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Enhanced adsorptive removal of ibuprofen from pharmaceutical effluent using TiO_2-coated multi-walled carbon nanotube

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Ibuprofen is one of the most widely used non-steroidal anti-inflammatory drugs (NSAID) and is frequently reported as a contaminant in aquatic systems because conventional wastewater treatments cannot fully eliminate it. This study presents the preparation of titanium dioxide–coated multi-walled carbon nanotubes (TiO_2-MWCNTs) and their application for Ibuprofen removal. Characterization techniques (FTIR, EDS, FESEM) confirmed uniform TiO_2 coating and surface modification of the nanotubes. Batch adsorption tests showed that TiO_2-MWCNTs achieved a maximum removal efficiency of 93.3% at 45 °C, which is higher than pristine MWCNTs. Kinetic modeling indicated that the adsorption followed a pseudo-second-order mechanism, while isotherm analysis fitted both Langmuir and Freundlich models, suggesting monolayer adsorption with some degree of surface heterogeneity. The maximum adsorption capacity was calculated as 125 mg/g. Furthermore, artificial neural network (ANN) modeling closely matched the experimental findings, confirming strong predictive capability ($R^2 > 0.98$). The results suggest that TiO_2-MWCNTs are promising adsorbents for the efficient removal of Ibuprofen from pharmaceutical wastewater.

Keywords*:* Adsorption, Ibuprofen, Nanomaterials, TiO_2-MWCNTs, Pharmaceutical wastewater

Introduction

Ibuprofen is one of the most widely used NSAIDs and is commonly prescribed for pain management, inflammation control, and fever reduction[1]. Its extensive use in both human and veterinary medicine, along with incomplete metabolism and improper disposal practices, has resulted in its frequent detection in different aquatic environments[2,3]. Wastewater treatment plants are often unable to eliminate ibuprofen completely, which means that residues persist in effluents and eventually enter rivers, lakes, soils, and groundwater[4]. Industrial discharges and sewage effluents further contribute to this contamination. The environmental persistence of ibuprofen is of concern because of its limited biodegradability and the formation of harmful transformation products during treatment, such as 1-(4-isobutylphenyl)-1-ethanol and 4-isobutyric-benzaldehyde[5,6,7]. Studies have shown that ibuprofen can bioaccumulate in aquatic species, causing oxidative stress, reproductive toxicity, and genotoxic effects[8,9]. While microbial degradation offers a potential treatment route, it requires precise control of environmental conditions such as pH, temperature, and nutrient availability, making large-scale application in wastewater treatment plants challenging[8,9]. Given these limitations, adsorption has been widely investigated as a robust and scalable method for the removal of pharmaceutical contaminants. Carbon-based nanomaterials, especially carbon nanotubes (CNTs), have shown promise due to their high surface area, strong physicochemical interactions, and favourable sorption capacity[10]. Among them, multi-walled carbon nanotubes (MWCNTs) are easier to modify than single-walled CNTs, and functionalization with groups such as hydroxyl (–OH) and carboxyl (–COOH) improves their dispersibility and adsorption efficiency[11]. In this study, titanium dioxide–coated MWCNTs (TiO_2-MWCNTs) were synthesized and evaluated for the adsorption of Ibuprofen from aqueous solution. The TiO_2 coating was expected to enhance adsorption by improving surface polarity and also by introducing hydroxyl groups, Along with experimental adsorption studies, artificial neural network (ANN) modeling was carried out to provide a predictive tool for adsorption performance and to complement mechanistic insights obtained from batch experiments.

Experimental Section

Chemicals and Reagents

The used chemicals and regents were MWCNT's (purity ~ 95%, length 10-20 μm, and outer diameter 10-20 nm, surface area ~230 m^2/g). Ibuprofen (Reagent grade – 99 % purity), H_2SO_4 and HNO_3 (99% purity), TTIP (purity 98%), Ethanol I.P (~ 99%), Acetic acid (~99%), Ammonium Hydroxide (25% aqueous solution). All Chemicals were of analytical grade and utilized without further purification.

Preparation of MWCNT

Catalyst Preparation

The Fe_2O_3/Al_2O_3 catalyst was prepared via coprecipitation to facilitate CNT growth. Aqueous solutions of $Fe(NO_3)_3 \cdot 9H_2O$ and $Al(NO_3)_3 \cdot 9H_2O$ were mixed under continuous stirring at 80 °C, followed by drying at 100 °C for 12 h. The dried precursor was ground, calcinated at 650 °C for 6 h, and sieved to obtain nanosized catalyst particles (15–20 nm). The alumina support promoted dispersion, minimized agglomeration, and enhanced catalytic activity during CNT synthesis.

Synthesis of multi-walled carbon nanotubes (MWCNT's)

The synthesis was conducted in a thermal chemical vapour deposition setup consisting a horizontal split-tube quartz furnace. The catalyst (0.1–0.5 g) was placed at the center of the furnace. The quartz tube was purged with argon (250 sccm) and heated at 15 °C/min to the target growth temperature (600–1000 °C). Once stabilized, hydrogen (100–250 sccm) and acetylene/ethylene (100 sc cm) were introduced simultaneously. Growth was sustained for 30–60 min depending on the run, after which the system was cooled to room temperature under argon flow.

Purification of MWCNT's

To remove residual metal catalysts and amorphous carbon, the as-grown MWCNTs were purified by acid treatment. One gm of MWCNT's was added to mixture of concentrated H_2SO_4 and HNO_3 taken in the ratio (v/v 3:1) at 40 °C for 3 h under ultrasonication. This treatment not only removed impurities but also introduced oxygen-containing groups on the nanotube surface[12]. The suspension was diluted with 300mL of deionized water, filtered through a PTFE membrane,and washed until neutral. The oxidized MWCNT's were dried at 70 °C for 6 h.

