

**ARTIFICIAL NEURAL NETWORK BASED ANALYSIS
OF OPERATING PARAMETERS IN METHYL ORANGE
PHOTODEGRADATION USING TiO_2 As A
PHOTOCATALYST**

A DISSERTATION REPORT

SUBMITTED IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE AWARD OF THE DEGREE

OF

MASTER OF SCIENCE

IN

CHEMISTRY

Submitted by

PANKAJ

(2k23/MSCCHE/80)

and

KHUSHI

(2k23/MSCCHE/22)

Under the Supervision of

DR. MANISH JAIN



**DEPARTMENT OF APPLIED CHEMISTRY
DELHI TECHNOLOGICAL UNIVERSITY**

(Formerly Delhi College of Engineering)
Bawana Road, Delhi-110042

JUNE, 2025



DELHI TECHNOLOGICAL UNIVERSITY
(Formerly Delhi College of Engineering)
Shahbad Daulatpur, Main Bawana Road, Delhi -110042

CANDIDATE'S DECLARATION

We, Pankaj (2k23/MSCCHE/80) and Khushi (2k23/MSCCHE/22) hereby certify that the work which is being presented in the Dissertation entitled “Artificial neural network based analysis of operating parameters in Methyl Orange photodegradation using TiO_2 as a photocatalyst” 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 my own work carried out during the period from June 2024 to May 2025 under the supervision of Dr. Manish Jain.

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

Place: Delhi

PANKAJ
(2k23/MSCCHE/80)

KHUSHI
(2k23/MSCCHE/22)

Date:20/06/2025



Department of Applied Chemistry
DELHI TECHNOLOGICAL UNIVERSITY
(Formerly Delhi College of Engineering)
Shahbad Daulatpur, Main Bawana Road,
Delhi -110042

SUPERVISOR'S CERTIFICATE

Certified that **Pankaj (2k23/MSCCHE/80)** and **Khushi (2k23/MSCCHE/22)** has carried out their search work presented in this thesis entitled “**Artificial Neural Network based analysis of operating parameters in Methyl Orange Photodegradation using TiO₂ as a Photocatalyst**” for the award of **Master of Science from** Department of Applied Chemistry, Delhi Technological University, Delhi, under my supervision. The dissertation embodies results of original work, and studies are carried out by the student themselves and the contents of the dissertation do not form the basis for the award of any other degree to the candidate or to anybody else from this or any other University.

Prof. Manish Jain
(Supervisor)

Place: Delhi

Date: 20/06/2025

ABSTRACT

Important operating parameters such dye concentration, light intensity, pH, and reaction duration have a big impact on photodegradation efficiency. An artificial neural network (ANN) model was used in this investigation to examine how these characteristics affected the degradation of methyl orange. An artificial neural network (ANN) was trained on 141 data points, optimizing the distribution of 33 neurons. With a mean squared error (MSE) value of 0.001438, the proposed model produced predictions that were correct. 3D surface plots were used to assess the fractional conversion of methyl orange and show how reaction time and crucial operating parameters relate to each other. According to the findings, fractional conversion falls as dye concentration rises, with lower MO concentrations (20–40 μM) showing the highest efficiency across longer time periods (100–160 minutes). While lower intensities by themselves do not achieve high degradation efficiency, higher light intensities ($>80 \text{ mW/cm}^2$) greatly increase conversion rates. Furthermore, pH has a significant impact on degradation performance; environments that are severely acidic ($\text{pH}<5$) or basic ($\text{pH}>10$) decrease efficiency, whereas neutral to slightly basic circumstances ($\text{pH } 7\text{--}9$) encourage the highest rates. The ANN model proved to be highly reliable in predicting deterioration trends, with a strong regression coefficient (R^2) of 0.98 and a relative error of less than 10%. The simulation results also highlighted how important it is to optimize the operating parameters, as this plays a key role in accurately controlling the efficiency of the photodegradation process.



DELHI TECHNOLOGICAL UNIVERSITY
(Formerly Delhi College of Engineering)
Shahbad Daulatpur, Main Bawana Road,
Delhi -110042

ACKNOWLEDGEMENT

With immense gratitude, first and foremost, we extend our sincere appreciation to our institutional guide, **Dr. Manish Jain (Assistant Professor, Department of Applied Chemistry, Delhi Technological University)**. His unwavering support, continuous motivation, and insightful suggestions have been instrumental in shaping the quality of this project report. Without his guidance and constructive criticism, this achievement would not have been possible.

We would also like to express our gratitude to all those who supported us throughout the completion of this project. We extend our heartfelt acknowledgement to the faculty and staff of the Department of Applied Chemistry for providing a conducive environment, facilities, and resources essential for our academic growth.

Furthermore, we are deeply thankful to our families and friends for their unconditional love, unwavering support, and constant encouragement during this academic pursuit. Their encouragement has been a source of strength and inspiration throughout this journey.

PANKAJ
(2k23/MSCCHE/80)

KHUSHI
(2k23/MSCCHE/22)



DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of Engineering)

Shahbad Daulatpur, Main Bawana Road,

Delhi -110042

PLAGIARISM VERIFICATION

Title of thesis “**Artificial Neural Network based analysis of operating parameters in Methyl Orange Photodegradation using TiO₂ as a Photocatalyst**”.

