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WATER PURIFICATION BY ADSORPTION CAPACITY OF CRYSTAL VIOLET DYE ON RAW AND MODIFIED AZADIRACHTA INDICA BIOMASS

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ABSTRACT

Green chemistry brought an additional focus to environmental security. Additionally, since dye contamination in aquatic systems has developed into a significant environmental issue, green synthetic plant-based adsorbents for the dye degradation have also garnered considerable attention. In detection of green research, common neem (Azadirachta indica) leaves has been used as an adsorbent to study its adsorption capacity on crystal violet dye. At various adsorbent dosages, adsorption times, dye concentrations, and pH levels of the solution, the ability of the adsorbent to adsorb CV dye was assessed. Batch adsorption studies were used to demonstrate the adsorbent's removal effectiveness for CV. Catalytic activity of the synthesized adsorbents was studied using CV dye, showing rapid degradation of CV in the first 90 min using raw neem biomass and after modifications with sulfanilamide and malonic acid its optimized time decreases to 60 min. The efficiency of adsorbent to remove CV dye was 90% with relatively low amount of biomass i.e.,

0.15 g using raw neem leaves. 0.1 g using AI modified with sulfanilamide and 0.08 g using AI modified with malonic acid. Studies showed that it has best adsorption capacity at high pH value. After optimized value of contact time, initial dye concentration, dose, and pH, further increase in dose, time or concentration decreases the adsorption rate as the active sites available by the adsorbent for dye molecule becomes filled. Studies also revealed that after modification of neem leaves with sulfanilamide and malonic acid, its adsorption capacity increases and sulfanilamide modification gives best results. All this reveals that neem leaves can be used as alternates of costly adsorbents for the CV dye removal from textile waste water and have high better adsorption capacity.

1. INTRODUCTION

Water is one of the most vital natural resources, indispensable for sustaining life, supporting ecosystems, and driving agricultural and industrial development [1]. However, rapid industrialization, urbanization, and population growth have placed enormous pressure on global water resources, both in terms of quality and availability [2]. Among the various forms of water pollution, contamination from synthetic dyes has emerged as a critical environmental challenge [3]. Synthetic dyes are extensively used in industries such as textiles, leather, paper, plastics, and cosmetics due to their vibrant colors, stability, and ease of application [4]. Unfortunately, their complex aromatic molecular structures make them highly resistant to biodegradation, leading to their persistence in aquatic systems [5].

The textile industry is recognized as one of the largest producers of colored wastewater, discharging substantial volumes of effluents containing toxic organic dyes into natural water bodies [6]. These colored discharges not only alter the aesthetic quality of water but also reduce light penetration, impairing photosynthesis in aquatic plants and disturbing the balance of aquatic ecosystems [7]. Furthermore, many dyes, including crystal violet (CV), are reported to have carcinogenic, mutagenic, and toxic effects on living organisms. CV, a triphenylmethane dye, is widely used as a biological stain, dermatological agent, and textile colorant. Its high stability and low biodegradability make it particularly challenging to remove through conventional wastewater treatment methods [8].

Various physical, chemical, and biological methods have been explored for dye removal, such as coagulation, oxidation, membrane filtration, and microbial degradation [9]. However, many of these approaches are costly, energy-intensive, or generate secondary pollutants. Among these methods, adsorption has gained significant attention due to its simplicity, high efficiency, and cost-effectiveness[10]. Activated carbon is the most commonly used adsorbent, but its high production and regeneration costs limit its large-scale application. As a result, researchers have been actively investigating low-cost, eco-friendly adsorbents derived from agricultural by-products and plant biomass [11].

Neem (Azadirachta indica) is a widely available plant known for its medicinal and antimicrobial properties [12]. Its leaves, seeds, and bark have been explored in environmental remediation due to their porous structure, high surface area, and abundance of functional groups that can bind pollutants[13]. Neem biomass is inexpensive, renewable, and

biodegradable, making it a promising alternative to commercial activated carbon for dye removal. Furthermore, chemical modification of neem biomass using agents such as sulfanilamide and malonic acid can enhance its surface functionality, thereby improving its adsorption capacity for dyes like CV[14].

