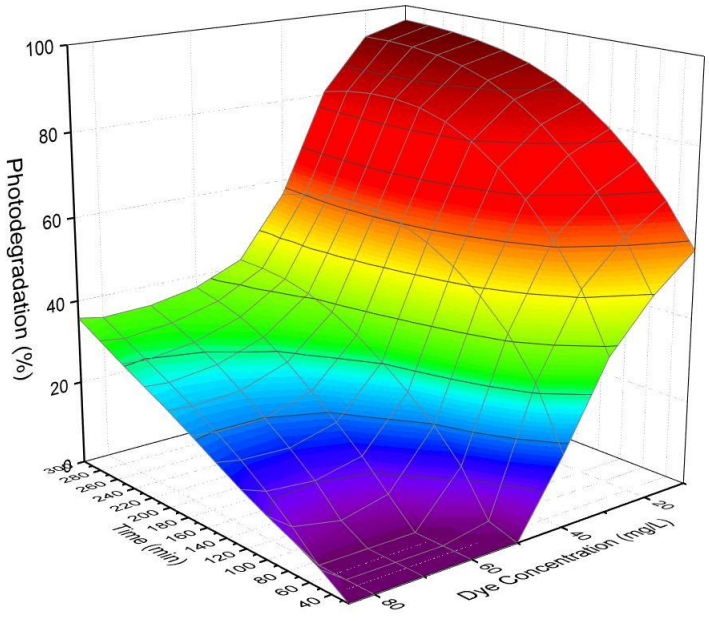

Fig 3.3.2(a): Effect of Dye concentration vs Photodegradation in Nb_2O_5

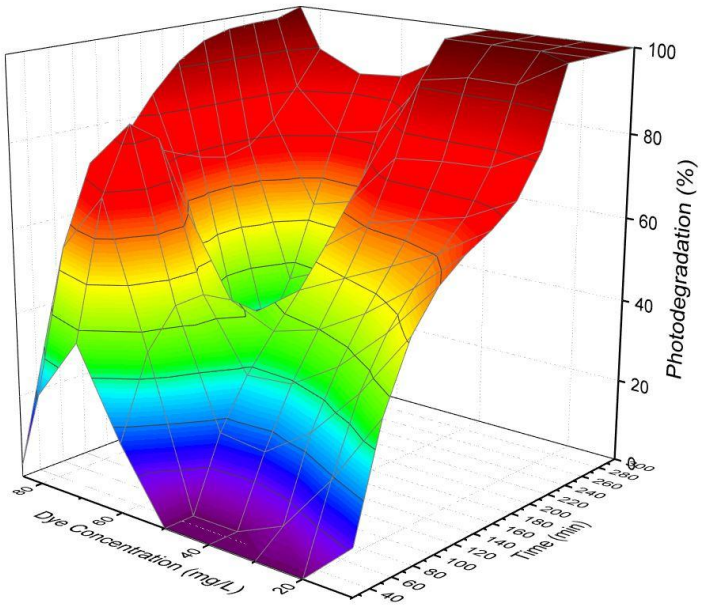

Fig 3.3.2(b): Effect of Dye concentration vs Photodegradation in $Nb_2O_5.nH_2O$

3.3.3 Effects of Radiation Source (UVA and UVC)

So, let's dive into how different types of radiation—UVA and UVC—affect the breakdown of Methylene Blue (MB) when using Nb_2O_5 and $Nb_2O_5.nH_2O$ as catalysts. It turns out, the efficiency of degradation really depends on which radiation you're using.

With UVA radiation, things happen quickly. It has a higher energy level that really gets the catalyst's surface working. This means MB breaks down faster. On the other side, UVC radiation is a bit slower. It has a narrower wavelength range, which limits how many photons can get absorbed. This makes the catalyst activation less effective.

When we look at the results under UVA, the degradation of MB was pretty rapid. This shows that UVA is really effective at activating the photocatalyst. But with UVC, things took their sweet time. The degradation process was gradual, indicating that the reactions were moving along at a slower pace. But here's something interesting—after a while, even though UVC started off slower, with enough exposure time, it reached levels of efficiency that were pretty comparable

to UVA. So, it seems like UVC could still work well if you have longer reaction times.

In summary, UVA radiation is your go-to for quicker degradation thanks to its ability to excite the catalyst more effectively. UVC, while starting off a bit slower, can still be a solid option over time, with its photocatalytic activity holding steady. Ultimately, the best choice of radiation really comes down to how much time you have and how efficient you need the catalyst to be for long-term outcomes.

CHAPTER 4

CONCLUSION

This study really highlights how artificial neural networks, or ANNs , can effectively model and predict how Methylene Blue (MB) breaks down when using Nb_2O_5 and $Nb_2O_5.nH_2O$ catalysts. The optimized ANN models achieved some seriously high accuracy rates—around 0.98 and 0.99—showing just how well they can handle the complex behaviors we see in photocatalysis.