This is to report that the above thesis was scanned for similarity detection. Process and outcome are given below:

Software used: **Turnitin**

Similarity Index: **10%**

Total Word Count: **4,447 Words**

Date: **20/06/2025**

PANKAJ
(2k23/MSCCHE/80)

KHUSHI
(2k23/MSCCHE/22)

Prof. Manish Jain
(Supervisor)

CONTENTS

Candidate's Declaration	ii
Supervisor's Certificate	iii
Abstract	iv
Acknowledgement	v
Plagiarism Verification	vi
Contents	vii
List of Tables	ix
List of Figures	x
List of Symbols, Abbreviations, and Nomenclature	xi
Chapter 1: Introduction	12-14
1.1 Background	
1.2 Significance	
Chapter 2: PROBLEM STATEMENT AND PROCEDURE	15-20
2.1 Problem Statement	
2.2 Research Objectives	
2.3 Data Collection	
2.4 Artificial Neural Network Approach (Procedure)	
2.4.1 Ann Architecture	
2.5 Experimental Procedure	
Chapter 3: RESULTS	21-25
3.1 Optimization and Number of Neurons	
3.2 Data Fitting and Model Validation Results	
3.3 Effect of Operating Parameters	
3.3.1 Effect of Dye Concentration	
3.3.2 Effect of Light Intensity	
3.3.3 Effect Of pH	
3.3.4 Effect of Reaction Time	
Chapter 4: CONCLUSION	26

APPENDICES	27-29
Appendix 1 Conference Attended	
Appendix 2 Conference registration proof	
REFERENCES	29-32
PLAGIARISM REPORT	33

LIST OF TABLES

Table 1: Experimental Data from [29]	16
---	----

LIST OF FIGURES

Fig 1.1: Structure of TiO₂	14
Fig 2.4.1: Architecture of ANN model	19
Fig 3.1: Impacts of changing a hidden layer's neurons on the study's MSE of the ANN model	21
Fig 3.2: Regression analysis of ANN model	22
Fig 3.3.1: Effect of Dye Concentration in Presence of Catalyst vs Fraction Conversion of MO	23
Fig 3.3.2: Effect of light intensity	24
Fig 3.3.3: Effect of pH	25

LIST OF SYMBOLS, ABBREVIATIONS, AND NOMENCLATURE

TiO ₂	Titanium Dioxide
MO	Methyl Orange
UV	Ultraviolet
ROS	Reactive Oxygen Species
MSE	Mean Squared Error
R ²	R-squared Value
ANN	Artificial Neural Network
pH	Potential of Hydrogen
mW/cm ²	Milliwatts per Square Centimeter
μM	Micromolar
L-M	Levenberg–Marquardt
R ²	Coefficient of Determination (also used as R-squared)
H ₂ O	Water
CO ₂	Carbon Dioxide
ANN	Artificial Neural Networks

CHAPTER 1

INTRODUCTION

Methyl orange is the orange color that azo dye produces. Due to its widespread use in coloring techniques, it ends up in the sewage of the paper, plastic, and textile sectors, among others. This region is stable due to azo-based (consisting of $-N=N-$ stable bond) MO dye, which necessitates the application of conventional physicochemical techniques [1][2]. Wastewater containing methyl orange may experience photodegradation, particularly photocatalysis. In order to produce reactive radicals that can break down complicated dye molecules into less hazardous and simpler compounds, photocatalysts usually use semiconducting materials like TiO_2 [3][4]. Photocatalysts are the favored methods for treating industrial wastewaters because of their various benefits, which include low cost, environmental friendliness, and the absence of secondary pollutants [4][5].

Numerous operating parameters, including initial dye concentration, solution pH, reaction duration, and light intensity, influence how well the photodegradation process works [5][6]. The overall degradation efficiency is influenced by the formation and lifetime of charge carriers in the photocatalyst, which also affects the efficiency of active species creation [7][8].

Titanium dioxide (TiO_2) was extensively researched as a photocatalyst for complex chemical compounds under light irradiation after the widely used azo dye methyl orange failed [4][9]. Photocatalytic degradation is a useful method for cleaning wastewater that contains harmful dyes like methyl orange. This process helps break down the dye into safe substances like carbon dioxide and water. How well this method works depends on several factors—such as how much dye is present, the amount of titanium dioxide (TiO_2) used, the pH level of the solution, and how long the water is exposed to light [9–12]. For

example, using more TiO_2 and keeping the pH at the right level can improve how the dye and the photocatalyst interact, which helps speed up the cleaning process [12][13].

TiO_2 is especially good at removing methyl orange from wastewater. Changing the structure of the photocatalyst and adjusting the conditions around it can make this process even more effective and help get rid of pollutants more completely [14].

To understand and predict how well this method works under different conditions, scientists often use models based on data. One common approach is to build a system that mimics how the human brain processes information. This system is made up of hidden layers, with each layer containing neurons that work together [15][16]. By changing how many layers are formed and neurons are used, the system can be made more accurate. Each neuron gives information, applies some rules to it, and then gives a result—helping to predict how well the wastewater treatment will work in different situations [16].

In this research, we have used the hyperbolic tangent sigmoid function as the transfer function. The evaluation of the performance of ANN is based on a loss function that assesses the difference between predicted outcomes and experimental data. The model is optimized by modifying the network weights through training called backpropagation. Standard backpropagation algorithms are gradient descent, Newton's method, conjugate gradient, Levenberg–Marquardt algorithm, and Quasi-Newton method. In this research, the Levenberg–Marquardt algorithm was the one chosen for the study because it is efficient at minimizing prediction errors while convergence speed is kept at an acceptable level [16][17].

The components of an artificial neural network (ANN) are organized into hierarchy levels, commonly referred to as the input, hidden, and output layers. The initial steps in the network learning process feature the setting of weights, determining the output to inputs, and adjusting weights which occur sequentially [15]. The forming of clusters happens through supervised and unsupervised learning, which allows ANN to go through many processes and learning cycles, effectively enhancing performance [16]. The use of ANN modeling permits researchers to easily deduce highly adaptable

photocatalytic systems using university-grade components for wastewater treatment systems [15][18-20].

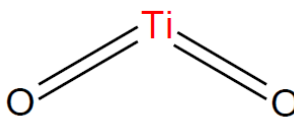


Fig 1.1: Structure of TiO₂.

1.1 BACKGROUND

TiO₂ is well known for its low cost, chemical stability, excellent photocatalytic activity, and non-toxicity. TiO₂ produces reactive oxygen species (ROS), including hydroxyl radicals, when exposed to ultraviolet (UV) light; these ROS can mineralize complex chemical molecules into innocuous byproducts like CO₂ and H₂O [14]. Notwithstanding its promise, operational factors—such as catalyst dose, initial dye concentration, solution pH, and irradiation duration—significantly affect the TiO₂-assisted photodegradation process's performance [12]. It is difficult to optimize the process using conventional empirical or statistical methods because of the intricate, nonlinear interactions between these parameters. Artificial neural networks have been shown to provide robust, accurate modeling of such nonlinear photocatalytic systems [21–23].