Preparation of TiO_2 Precursor Solution

TTIP and acetic acid were added to 15 mL of ethanol and was kept under stirring for 0.5 h. The stirring resulted in precipitates of TiO_2 in the solution. The prepared TiO_2 precursor solution was further used to coat MWCNT's with TiO_2.

Synthesis of TiO_2 coated MWCNT's

One gram of o-MWCNT's was dispersed in 100 mL of purified water by sonication to obtain a stable suspension. The TiO_2 precursor solution was added dropwise under continuous stirring for 2 h to achieve uniform coating. The suspension pH was adjusted to 9 with ammonium hydroxide to facilitate TiO_2 deposition, followed by the addition of 10 mL ethanol and further stirring for 30 min. The resulting product was filtered, wash away with 150 mL of ethanol and dried in hot air oven at 70 °C for 8 h. Successful coating was later confirmed using FESEM imaging and EDS analysis.

Adsorption experiment

A stock ibuprofen solution (50 mg/L) was prepared and diluted for adsorption studies. Batch experiments were conducted in a Temperature Controlled Magnetic Stirrer. 0.03 g of adsorbent with 40 mL of stock solution. Parameters such as temperature, contact time and pH were systematically varied. After adsorption, the suspension was filtered and the residual Ibuprofen concentration was measured using UV-Vis Spectrophotometer at λ_{max}=264 nm. The adsorption capacity (Q mg/g) was calculated using:

$$Q = (C_0 - Ci)\frac{V}{M} \quad \ldots (1)$$

Where Q (mg/g) is the amount of Ibuprofen adsorbed, Co (mg/L) is the initial Concentration of ibuprofen, C_i is the residual concentration of ibuprofen, V (L) is the solution volume and M (g) is the amount of adsorbent[13].

Results and Discussion

Characterization of TiO_2 coated MWCNT's

The prepared adsorbent was characterized to identify the presence of functional groups and successful TiO_2 coating.

Fourier transform infrared analysis (FTIR)

FTIR spectrometer (Shimadzu, Japan) was used to validate the introduction of oxygen functional group arranged on the surface of the adsorbent. The spectrum is shown in Fig 1. The broad peak at 3199 cm^{-1} confirms OH stretching vibrations and suggest the presence of hydroxyl group on the surface of MWCNT's. The peaks at 1534 cm^{-1} and 1537.81 cm^{-1} correspond to C=O and C=C stretching vibrations due to the presence of carboxyl groups formed during functionalization[14]. C-O

stretching is also observed at 1404.25 cm^{-1}. These peaks indicate the introduction of oxygen functional group on the surface of MWCNT's. The peak at 618 cm^{-1} indicates the characteristic Ti-O-Ti stretching vibrations and slight shift in this region also suggests Ti-O-C bonding and signifies the interaction between TiO_2 and MWCNT surface. The observed peaks indicate the successful functionalisation of oxygen functional group and surface modification of MWCNT's by TiO_2.

Energy dispersive spectroscopy (EDS)

The EDS spectrum (Fig. 2a) shows strong, distinct peaks corresponding to Titanium at approximately 4.5-5 keV and oxygen at 0.5 keV. The normalized weight percentage of Ti and O were reported to be 66.8% and 33.12%, respectively. The surface modification by TiO_2 is evident from significant Ti and O peaks. Their atomic percentages also confirm the same.

Field emission scanning electron microscope (FESEM)

The FESEM micrographs at varying magnifications showed rough, irregular surfaces associated with TiO_2 deposition on the nanotube network (FESEM ZEISS (SIGMA), FEI/Thermo Fisher Scientific, USA) (Fig. 2b-d). The coated CNTs exhibited agglomerated TiO_2 particles, indicating successful surface modification compared to pristine MWCNT's.