Although neem biomass has been studied for the adsorption of certain pollutants, there is limited research on its efficiency in removing crystal violet dye, especially when chemically modified to improve adsorption performance[15]. Most existing studies focus on raw biomass, leaving a knowledge gap regarding the comparative performance of raw versus modified neem leaves under optimized operational conditions. Additionally, there is insufficient experimental data on the influence of key parameters such as adsorbent dosage, contact time, initial dye concentration, and pH on the CV removal efficiency using modified neem biomass [16]. Addressing this gap is essential to develop sustainable, low-cost, and scalable solutions for treating dye-contaminated wastewater [17]. The primary objective of this study is to evaluate the potential of neem (Azadirachta indica) biomass as a sustainable, low-cost adsorbent for the removal of crystal violet dye from aqueous solutions. The research focuses on assessing the adsorption efficiency of both raw and chemically modified neem biomass, with modifications carried out using sulfanilamide and malonic acid to enhance surface functionality and adsorption performance. In doing so, the study aims to compare the removal efficiencies of the raw and modified forms under varying operational conditions, including changes in adsorbent dosage, contact time, initial dye concentration, and solution pH. Furthermore, it seeks to determine the optimal conditions for maximum dye removal and analyze the impact of chemical modification on adsorption kinetics and overall efficiency. Ultimately, the work intends to demonstrate the feasibility of neem biomass as an eco-friendly alternative to conventional adsorbents, offering an effective solution for the treatment of dye-contaminated wastewater, particularly from textile industries.

2 Materials and Methods

2.1 Materials and Methods

2.1.1 Chemicals and Reagents

Crystal violet (CV) dye, a cationic triphenylmethane dye, was selected as the model contaminant due to its widespread industrial use and environmental persistence. The dye was obtained in analytical grade form and used without further purification. Sulfanilamide and malonic acid, also of analytical grade, were purchased and employed as modifying agents for neem biomass. Sodium hydroxide (NaOH, 0.1 M) and hydrochloric acid (HCl, 0.1 M) were prepared freshly for pH adjustment during experiments. All solutions were prepared using distilled water to avoid interference from dissolved impurities.

2.2 Collection and Preparation of Adsorbent

Fresh leaves of neem (Azadirachta indica) were collected from local trees in Multan, Pakistan. The leaves were first rinsed thoroughly with tap water to remove surface dust and adhered particulates, followed by repeated washing with distilled water to eliminate any remaining soluble impurities. The cleaned leaves were air-dried at room temperature for several days until they became crisp, ensuring moisture removal without degrading their surface functional groups. The dried leaves were then ground into a fine powder using a laboratory-scale mechanical grinder and sieved to obtain uniform particle size (<250 μm). The powdered neem leaf biomass was stored in airtight polyethylene containers to prevent moisture absorption before use.