1.2 SIGNIFICANCE

This study intends to close the gap between experimental research and real-world application of photocatalytic wastewater treatment by utilizing the power of artificial neural networks. The creation of a trustworthy predictive model can greatly cut down on the need for expensive and time-consuming tests, allowing for more effective process design, optimization, and scaling up. Previous work has successfully applied ANN models to predict degradation kinetics in TiO₂-based photocatalytic systems, demonstrating high accuracy and generalizability [21]. In addition to boosting environmental engineering, this study shows how artificial intelligence is increasingly being used to develop sustainable solutions [22][24].

CHAPTER 2

PROBLEM STATEMENT AND PROCEDURE

2.1 PROBLEM STATEMENT

The textile, printing, and leather industries' release of artificial dyes like Methyl Orange (MO) into natural water bodies is a serious environmental and public health risk. In addition to being aesthetically unpleasing, these dyes are poisonous, chemically stable, and biodegradable [1][4]. Because of its effectiveness in converting complex organic molecules into less hazardous byproducts, photocatalysis employing titanium dioxide (TiO_2) under ultraviolet (UV) light has drawn a lot of interest among the several treatment methods [14][21]. The efficiency of the photocatalytic process depends on several factors, like dye concentration, amount of catalyst used, pH level, and how long the material is exposed to light [12][14].

Finding the best conditions using traditional experiments can take a lot of time and money, especially when dealing with complex systems that have many variables. This is where Artificial Neural Networks (ANNs) can be a great alternative [15][21].

ANNs are useful for modeling environmental systems, but they haven't been widely used for predicting how dyes like methyl orange break down through photocatalysis. To make full use of this technology, a reliable ANN-based predictive model needs to be developed. Such a model can quickly estimate photodegradation efficiency under different conditions. This helps improve the process, making it more cost-effective and eco-friendlier for wastewater treatment [22][25].

2.2 RESEARCH OBJECTIVES

This study aims to develop and test an Artificial Neural Network (ANN) model to predict how efficiently methyl orange can be broken down using titanium dioxide (TiO_2) and ultraviolet (UV) light. By using ANN, we analyze key factors like catalyst concentration, dye concentration, solution pH, and irradiation time to find the best conditions for degradation. The results show that ANN is a powerful and accurate tool for understanding complex environmental processes, helping researchers reduce

experimental workload and improve wastewater treatment methods in a more cost-effective and efficient way.

2.3 DATA COLLECTION

To properly break down methyl orange, having reliable experimental data is essential. This data helps understand how the catalyst reacts under different conditions. However, while many studies focus on the degradation of methyl orange using heterogeneous catalysts, only a few provide detailed insights into how factors like dye concentration, radiation source, or natural pH affect the process. Without this information, it becomes harder to optimize the reaction for better efficiency. In this work, the photocatalytic efficacy of TiO₂ with Methyl Orange at natural pH 6 is assessed. Since light intensity affects reaction kinetics and overall treatment effectiveness, it is crucial for attaining ideal photodegradation rates.

To forecast MO degradation efficiency across a range of light intensities, dye concentrations, and pH levels, the ANN model was trained using the parametric data given in. Table 1 compares ANN predictions and experimental results, allowing for a systematic evaluation of the effects of light intensity and TiO₂ characteristics on degrading performance.

Table 2.1: Experimental Data from [29]

S.No.	Light Intensity(mW/cm ²)	Dye Concentration(μ M)	pH	Time(min)	Fractional Conversion of MO
1	3	20	6	19.84615816	0.028378347
2	3	20	6	39.69230751	0.038888857
3	3	20	6	60.23077157	0.047297298
4	3	20	6	80.30768662	0.058858843
5	3	20	6	100.1538536	0.071471504
6	3	20	6	120.6923	0.090390375
7	3	20	6	140.3076837	0.096696665
8	3	20	6	159.4615536	0.105105106
9	3	20	6	180	0.111411396
10	16	20	6	20.30768955	0.023123091
11	16	20	6	40.38462221	0.052552553
12	16	20	6	60.23077157	0.068318319
13	16	20	6	79.84615522	0.096696665
14	16	20	6	100.1538536	0.109309326
15	16	20	6	120.2307686	0.126126127
16	16	20	6	140.076918	0.134534568
17	16	20	6	159.6923016	0.148198224
18	16	20	6	180	0.161861879