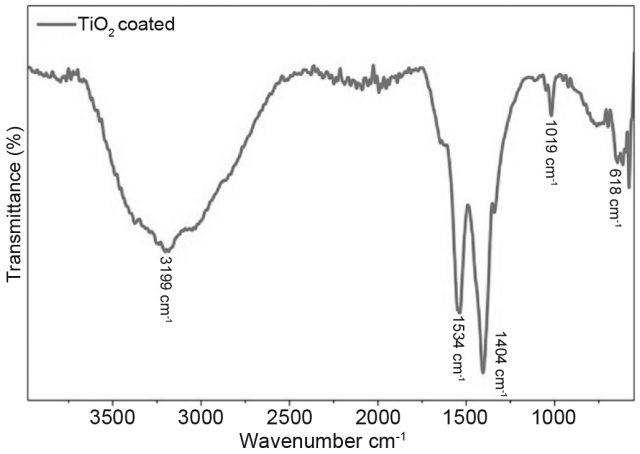

Fig. 1 — FTIR spectrum of TiO_2-MWCNT

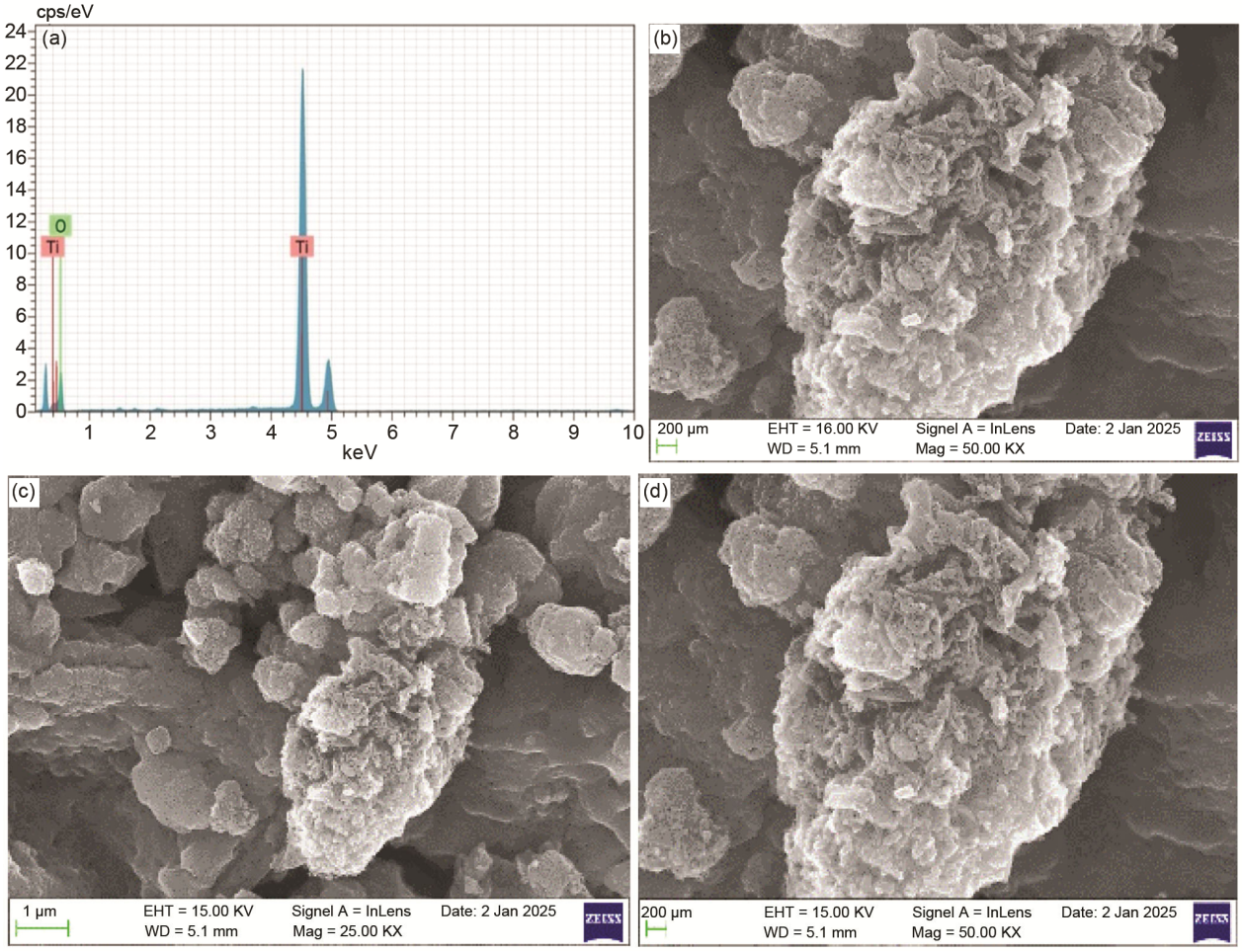

Fig. 2 — (a) EDS spectrum and (b-d) FESEM images of TiO_2-MWCNT

Table 1 — Absorbance value *vs* removal % of Ibuprofen

Influence of Temperature						
	Absorbance		Final concentration (mg/L)		Removal % of Ibuprofen	
Temperature (°C)	Pristine MWCNT's	TiO_2 coated MWCNT's	Pristine MWCNT's	TiO_2 coated MWCNT's	Pristine MWCNT's	TiO_2 coated MWCNT's
15	1.886	1.785	37.34	35.33	25.32	29.34
28	1.259	1.120	24.92	22.17	50.16	55.66
35	0.754	0.574	14.93	11.36	70.13	77.28
45	0.250	0.169	4.95	3.34	90.1	93.32
55	0.219	0.168	4.33	3.32	91.33	93.36
Influence of Contact time						
Contact time (min)	Pristine MWCNT's	TiO_2 coated MWCNT's	Pristine MWCNT's	TiO_2 coated MWCNT's	Pristine MWCNT's	TiO_2 coated MWCNT's
30	1.889	1.746	37.39	34.56	25.22	30.88
60	1.026	0.978	20.31	19.36	59.38	61.28
90	0.721	0.568	14.27	11.25	71.45	77.5
120	0.361	0.229	7.15	4.54	85.69	90.92
150	0.343	0.229	6.78	4.53	86.43	90.94
180	0.306	0.229	6.06	4.53	87.88	90.94
Influence of pH						
pH	Pristine MWCNT's	TiO_2 coated MWCNT's	Pristine MWCNT's	TiO_2 coated MWCNT's	Pristine MWCNT's	TiO_2 coated MWCNT's
2	0.739	0.562	14.62	10.98	70.76	78.04
4	0.612	0.412	12.11	4.53	75.77	90.94
6	0.809	0.229	16.02	5.79	67.96	88.42
8	1.714	0.393	33.93	20.63	32.14	58.74
10	1.880	0.534	37.22	24.71	25.55	50.58

Adsorption studies

The effective removal percentage of Ibuprofen was analysed using UV-visible spectrophotometer. It is mathematically expressed as follows[15]

$$RemovalPercentage(\%) = \frac{(c_0 - c_i)}{c_0} * 100 \quad \ldots (2)$$

Where C_o and C_i have their usual meaning. Temperature (15 °C to 55 °C) and Contact time (30 to 180 min) was studied to identify the optimum conditions for maximum removal rate. A comparative analysis was conducted to analyse the adsorption efficiency between pristine MWCNT's and TiO_2 MWCNT's. As per literature, the λ_{max} for Ibuprofen is identified at 264 nm[16] and the absorbance for 50 ppm (mg/L) Ibuprofen solution is 2.414. Table 1 represents the recorded absorbance value for every resulting solution obtained in the batch experiments.