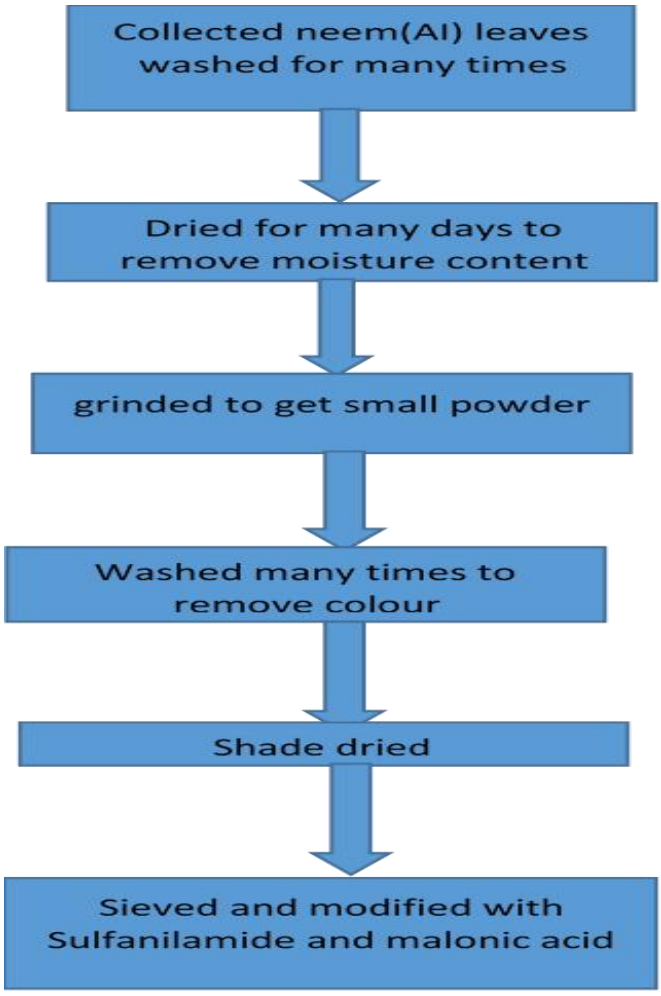


Figure 2.1*:* Preparation of biomass

2.3 Chemical Modification of Neem Biomass

To enhance the adsorption properties of neem biomass, two chemical modification processes were performed. In the first method, sulfanilamide modification, a measured quantity of neem leaf powder was immersed in an aqueous sulfanilamide solution under controlled stirring conditions to facilitate surface reactions between sulfanilamide molecules and the functional groups present on the biomass. After the required contact time, the treated biomass was filtered, thoroughly rinsed with distilled water to remove any unreacted chemicals, and then oven-dried at 60 °C until a constant weight was achieved. In the second method, malonic acid modification, neem leaf powder was treated in a similar manner using an aqueous malonic acid solution. This process also involved continuous stirring for a specific duration, followed by filtration, repeated washing with distilled water, and oven-drying at 60 °C. The chemically modified adsorbents obtained from these procedures were designated as AI-sulfanilamide and AI-malonic acid, respectively, while the untreated neem leaf powder was referred to as raw AI.

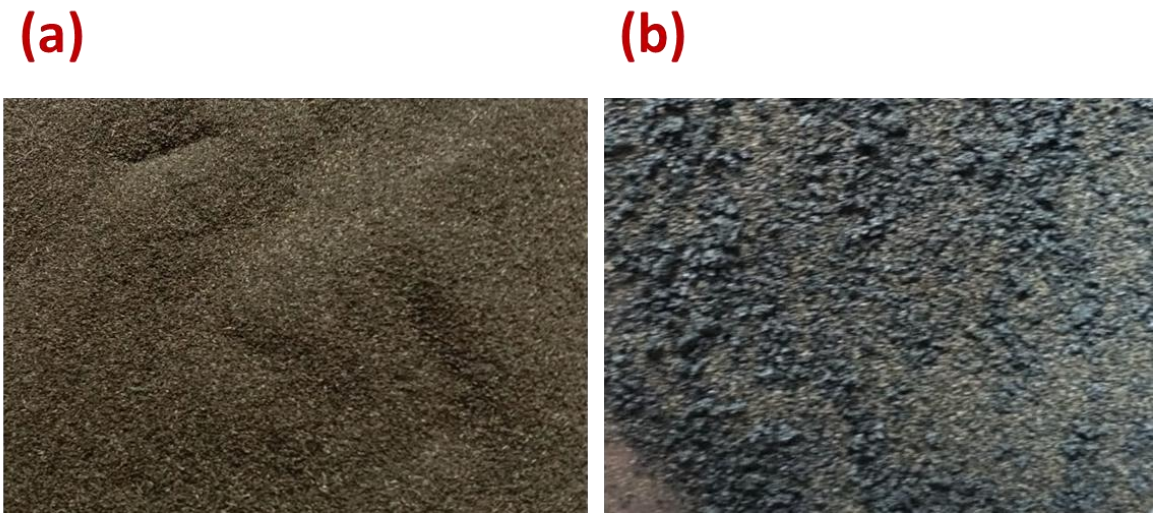


Figure 2.2: ***(a)*** AI biomass prepared **(b) AI modified with sulfanilamide**

2.4 Preparation of Dye Solutions

A stock solution of CV dye (1000 mg/L) was prepared by dissolving an accurately weighed amount of CV powder in distilled water. Working solutions of desired concentrations (10–50 mg/L) were prepared by serial dilution of the stock solution immediately before use to ensure stability. All glassware used for dye preparation was rinsed with distilled water before and after each use to prevent cross-contamination.