19	37	20	6	19.84615816	0.036786787
20	37	20	6	40.15385651	0.08513512
21	37	20	6	60.46153727	0.143993923
22	37	20	6	80.30768662	0.199699701
23	37	20	6	100.1538536	0.26171173
24	37	20	6	120.2307686	0.289039042
25	37	20	6	140.3076837	0.301651662
26	37	20	6	160.153833	0.311111138
27	37	20	6	180	0.318468463
28	92	20	6	19.84615816	0.049399368
29	92	20	6	40.38462221	0.122972942
30	92	20	6	59.53845687	0.201801731
31	92	20	6	80.30768662	0.282732751
32	92	20	6	99.69230458	0.369969981
33	92	20	6	120.0000029	0.456156176
34	92	20	6	140.076918	0.503453474
35	92	20	6	160.3846163	0.552852862
36	92	20	6	180	0.589639649
37	165	20	6	19.84615816	0.117717687
38	165	20	6	39.46154181	0.200750777
39	165	20	6	60.23077157	0.269069095
40	165	20	6	78.69230913	0.334234229
41	165	20	6	99.69230458	0.386786782
42	165	20	6	119.7692372	0.455105101
43	165	20	6	139.8461523	0.524474495
44	165	20	6	159.6923016	0.582282303
45	165	20	6	180	0.603303325
46	165	2.5	6	19.726024	0.25931447
47	165	2.5	6	39.67621251	0.630402408
48	165	2.5	6	60.07471295	1
49	165	5	6	20.17433593	0.2011923
50	165	5	6	39.90036848	0.459016423
51	165	5	6	59.178072	0.597615513
52	165	5	6	79.8007455	0.789865873
53	165	5	6	99.75091692	0.979135625
54	165	10	6	20.17433593	0.157973146
55	165	10	6	39.22788349	0.460506713
56	165	10	6	59.62640103	0.655737711
57	165	10	6	80.02490147	0.75260805
58	165	10	6	100.1992459	0.839046217
59	165	10	6	119.9252614	0.989567812
60	165	20	6	19.95017996	0.117734743
61	165	20	6	39.67621251	0.198211663
62	165	20	6	60.07471295	0.271236962
63	165	20	6	80.02490147	0.333830116
64	165	20	6	99.30260499	0.384500778
65	165	20	6	119.2527935	0.456035786
66	165	20	6	139.427138	0.502235464
67	165	20	6	159.8256555	0.551415835
68	165	20	6	180	0.587183311
69	165	40	6	20.39850899	0.055141646
70	165	40	6	40.12452444	0.108792888
71	165	40	6	59.85055699	0.140089437
72	165	40	6	80.02490147	0.180327783
73	165	40	6	100.6475579	0.230998559

74	165	40	6	119.4769495	0.284649687
75	165	40	6	139.8754499	0.345752608
76	165	40	6	160.0497944	0.38301043
77	165	40	6	179.7758269	0.423248891
78	165	60	6	19.50186804	0.028315968
79	165	60	6	39.67621251	0.044709387
80	165	60	6	60.29886892	0.070044775
81	165	60	6	80.24905743	0.092399469
82	165	60	6	100.4234019	0.116244453
83	165	60	6	119.0286375	0.143070017
84	165	60	6	139.8754499	0.171385985
85	165	60	6	160.7222794	0.204172881
86	165	60	6	180	0.232488735
87	165	80	6	21.74346187	0.350223592
88	165	80	6	19.27771207	0.016393419
89	165	80	6	39.45205655	0.022354694
90	165	80	6	60.52302488	0.034277243
91	165	80	6	79.8007455	0.040238517
92	165	80	6	100.1992459	0.058122226
93	165	80	6	119.4769495	0.076005936
94	165	80	6	139.6512939	0.086438195
95	165	80	6	160.4981063	0.107302598
96	165	80	6	180	0.128166888
97	165	100	6	20.62266495	0.007451565
98	165	100	6	39.90036848	0.010432259
99	165	100	6	59.85055699	0.016393419
100	165	100	6	79.8007455	0.025335388
101	165	100	6	99.97508998	0.031296548
102	165	100	6	119.9252614	0.050670662
103	165	100	6	139.8754499	0.059612517
104	165	100	6	159.8256555	0.0834575
105	165	100	6	179.7758269	0.089418775
106	165	20	6	20.07967601	0.110400024
107	165	20	6	40.39840131	0.201599976
108	165	20	6	60.95618504	0.267200012
109	165	20	6	79.60159261	0.334399963
110	165	20	6	99.92031791	0.388799988
111	165	20	6	119.7609629	0.454399963
112	165	20	6	139.840648	0.508799988
113	165	20	6	159.9203331	0.550399963
114	165	20	6	180	0.584
115	165	20	7	20.07967601	0.065599976
116	165	20	7	40.15936113	0.168
117	165	20	7	59.7609659	0.241599976
118	165	20	7	79.60159261	0.307200012
119	165	20	7	99.68127773	0.377599976
120	165	20	7	119.5219227	0.427200012
121	165	20	7	140.0796882	0.483200012
122	165	20	7	160.3984135	0.521599976
123	165	20	7	180	0.566399963
124	165	20	9	20.07967601	0.084799927
125	165	20	9	39.44224059	0.203200012
126	165	20	9	60.00000608	0.299200012
127	165	20	9	79.84063279	0.387200012
128	165	20	9	100.1593581	0.473599976

129	165	20	9	119.7609629	0.536
130	165	20	9	139.6015896	0.603200012
131	165	20	9	160.3984135	0.667200012
132	165	20	9	180	0.707199982
133	165	20	11	19.84063583	0.145599976
134	165	20	11	40.15936113	0.329599976
135	165	20	11	60.00000608	0.465599976
136	165	20	11	79.60159261	0.584
137	165	20	11	99.92031791	0.673599976
138	165	20	11	120.000003	0.747199982
139	165	20	11	139.6015896	0.809599976
140	165	20	11	160.1593551	0.84
141	165	20	11	180	0.870399994

2.4 ARTIFICIAL NEURAL NETWORK APPROACH (PROCEDURE)

2.4.1 ANN ARCHITECTURE

The ANN model developed for this study consists of an input layer, hidden layers, and an output layer. The input layer has three neurons, each representing one of the input parameters: run duration, instantaneous flux, and time. The output layer contains a single neuron corresponding to TMP. One or more hidden layers with varying numbers of neurons are used to capture the complex relationships between the inputs and the output. The optimal architecture, including the number of hidden layers and neurons, is determined through experimentation and validation [15][16][26].