Effect of temperature

At lower temperatures (15–28 °C), removal efficiencies were relatively modest, with pristine MWCNTs achieving 25–50% and TiO_2-coated MWCNTs showing slightly higher efficiencies of 29–56% shown in Fig. 3a. This can be attributed to reduced molecular mobility and lower diffusion rates of Ibuprofen in aqueous solution at lower thermal energies, which limit the accessibility of adsorption sites. As the temperature increased to 35–45 °C, the removal percentages rose sharply to ~70–90% for pristine MWCNTs and ~77–93% for TiO2-coated MWCNTs. This enhancement suggests that adsorption is endothermic in nature, where elevated temperature promotes increased ibuprofen solubility and facilitates intraparticle diffusion onto the sorbent surfaces.

Above 45 °C, the removal efficiency plateaued for both materials (~91–93%), indicating that adsorption sites approached saturation. At this stage, further increases in temperature did not significantly enhance Ibuprofen uptake, suggesting that equilibrium adsorption had been achieved. The TiO_2 coating introduces additional active sites, including surface hydroxyl groups, which facilitate stronger hydrogen bonding and electrostatic interactions with ibuprofen molecules. Furthermore, TiO_2 increases the surface polarity, thereby improving the wettability and dispersion of the nanotubes in aqueous solution, which enhances accessibility of ibuprofen to the adsorption sites. These combined effects result in higher removal efficiency at all tested temperatures, particularly noticeable in the dynamic adsorption phase (28–35 °C).

Effect of contact time

From Fig. 3b, it can be noted that at short contact times (30 min), removal was relatively low (25.22% for pristine MWCNTs and 30.88% for TiO_2-coated MWCNTs), reflecting the limited interaction between sorbent surfaces and Ibuprofen molecules. As the contact time increased to 60 and 90 min, adsorption improved substantially, reaching 59–71% for pristine MWCNTs and 61–77% for TiO_2-coated MWCNTs. This rapid uptake during the initial stage can be attributed to the abundant availability of active sites on the sorbents and the strong affinity between ibuprofen molecules and CNT surfaces.

Equilibrium was attained at approximately 120 min, with pristine MWCNTs and TiO_2-coated MWCNTs achieving 85.69% and 90.92% removal, respectively. The improved performance of the composite was attributed to increased wettability and dispersion, which promoted greater accessibility of active sites.

Effect of pH

At acidic pH (pH 2–4), both pristine and TiO_2-coated MWCNTs exhibited high adsorption efficiency, with the TiO_2-coated MWCNTs consistently outperforming the pristine samples. At pH 4, the TiO_2-coated MWCNTs achieved the maximum ibuprofen removal of 90.94%, compared to 75.77% for pristine MWCNTs.

The pH strongly influenced adsorption efficiency (Table 1, Fig. 3c). Maximum ibuprofen removal occurred at mildly acidic conditions (pH 4), with TiO_2-coated MWCNTs achieving 90.94% compared to 75.77% for pristine MWCNTs. At alkaline (pH>8), removal efficiency declined significantly due to electrostatic repulsion between negatively charged Ibuprofen (pKa ≈ 4.9) and the deprotonated adsorbent surface. The enhancement by TiO_2 coatings at acidic pH was linked to additional surface hydroxyl groups that strengthened hydrogen bonding.

Adsorption kinetics

Adsorption kinetics was used to obtain kinetic parameters for pseudo first order kinetics, pseudo second order kinetics and Intra-particle diffusion to determine the mechanism of the adsorption process. The kinetic equations and derived parameters are shown in Table 2.

Pseudo first-order model

The pseudo-first-order kinetic model was applied to evaluate the adsorption of ibuprofen onto TiO_2-coated MWCNTs. The linearized plot of $\log(q_e - q_t)$ versus t yielded a correlation coefficient (R^2) of 0.64, indicating poor conformity of the experimental data to the pseudo-first-order model (Fig. 4a). Furthermore, the q_e value

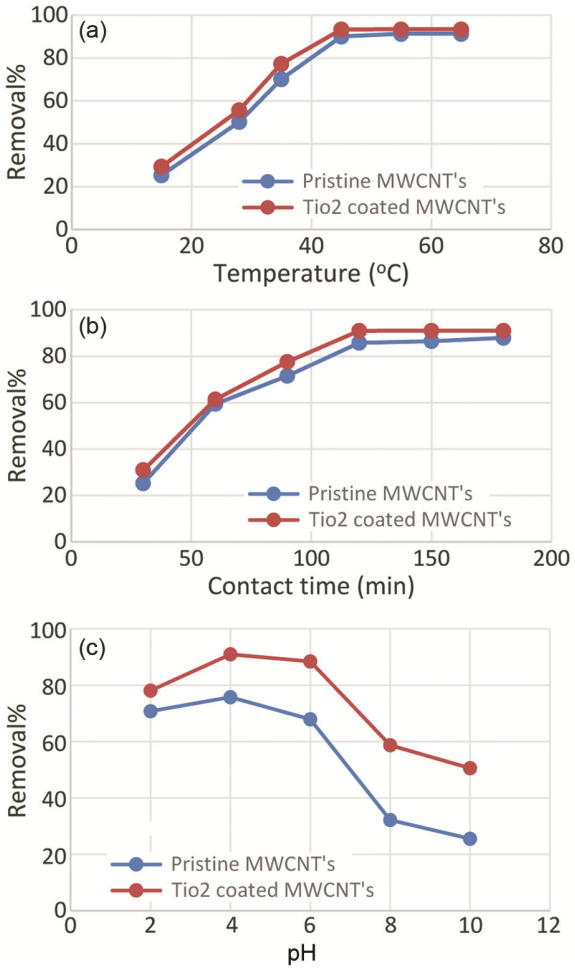

Fig. 3 — Effect of (a) temperature, (b) contact time and (c) pH on removal % of Ibuprofen