2.5 Batch Adsorption Experiments

Adsorption experiments were performed in batch mode to assess the removal efficiency of both raw and chemically modified neem biomass for crystal violet (CV) dye. In each trial, a measured quantity of adsorbent (ranging from 0.05 to 0.20 g) was added to 50 mL of dye solution contained in 100 mL Erlenmeyer flasks. The flasks were placed on an orbital shaker and agitated at a constant speed to maintain a uniform suspension and ensure effective contact between dye molecules and the adsorbent surface. The influence of various operational parameters was investigated by altering one factor at a time while keeping the others constant. The parameters studied included adsorbent dosage (0.05, 0.08, 0.10, 0.15, and 0.20 g), contact time (30, 60, 90, and 120 minutes), initial dye concentration (10, 20, 30, 40, and 50 mg/L), and solution pH (2, 4, 6, 8, and 10), with pH adjustments made using 0.1 M NaOH or 0.1 M HCl. At predetermined intervals, samples were withdrawn from the flasks, filtered through Whatman No. 42 filter paper to remove suspended adsorbent particles, and the resulting filtrate was analyzed to determine the residual dye concentration.

2.6 Analytical Measurements

The concentration of CV dye in the filtrates was determined using a UV–Visible spectrophotometer (λ_max = 585 nm). Calibration curves were prepared from standard solutions of known concentrations to ensure measurement accuracy. The percentage removal of dye was calculated using the equation:

$$\%\text{Removal} = \frac{C_0 - Ct}{C_0} \times 100$$

C0 (mg/L) = the initial dye concentration
C_t(mg/L) = Concentration at time t.

2.7 Solution preparation

2.7.1 Stock solution

Stock solution was prepared by taking 1g crystal violet dye and dissolve it in minimum amount of water and then make volume of measuring flask upto 1000 mL with distilled water. Stock solution was covered and stored in the dark for further use. All working solutions were prepared from this. As a blank reagent, distilled water was used to calibrate the instrument before using each sample solution in UV-visible spectrophotometer.

2.8 Working solution of crystal violet dye

Working solution was prepared from the stock solution by using the dilution formula,

$$C1V1 = C2v2$$
$$1000 \times V1 = 100 \times 100$$
$$V1 = 100 \times 100 \div 1000$$
$$V1 = 10 \text{ mL}$$

So, we take 10 mL of stock solution and dilute it upto 100 mL to make 100 mg/L solution in 100 mL. This working solution is then used in further process.

2.9 Sodium hydroxide (0.1M) solution

0.1M NaOH solution was prepared by using a formula,

$$\text{Molarity} = \frac{\text{mass of solute}}{\text{molar mass of solute}} \times \frac{1}{\text{volume of solution in litre}}$$

$$\text{Mass of solute} = \frac{\textit{molarity} \times \textit{molar mass} \times 100}{1000}$$

$$\text{Mass of NaOH} = \frac{0.1 \times 40 \times 100}{100}$$

$$\text{Mass of NaOH} = 0.4\text{g}$$

0.1M NaOH was prepared from this formula by adding 0.4g NaOH in 100 mL of distilled water. This solution is used in pH maintenance study.

2.8.1 Hydrochloric acid (0.1M) solution

8.6 mL concentrated hydrochloric acid was taken and diluted with distilled water upto 100 mL to prepare 0.1M HCl solution for pH maintenance study.

2.8.2 wavelength scan (λmax) of crystal violet dye

50 mg/L solution is prepared from stock solution, and then absorbance of wavelength 400nm to 750nm was observed. The maximum absorbance of dye was observed at 585nm.