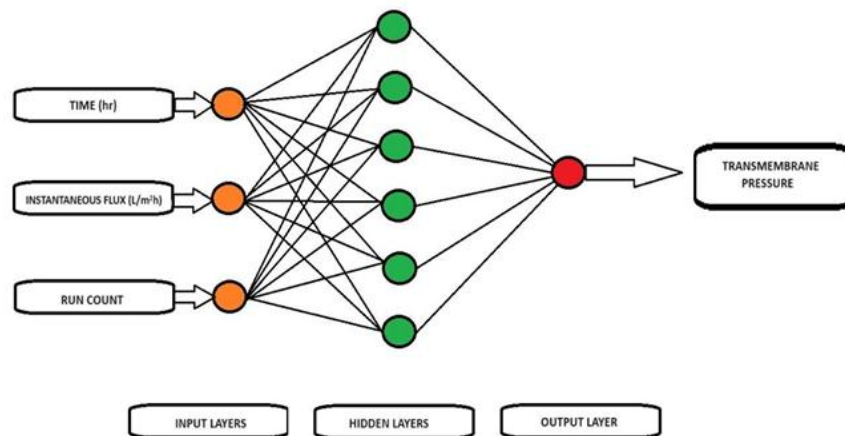


Fig 2.4.1: Architecture of ANN Model

2.4.2 TRAINING AND VALIDATION

The ANN is trained by transmitting the input data into the network and judging the prediction error while tuning the weights. This is where the Levenberg–Marquardt (L-

M) algorithm is used because of its effectiveness in solving nonlinear optimization problems [16][17][27]. The dataset is divided into training and validation as the training set to train the model and validation set to evaluate its performance. The model's performance is measured with metrics like Mean Squared Error (MSE) and R-squared value (R^2) [15][28]

2.5 EXPERIMENTAL PROCEDURE

Under ultraviolet (UV) light, titanium dioxide (TiO_2) was used as a catalyst in an experiment meant to investigate the photocatalytic degradation of methyl orange (MO). To assess the impact of different operating settings on the degrading efficiency, a number of batch tests were carried out in a controlled laboratory environment. A 250 mL cylindrical glass reactor with a UV light source was used for all tests, which were conducted at room temperature to guarantee constant irradiation.

TiO_2 powder (photocatalyst) was further placed into the mixture at the point of light application after weighing. Adsorption desorption equilibrium was reached, between dye molecules and surface of the catalyst, by stirring the slurry in dark for 0.5 h. Upon the equilibration period, the UV irradiation was turned on to initiate the photocatalytic reaction. Samples were withdrawn during irradiation at predetermined time intervals and immediately centrifuged or filtered to remove the TiO_2 particles. The photodegradation efficiency was calculated by taking ratio of breakdown of initial and final concentration of dye.

- Dye concentration (0.1 - 1.0 μM)
- pH (3 – 11)
- Irradiation time (10 – 120 min)
- Light intensity (3-165 mW/cm^2)

CHAPTER 3

RESULTS

3.1 OPTIMIZATION AND NUMBER OF NEURONS

Through a rigorous trial and error process, we were able to discover the appropriate number of neurons to inhabit the hidden layer of the ANN. The performance of multiple network architectures trained, each with a different number of hidden layer neurons, was compared based on the model predicted Mean Squared Error (MSE). Considering the better prediction accuracy and generalization ability of the model for the TiO_2 catalyzed Methyl Orange photodegradation system, the model with 33 neurons was also chosen. The performance of a set of network topologies that we trained, with different number of neurons in the hidden layer, were evaluated using the Mean Squared Error (MSE) measured on the model predictions. With 33 neurons in the hidden layer, the model achieved its best performance, reducing the Mean Squared Error (MSE) to just 0.001438 for the TiO_2 -based degradation of methyl orange. This shows that the selected number of neurons helped improve accuracy and efficiency in predicting the breakdown process.

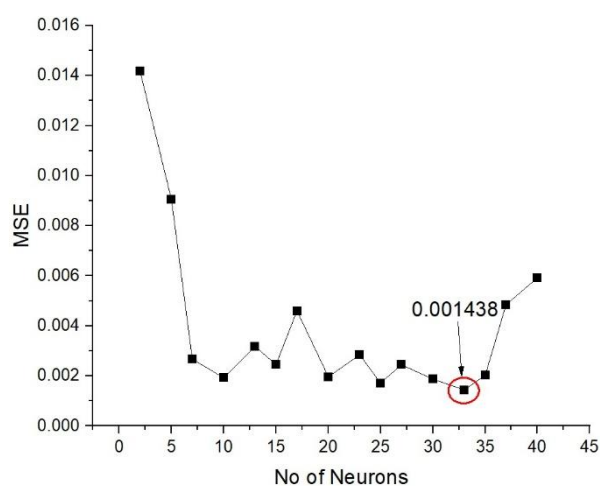


Fig 3.1 : Impacts of Changing a Hidden Layer's Neurons on the Study's MSE of the ANN Model

3.2 DATA FITTING AND MODEL VALIDATION RESULTS

Using 33 neurons, the ANN model could still make good predictions and helped improve how TiO₂ breaks down methyl orange. Figure 2 shows that the ANN's predictions are very close to the real results, with an R² of 0.98, which means the model works well and can be trusted. An MSE of 0.001438 means the model predicted the efficiency of degradation very accurately, with only a small gap between expected and actual values. The independence of the ANN model in modeling the photocatalytic degradation process with TiO₂ is confirmed by the high R² value, which is near 1. This value gives a great correlation between the predicted and experimental results. ANN has proven to be a reliable tool for accurately modeling and optimizing methyl orange degradation in various conditions.