Table 2 — Parameters for kinetic models

Pseudo first order[17]				Pseudo second order[18]			Intra-particle diffusion model[19]		
$log(q_e - q_t) = \log q_e - \left(\frac{k_1}{2.303}\right)t$				$\frac{t}{q_t} = \frac{t}{q_e} + \frac{1}{k_2 q_e^2}$			$q_t = k_{id}t^{0.5} + C$		
q_e exp (mg/g)	q_e Calc (mg/g)	K_1 (1/min)	R^2	q_e	K_2 (g/mg·min)	R^2	K_{id} (mg/g·min$^{0.5}$)	R^2	C (mg/g)
62.5	181	0.014	0.64	65.78	1.36×10^{-3}	0.98	1.63	0.742	42.5

calculated from the intercept (181 mg g^{-1}) was considerably higher than the experimental equilibrium capacity (62.5 mg g^{-1}), highlighting a significant deviation between predicted and observed values. This deviation in values suggests that the adsorption kinetics are not governed by a simple first-order rate process.

Pseudo-second order model

A strong linear correlation (R^2=0.98) was obtained using pseudo-second order model (Fig. 4b). The calculated q_e (65.78 mg g^{-1}) closely matched the experimental q_e (62.5 mg g^{-1}) confirming chemisorptions as the dominant mechanism.

Intraparticle diffusion model

A multi-layer plot (R^2=0.742) suggested that intraparticle diffusion contributed but was not the sole rate limiting step (Fig. 4c). The positive intercept indicated boundary layer effects.

Adsorption isotherms

The adsorption isotherm data was analyzed using Langmuir, Freundlich and Dubinin-Radushkevich Isotherm models. The modelling was done using Microsoft Excel® and Table 3 presents corresponding modeling equations and outcomes of the mathematical simulations. The isotherm data was generated through a series of batch experiments conducted with varying initial concentrations of ibuprofen. These experiments were performed under optimized conditions determined from earlier batch studies; T= 45 °C and t= 120 min and pH=4.

The equilibrium amount of ibuprofen adsorbed was calculated using the following equation

$$q_e = (C_0 - C_e)\left(\frac{v}{m}\right) \quad \ldots (3)$$

Where, Co is the initial concentration (mg/L), Ce is the final concentration (mg/L), V is the volume of solution (L), and m is the mass of adsorbent (g). qe is the amount of Ibuprofen adsorbed per unit mass of adsorbent(mg/g).

The Langmuir isotherm assumes monolayer adsorption onto a surface with a finite number of identical sites. The isotherm data was plotted between $1/C_e$ and $1/q_e$ (Fig. 5a). The linearized form of Langmuir plot shows high degree of linearity with R^2 value of 0.9779. The values of q_{max} and K_L were determined to be 125 mg/g and 0.187 L/mg, respectively. The relatively high q_{max} suggests good

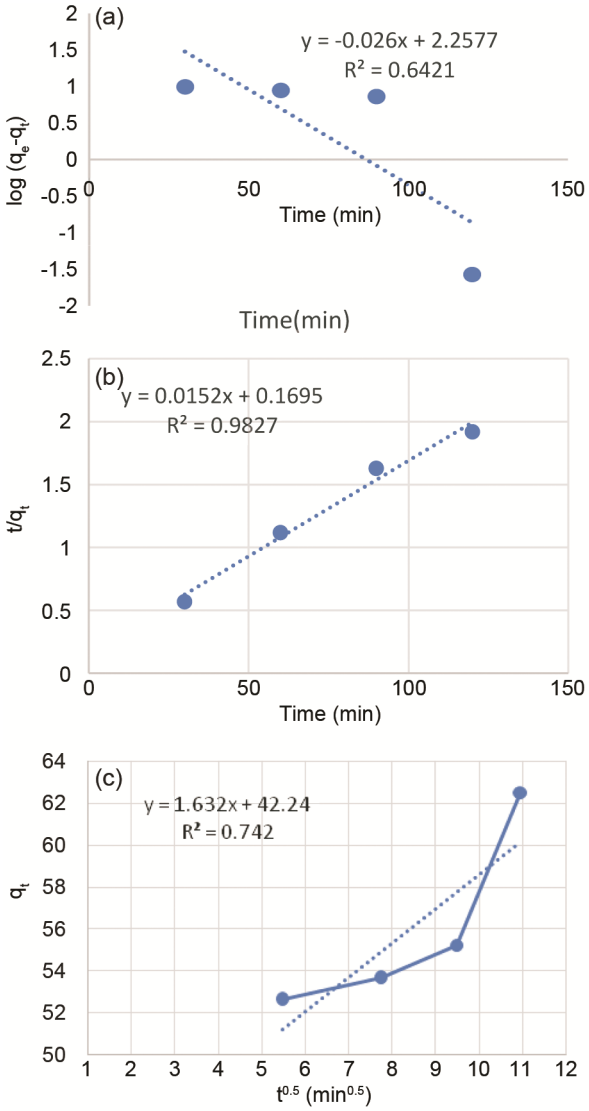

Fig. 4 —Plots for (a) pseudo first order kinetics, (b) pseudo second order kinetics and (c) intra-particle diffusion model