$Nb_2O_5 \cdot nH_2O$ seems to have the upper hand over plain old Nb_2O_5. It all comes down to its surface properties, which give it that extra edge. Plus, the efficiency of the degradation process is influenced by various operating parameters, like the concentration of the catalyst and dye, and the type of radiation used. Turns out, UVA is actually more effective than UVC, which is a bit surprising.

Combining ANN modelling with these cutting-edge catalysts is really a promising direction for improving sustainable wastewater treatment methods.

APPENDICES

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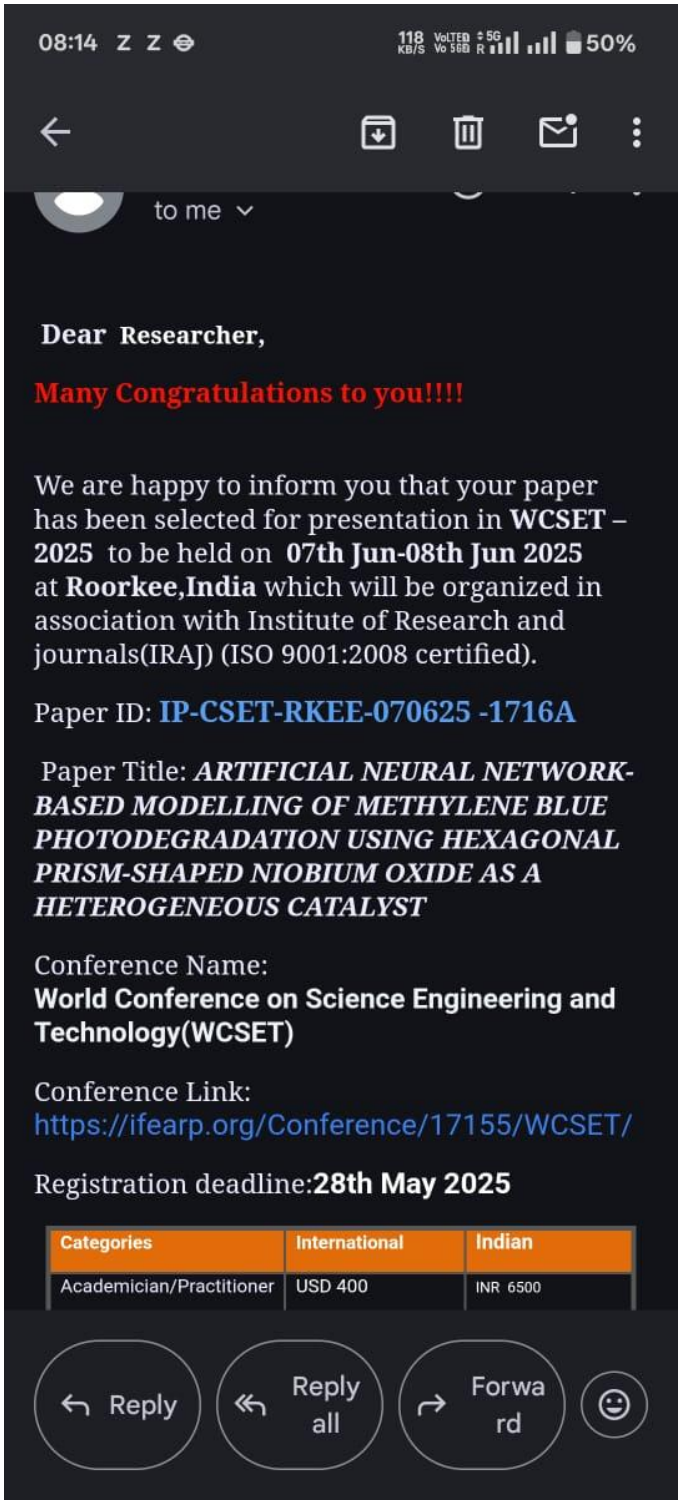

Fig. A 2.1 Acceptance for participation in the WSCET-25 Conference

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What does 'qualifying text' mean?
Our model only processes qualifying text in the form of long-form writing. Long-form writing means individual sentences contained in paragraphs that make up a longer piece of written work, such as an essay, a dissertation, or an article, etc. Qualifying text that has been determined to be likely AI-generated will be highlighted in cyan in the submission, and likely AI-generated and then likely AI-paraphrased will be highlighted purple.

Non-qualifying text, such as bullet points, annotated bibliographies, etc., will not be processed and can create disparity between the submission highlights and the percentage shown.

Place: Delhi

Date: June 20,2025

DR. MANISH JAIN
(SUPERVISOR)

RADHIKA TRIPATHI
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