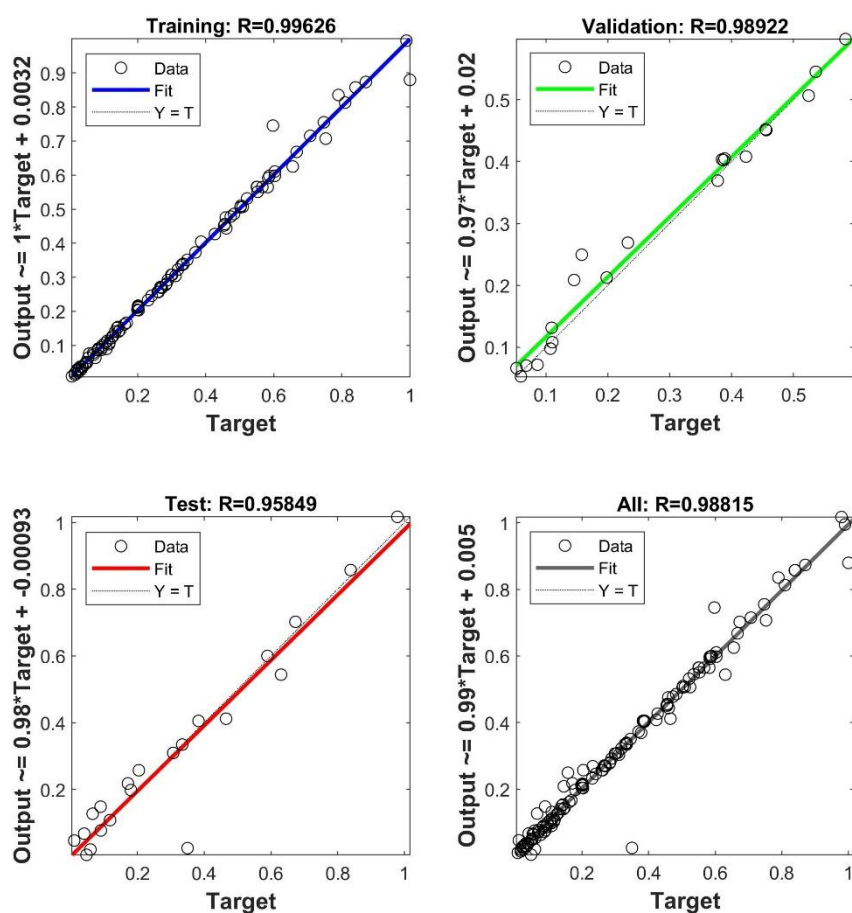


Fig 3.2: Regression Analysis of ANN Model

3.3 EFFECT OF OPERATING PARAMETERS

3.3.1 Effect of dye concentration

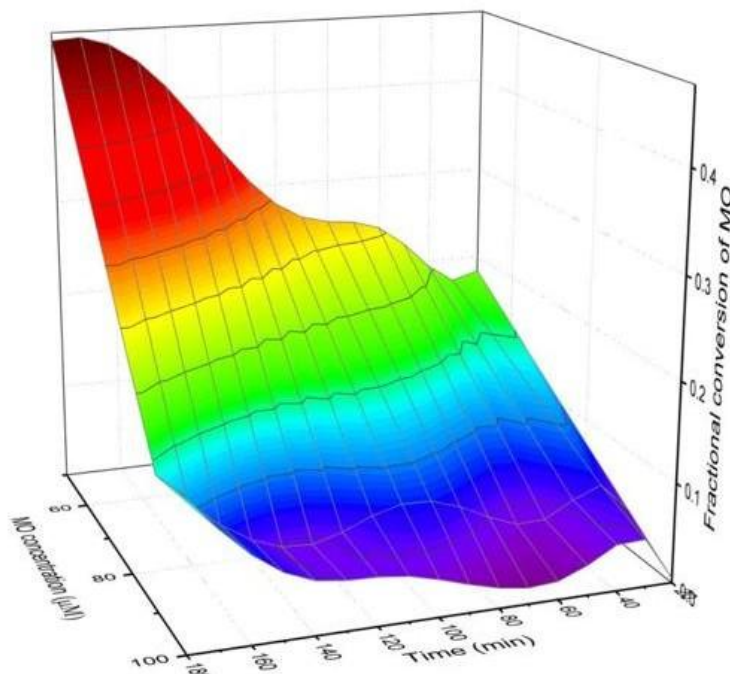


Fig 3.3.1: Effect of Dye Concentration in Presence of Catalyst vs Fraction Conversion of MO

- Dye molecules may obstruct the TiO_2 active sites, decreasing catalytic performance; higher dye concentrations enhance solution color, restricting light penetration to the catalyst.
- Low concentrations (20–40 μM) enhance the rate of reaction by allowing more light to activate the catalyst.
- Light shielding and decreased active surface availability cause the conversion rate to decrease over 40 μM .

3.3.2 Effect of light intensity

- On the catalyst, the rate at which electron-hole pairs are generated is determined by the intensity of the light.
- Degradation is accelerated by greater intensity (over 80 mW/cm^2), which increases radical production.

- Poor conversion results from low intensity because it does not activate enough catalytic sites.
- Without using too much energy, optimal intensity strikes a balance between energy input and deterioration yield.

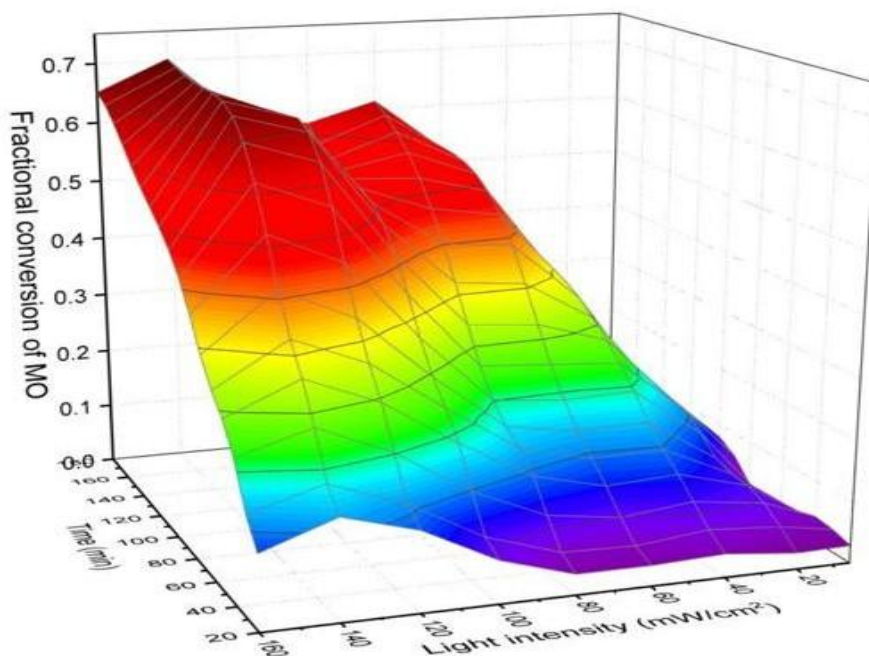


Fig 3.3.2: Effect of light intensity

3.3.3 Effect of pH

- The pH affects the surface charge and dye ionization of TiO_2 .
- The surface becomes positively charged at low pH (<5), which repels protonated MO.
- Excess OH^- scavenges reactive radicals and decreases reaction efficiency at high pH values (>10).
- The optimal pH range is 7–9, which is neutral to slightly basic and promotes maximal breakdown efficiency.