Table 3 —Adsorption isotherm-linear regression

Isotherm Model	Linear model Expression	R^2	q_{max}(mg/g)	K_L(L/mg)
Langmuir	$\frac{1}{q_e} = \frac{1}{q_{\max} k_L}\frac{1}{C_e} + \frac{1}{q_{max}}$	0.9779	125	0.187
		R^2	n (Dimensionless)	K_F (mg/g) (L/mg)$^{(1/n)}$
Freundlich	$ln\, q_e = \ln K_F + \frac{1}{n}\ln C_e$	0.9884	1.55	3.874
		R^2	q_s (mg/g)	E (kJ/mol)
Dubinin-Radushkevich	$ln\, q_e = \ln q_S - k_D\varepsilon^2$	0.9143	63.307	1

adsorption capacity, while the moderate K_L indicates significant affinity of Ibuprofen molecules to the adsorbent surface[20,21]. These findings are characteristic of a physisorption-dominated process. The strong linear correlation implies that the adsorption occurred on a homogeneous surface with equivalent energy sites, consistent with Langmuir assumptions. To account for adsorption on a heterogeneous surface and the possibility of multilayer formation, the equilibrium data were further evaluated using the Freundlich isotherm[20,22,23] (Fig. 5b). The linear regression plot of log q_e Vs log C_e resulted in R^2 value of 0.9884.The value of n (favourability of adsorption) was 1.55, indicating adsorption is favourable and efficient. Unlike Langmuir and Freundlich isotherm, Dubinin-Radushkevich isotherm model does not assume a homogeneous surface or constant adsorption potential. Instead, it provides insight into the porosity of the adsorbent and physical or chemical nature of adsorption through the estimation of mean adsorption energy[24]. A plot between q_e *vs* ε^2 corresponds to a R^2 value of 0.9143 (Fig. 5c). The mean free energy of adsorption was determined to be 1 kJ/mol and this suggests that the adsorption process is predominantly physical in nature.

Artificial neural network studies for adsorption

Artificial Neural Networks (ANNs) are computational models inspired by the biological nervous system, particularly the way the human brain processes and learns from information. Unlike conventional mathematical models, which often struggle to capture the complexity and non-linearity of adsorption processes, ANN models excel at recognizing patterns and mapping nonlinear relationships between input and output parameters. This makes them particularly valuable in adsorption research, where multiple interacting factors such as pH, temperature, adsorbent dose, and contact time govern pollutant removal efficiency.

In environmental engineering, ANNs have been successfully applied to simulate adsorption kinetics, predict equilibrium capacities, and optimize process conditions. A typical ANN consists of three main layers: an input layer (representing process variables), one or more hidden layers (responsible for nonlinear transformations), and an output layer (representing predicted adsorption efficiency or capacity). During training, experimental data are used to adjust the weights between neurons, enabling the network to

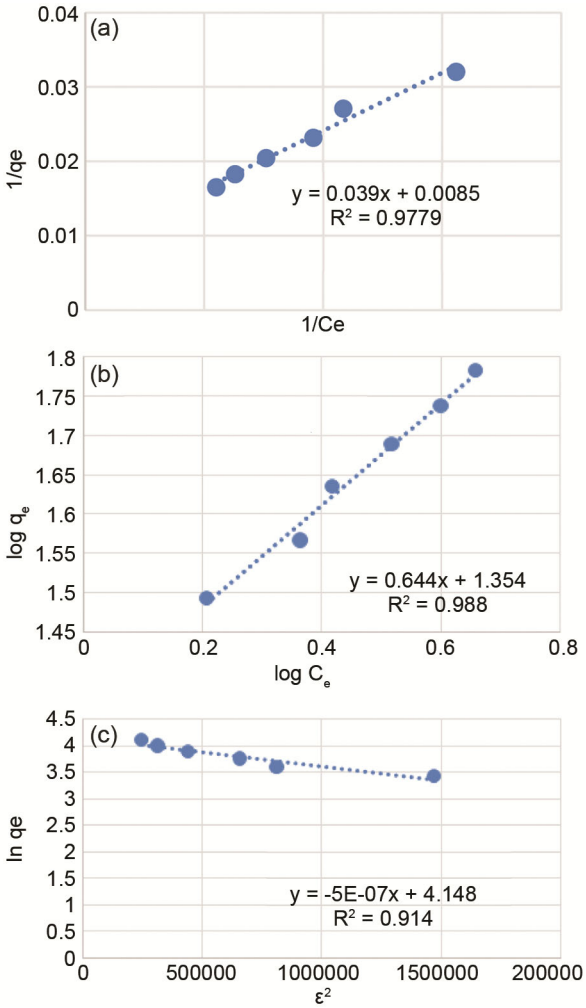

Fig. 5 — Plots for (a) Langmuir, (b) Freundlich and (c) Dubinin-Radushkevich isotherm

"learn" and provide accurate predictions for new or unseen conditions.

In the present study, ANN modeling (Fig. 6) was employed to predict ibuprofen adsorption on TiO_2-coated multi-walled carbon nanotubes (TiO_2-MWCNTs), a novel adsorbent designed to enhance removal efficiency through increased surface polarity and additional hydroxyl groups. Experimental adsorption data under varying pH (2–10), temperature (15–65 °C), contact time (30–180 min), and adsorbent dosage (10–40 mg) were used as inputs for training the ANN model. The back propagation-trained ANN demonstrated excellent predictive performance, with low mean squared errors (MSE < 0.5) and high coefficients of determination ($R^2 > 0.99$), confirming its robustness in capturing the nonlinear adsorption behaviour. The ANN results closely matched the experimental profiles across all conditions. For