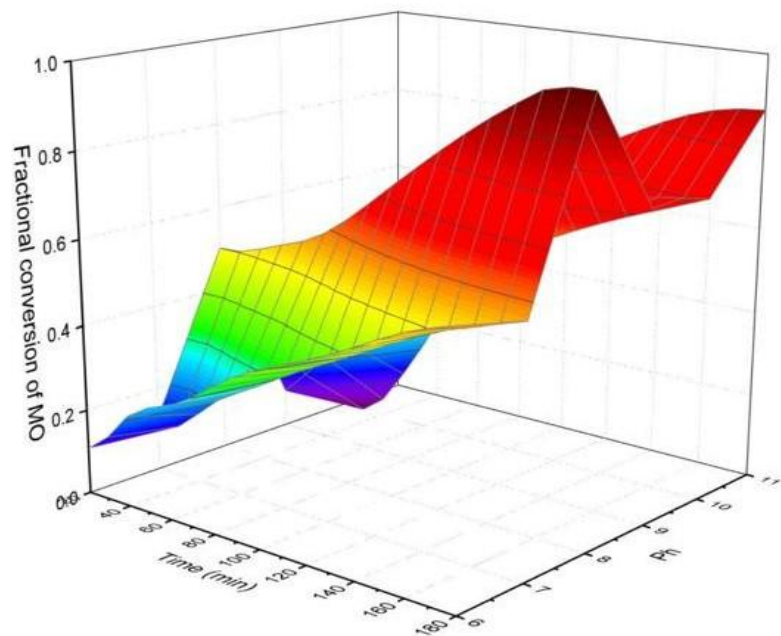


Fig 3.3.3 Effect of pH

3.3.4 Effect of reaction time

- Because photocatalytic degradation is cumulative, more dye breakdown occurs over time.
- Sustained radical production from prolonged exposure (100–160 min) increases conversion.
- While very lengthy times provide declining results, very short times result in incomplete reactions.
- According to the study, the ideal time-efficiency trade-off is between 120 and 140 minutes.

CHAPTER 4

CONCLUSION

In this report, ANN was used to see how well TiO_2 can remove methyl orange in different situations. We trained an ANN model with 33 hidden neurons and 141 data points. This produced a very good correlation between the actual and predicted data ($R^2 = 0.98$) and good predictive accuracy (relative mean square error 0.001438). Additionally, we discovered that while lower light intensity did not perform as well, higher light intensity (above 80 mW/cm^2) increased the MO removal rate. Additionally, we observed that the degradation rate was enhanced by a decreased dye concentration, ranging from 20 to $40 \mu\text{M}$.

We did observe that excessively acidic or basic pH decreased effectiveness, and that the greatest results were obtained around neutral to basic pH values (pH 7–9). Additionally, we observed that the majority of the dye degraded during the first 100–160 minutes. To put it briefly, we created a model that demonstrated the various aspects that contribute to MO degradation, making it simple to choose the ideal treatment settings. Our method enhances the way we use photocatalysis to treat dye-contaminated water while saving time and effort in the lab.

APPENDICES

APPENDIX 1 CONFERENCE ATTENDED



Fig. A 1.1 Certificate of participation in the WSCET-25 Conference

APPENDIX 1 CONFERENCE ATTENDED



Fig. A 1.2 Certificate of participation in the WSCET-25 Conference

APPENDIX 2 CONFERENCE REGISTRATION PROOF



Acceptance for participation in the WSCET-25 Conference

REFERENCES


- [1] H. Zollinger, *Color Chemistry: Syntheses, Properties, and Applications of Organic Dyes and Pigments*, 3rd ed. Wiley-VCH, 2003.
- [2] T. Robinson, G. McMullan, R. Marchant, and P. Nigam, "Remediation of dyes in textile effluent: a critical review on current treatment technologies with a proposed alternative," *Bioresour. Technol.*, vol. 77, no. 3, pp. 247–255, 2001.
- [3] A. Fujishima and K. Honda, "Electrochemical photolysis of water at a semiconductor electrode," *Nature*, vol. 238, pp. 37–38, 1972.
- [4] M. R. Hoffmann, S. T. Martin, W. Choi, and D. W. Bahnemann, "Environmental applications of semiconductor photocatalysis," *Chem. Rev.*, vol. 95, no. 1, pp. 69–96, 1995.
- [5] A. K. Verma, R. R. Dash, and P. Bhunia, "A review on chemical coagulation/flocculation technologies for removal of colour from textile wastewaters," *J. Environ. Manage.*, vol. 93, no. 1, pp. 154–168, 2012.
- [6] J. Yu, W. Wang, B. Cheng, and M. Zhou, "Effects of calcination temperature on the microstructures and photocatalytic activity of anatase TiO₂ hollow spheres," *J. Mol. Catal. A Chem.*, vol. 258, no. 1–2, pp. 104–110, 2006.
- [7] M. Pelaez et al., "A review on the visible light active titanium dioxide photocatalysts for environmental applications," *Appl. Catal. B Environ.*, vol. 125, pp. 331–349, 2012.
- [8] A. A. Umar et al., "Photocatalytic degradation of methyl orange using titanium dioxide nanoparticles in aqueous suspension," *J. Nanomater.*, vol. 2013, Article ID 401291, 2013.
- [9] D. D. Dionysiou et al., "Photocatalytic treatment of organic contaminants in water," *Crit. Rev. Environ. Sci. Technol.*, vol. 34, no. 3, pp. 231–292, 2004.
- [10] N. Daneshvar, D. Salari, and A. R. Khataee, "Photocatalytic degradation of azo dye acid red 14 in water: investigation of the effect of operational parameters," *J. Photochem. Photobiol. A Chem.*, vol. 157, no. 1, pp. 111–116, 2003.
- [11] M. A. Rauf and S. S. Ashraf, "Fundamental principles and application of heterogeneous photocatalytic degradation of dyes in solution," *Chem. Eng. J.*, vol. 151, no. 1–3, pp. 10–18, 2009.

- [12] A. N. Fernandes et al., "Evaluation of advanced oxidation processes for water and wastewater treatment—a critical review," *Water Res.*, vol. 46, no. 13, pp. 3925–3936, 2012.
- [13] S. S. Bhagwat et al., "Optimizing pH and catalyst concentration for the photocatalytic degradation of methyl orange," *Desalination Water Treat.*, vol. 57, no. 21, pp. 9805–9813, 2016.
- [14] X. Chen and S. S. Mao, "Titanium dioxide nanomaterials: synthesis, properties, modifications and applications," *Chem. Rev.*, vol. 107, no. 7, pp. 2891–2959, 2007.
- [15] S. Haykin, *Neural Networks and Learning Machines*, 3rd ed. Pearson, 2009.
- [16] M. T. Hagan, H. B. Demuth, and M. H. Beale, *Neural Network Design*, 2nd ed. Martin Hagan, 2014.
- [17] M. A. Al-Garni, "Application of the Levenberg-Marquardt algorithm for neural networks training," *J. Eng. Appl. Sci.*, vol. 5, no. 6, pp. 409–414, 2010.
- [18] A. Kaur and S. Singh, "Modeling and simulation of wastewater treatment plant using ANN technique," *Int. J. Comput. Appl.*, vol. 97, no. 2, pp. 1–4, 2014.
- [19] G. R. Loura and P. B. Vidyasagar, "ANN modeling of photocatalytic degradation of methyl orange dye using TiO_2 ," *Int. J. Eng. Technol.*, vol. 7, no. 3, pp. 1238–1242, 2018.
- [20] A. K. Mittal et al., "Artificial neural network modeling for predicting the removal of dye from wastewater by adsorption," *Appl. Water Sci.*, vol. 7, no. 6, pp. 3191–3200, 2017.
- [21] G. R. Loura and P. B. Vidyasagar, "ANN modeling of photocatalytic degradation of methyl orange dye using TiO_2 ," *Int. J. Eng. Technol.*, vol. 7, no. 3, pp. 1238–1242, 2018.
- [22] A. K. Mittal et al., "Artificial neural network modeling for predicting the removal of dye from wastewater by adsorption," *Appl. Water Sci.*, vol. 7, no. 6, pp. 3191–3200, Jun. 2017.
- [23] S. K. Bhatia, H. Kim, and R. Meena, "Artificial neural networks: An overview for environmental applications," *Environ. Eng. Res.*, vol. 25, no. 3, pp. 363–377, Jul. 2020.
- [24] A. A. Ezugbe and S. Rathilal, "Membrane technologies in wastewater treatment: A review," *Membranes*, vol. 10, no. 5, p. 47, May 2020.
- [25] R. Singh, M. Srivastava, and A. S. Rathore, "Artificial intelligence in environmental monitoring and wastewater treatment: recent developments and future prospects," *Environ. Sci. Water Res. Technol.*, vol. 8, no. 3, pp. 531–548, 2022.

- [26] D. F. Specht, "A general regression neural network," *IEEE Trans. Neural Netw.*, vol. 2, no. 6, pp. 568–576, Nov. 1991.
- [27] M. Beale, M. T. Hagan, and H. Demuth, *Neural Network Toolbox™ User's Guide*, MathWorks, 2019.
- [28] D. W. Marquardt, "An Algorithm for Least-Squares Estimation of Nonlinear Parameters," *J. Soc. Ind. Appl. Math.*, vol. 11, no. 2, pp. 431–441, Jun. 1963.
- [29] Y.R. Smith, A. Kar, and V. Subramanian, "Investigation of Physicochemical Parameters That Influence Photocatalytic Degradation of Methyl Orange over TiO₂ Nanotubes," *Ind. Eng. Chem. Res.*, vol. 48, no. 23, pp. 10268–10276, 2009. DOI: 10.1021/ie801851p.

PLAGIARISM REPORT

pankaj thesis final (1).pdf

 Delhi Technological University

Document Details

Submission ID

trn:oid::27535:101684657

Submission Date

Jun 19, 2025, 7:15 PM GMT+5:30

Download Date

Jun 19, 2025, 7:17 PM GMT+5:30

File Name

pankaj thesis final (1).pdf

File Size

671.8 KB

18 Pages

4,447 Words

22,664 Characters



Page 2 of 23 - Integrity Overview

Submission ID trn:oid::27535:101684657





10% Overall Similarity

The combined total of all matches, including overlapping sources, for each database.




Filtered from the Report

▸ Bibliography

Match Groups

-  **30 Not Cited or Quoted 8%**
Matches with neither in-text citation nor quotation marks
-  **11 Missing Quotations 2%**
Matches that are still very similar to source material
-  **0 Missing Citation 0%**
Matches that have quotation marks, but no in-text citation
-  **0 Cited and Quoted 0%**
Matches with in-text citation present, but no quotation marks

Top Sources

- 5%  Internet sources
- 5%  Publications
- 7%  Submitted works (Student Papers)

Integrity Flags

0 Integrity Flags for Review

No suspicious text manipulations found.

Our system's algorithms look deeply at a document for any inconsistencies that would set it apart from a normal submission. If we notice something strange, we flag it for you to review.

A Flag is not necessarily an indicator of a problem. However, we'd recommend you focus your attention there for further review.

Place: Delhi

Date: June 20, 2025

DR. MANISH JAIN
(SUPERVISOR)

PANKAJ
(23/MSCCHE/80)

KHUSHI
(23/MSCCHE/22)