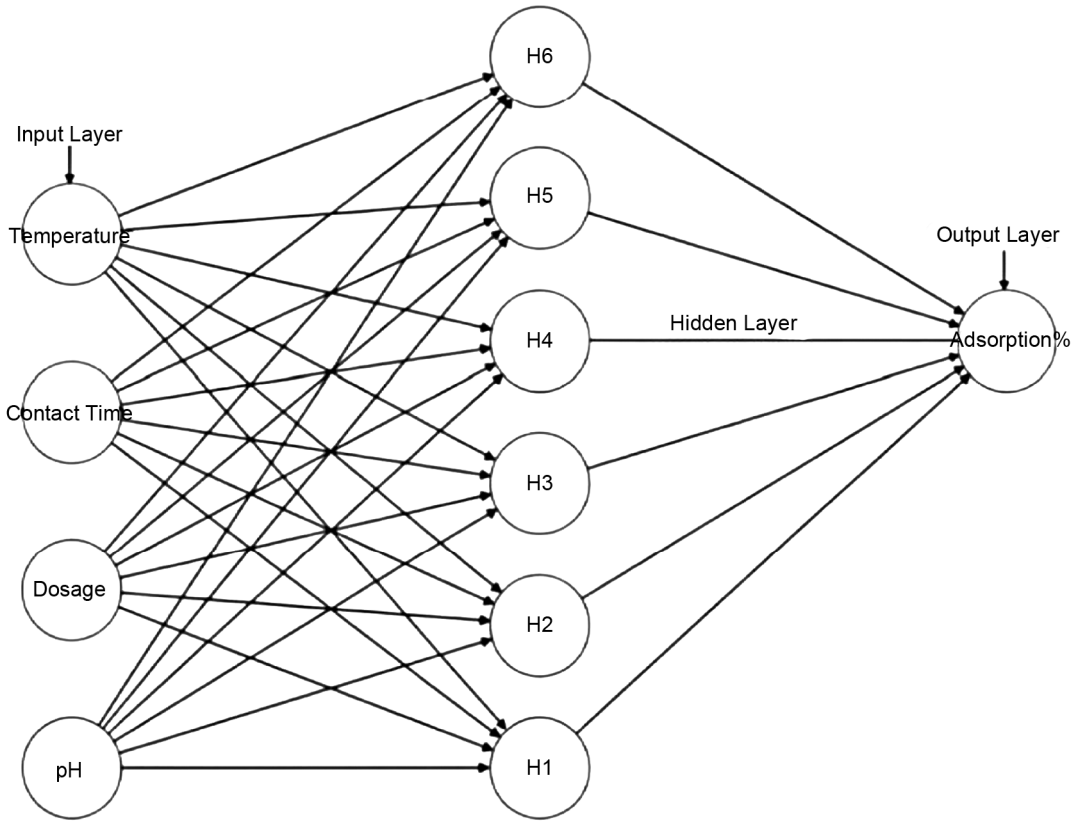

Fig. 6 — ANN architecture for TiO_2-MWCNT adsorption

instance, the model accurately reflected the sharp increase in ibuprofen removal at optimal pH (~6), the endothermic nature of adsorption with rising temperature, the saturation trend at equilibrium contact time (~120 min), and the enhancement in efficiency with higher adsorbent dosage. This indicates that ANN is not only capable of fitting the experimental data but also of simulating the thermodynamic, kinetic, and equilibrium aspects of the adsorption system[25,26].

Temperature effects

The influence of temperature on adsorption efficiency is shown in Fig. 7a. Experimental results revealed that adsorption increased significantly with temperature up to 45 °C, beyond which it plateaued, suggesting endothermic behavior with equilibrium stability at higher temperatures. The ANN model closely followed the experimental trend, with predicted values overlapping experimental ones in most cases. The minor differences at higher temperatures are attributed to slight experimental fluctuations rather than modeling inaccuracies, confirming the reliability of the ANN in thermal response prediction.

Dose effects

Fig. 7b illustrates the variation between experimental and ANN-predicted removal efficiencies at different adsorbent dosages ranging from 0.01 g to 0.04 g. Both experimental and predicted results showed a consistent increasing trend, confirming that higher adsorbent loading provided more active sites for adsorption. The ANN predictions exhibited a high degree of correlation with the experimental data, with only minor deviations observed at higher dosages. This indicates that the model successfully captured the non-linear relationship between dosage and adsorption efficiency.

pH effects

The effect of solution pH on adsorption efficiency is presented in Fig. 7c. Experimental results demonstrated that maximum adsorption occurred at pH 6, beyond which adsorption efficiency declined. This is consistent with the influence of electrostatic interactions between the adsorbent surface and ibuprofen molecules under varying protonation states. The ANN predictions accurately reflected this behaviour, showing only marginal deviations at extreme pH values. The strong correlation between

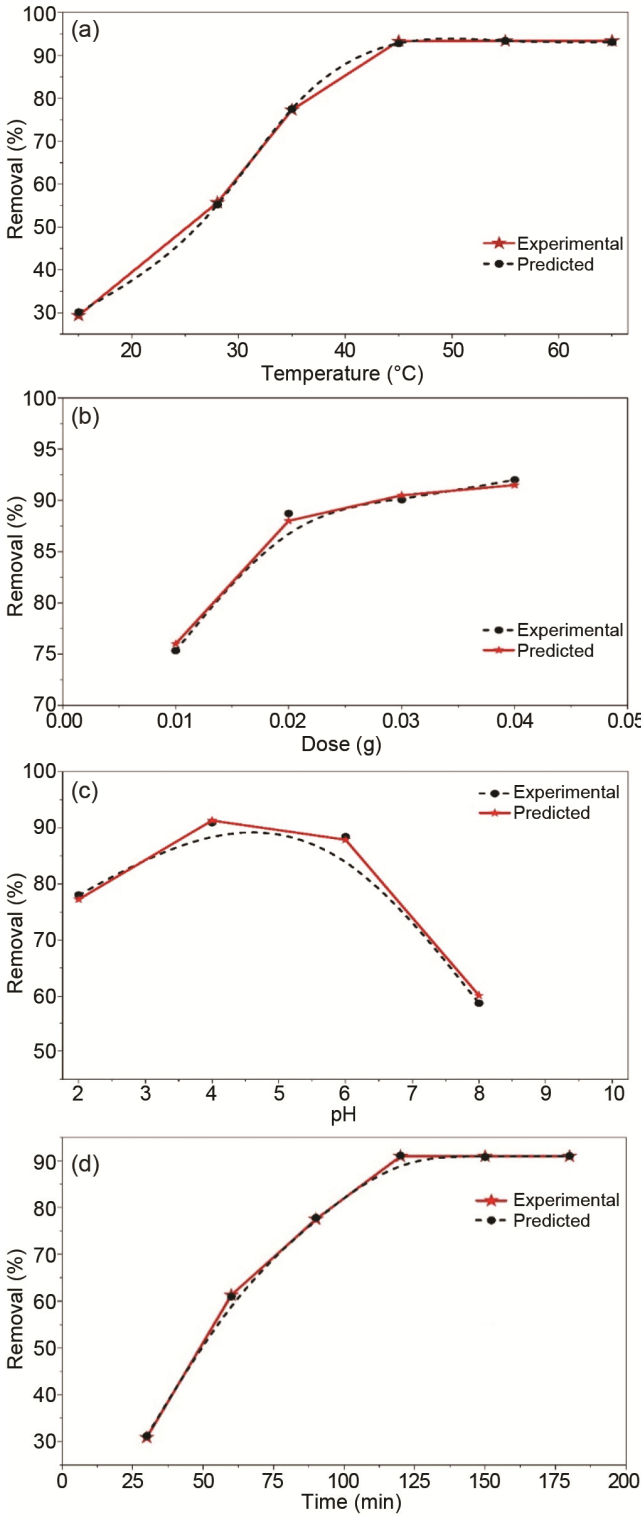

Fig. 7 — Effect of (a) temperature, (b) dose, (c) pH and (d) contact time with its experimental and predicted values

predicted and experimental values highlights the ANN's ability to capture the complex pH-dependent adsorption phenomena.

Table 4 — MSE and R^2 with its observation for TiO_2-MWCNT

Parameter	MSE	R^2	Observation
Adsorbent dosage	0.0018	0.9921	Excellent agreement between experimental and predicted values
Temperature	0.0021	0.9878	Very high predictive accuracy; minor deviation observed at higher temperatures
Contact time	0.0015	0.9934	Best fit; ANN effectively captured the equilibrium adsorption stage
pH	0.0024	0.9865	High accuracy; slight deviation at extreme pH conditions

Contact time effect

Fig. 7d compares the experimental and predicted removal percentages as a function of contact time (30–180 min). Both results indicated a rapid increase in adsorption up to 120 min, after which the curve stabilized, demonstrating attainment of adsorption equilibrium. The ANN-predicted values showed excellent agreement with the experimental data, effectively capturing both the rapid initial adsorption phase and the equilibrium region. This validates the robustness of the ANN model in time-dependent adsorption studies.

ANN modeling was employed to evaluate the adsorption performance of ibuprofen under different process parameters. For adsorbent dosage, the ANN architecture consisted of 10 hidden neurons and one output neuron with a ReLU/Linear activation function, achieving an MSE of 0.0018 and an R^2 of 0.9921, indicating excellent predictive accuracy. Temperature modeling was performed using 12 hidden neurons and one output neuron with the same activation function, yielding an MSE of 0.0021 and R^2 of 0.9878, with only minor deviations observed at higher temperatures. Contact time prediction employed 8 hidden neurons and one output neuron, resulting in the best performance among the tested parameters, with an MSE of 0.0015 and R^2 of 0.9934, effectively capturing the equilibrium adsorption stage. For pH, the ANN model utilized 9 hidden neurons and one output neuron, giving an MSE of 0.0024 and R^2 of 0.9865, which are mentioned in Table 4.Values are with high accuracy but slight deviations under extreme acidic or alkaline conditions. Overall, the ANN results demonstrated strong agreement with experimental data, confirming its effectiveness as a predictive tool for adsorption studies.

Conclusion

This study demonstrated the successful synthesis and application of TiO_2-coated multi-walled carbon

nanotubes (MWCNTs) as efficient adsorbents for the removal of ibuprofen from aqueous media. Characterization results (FTIR, EDS, FESEM) confirmed uniform TiO_2 deposition and the introduction of oxygen-containing functional groups, which enhanced surface polarity and adsorption capability. Compared to pristine MWCNTs, the TiO_2-modified material exhibited superior performance, achieving a maximum removal efficiency of 93.3% at 45 °C and equilibrium within 120 min. Optimum adsorption was observed at acidic pH conditions, whereas alkaline environments reduced efficiency due to electrostatic repulsion, consistent with earlier reports on ibuprofen behaviour in aqueous systems. Kinetic modeling showed that the pseudo-second-order model best described the process, suggesting chemisorption as the dominant mechanism, with intraparticle diffusion contributing to the overall adsorption pathway. Isotherm analysis revealed strong agreement with both Langmuir and Freundlich models, with a maximum adsorption capacity of 125 mg/g, confirming the high sorption potential of TiO_2-MWCNTs. In addition, artificial neural network (ANN) modeling provided excellent predictive capability, showing strong correlation ($R^2 > 0.98$) with experimental results. This approach highlights the potential of combining experimental data with computational tools for reliable prediction and optimization of adsorption processes. Overall, TiO_2-coated MWCNTs are shown to be promising candidates for the treatment of pharmaceutical wastewater, offering improved adsorption efficiency and a strong basis for integrating nanomaterials with data-driven modeling in environmental remediation

Conflict of Interest

The authors declare no conflict of interest.

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