Table2.1: *Wavelength scan of CV*

Sr. no.	Wavelength(nm)	Absorbance(nm)
1	400	0.1
2	450	0.15
3	500	0.25
4	550	0.37
5	585	0.45
6	600	0.35
7	650	0.2
8	700	0.15
9	750	0.11

Table2.2: Materials and Methods

Category	Details
Adsorbent Source	Neem (Azadirachta indica) leaves collected locally (Multan, Pakistan), washed with tap and distilled water, air-dried, ground, and sieved (<250 μm).
Chemical Modifications	- **Sulfanilamide modification:** Neem leaf powder treated with aqueous sulfanilamide solution, washed, and oven-dried at 60 °C. - **Malonic acid modification:** Neem leaf powder treated with aqueous malonic acid solution, washed, and oven-dried at 60 °C.
Dye Used	Crystal violet (CV), analytical grade, λ_max = 585 nm, molar mass 407.99 g/mol.
Chemicals for pH Adjustment	Sodium hydroxide (NaOH, 0.1 M) and hydrochloric acid (HCl, 0.1 M).
Stock Solution	1000 mg/L CV prepared in distilled water; working solutions (10–50 mg/L) prepared by dilution.
Batch Adsorption Setup	50 mL dye solution in 100 mL Erlenmeyer flask, adsorbent dosage 0.05–0.20 g, agitated on orbital shaker at room temperature.
Parameters Studied	- Adsorbent dosage: 0.05, 0.08, 0.10, 0.15, 0.20 g - Contact time: 30, 60, 90, 120 min - Initial dye concentration: 10, 20, 30, 40, 50 mg/L - pH: 2, 4, 6, 8, 10
Analysis Method	UV–Visible spectrophotometer at λ_max = 585 nm; calibration curve prepared from standard CV solutions.
Removal Calculation	$\%\text{Removal} = \frac{C_0 - Ct}{C_0} \times 100$
Reproducibility	All experiments conducted in triplicate; mean values and standard deviations calculated.

3 Results and Discussion:

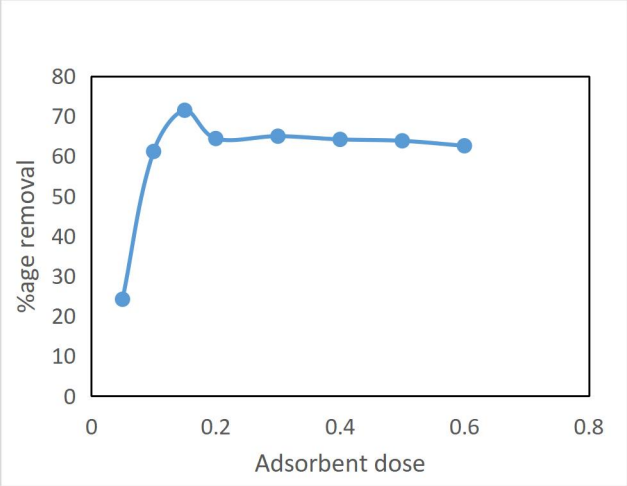
3.1 Effect of Adsorbent Dosage

The removal efficiency of crystal violet (CV) increased with an increase in adsorbent dosage for all three adsorbents raw neem biomass (AI), sulfanilamide-modified AI, and malonic acid–modified AI. This trend is attributed to the greater availability of active binding sites as more adsorbent mass is introduced into the system. The maximum removal for raw AI (90%) was achieved at 0.15 g dosage, while AI-sulfanilamide reached ~95% removal at 0.10 g, and AI-malonic acid achieved ~94% at 0.08 g. Beyond these optimal dosages, the removal percentage plateaued or slightly decreased, likely due to particle aggregation leading to a reduction in effective surface area, as reported in similar adsorption studies [18].

Table 3.1: Optimization of adsorbent dose (raw neem)

Initial dye concentration =100 mg/L
Volume of dye used = 40 mL
Particle size <100 um

Sr. no.	Adsorbent dose	Initial absorbance	Final absorbance	Final concentration	%age removal
1	0.05	2.251	1.707	75.83296313	24.16703687
2	0.1	2.251	0.875	38.87161262	61.12838738
3	0.15	2.251	0.643	28.56508219	71.43491781
4	0.2	2.251	0.802	35.62860951	64.37139049
5	0.3	2.251	0.789	35.05108841	64.94891159
6	0.4	2.251	0.807	35.85073301	64.14926699
7	0.5	2.251	0.815	36.20613061	63.79386939
8	0.6	2.251	0.843	37.45002221	62.54997779



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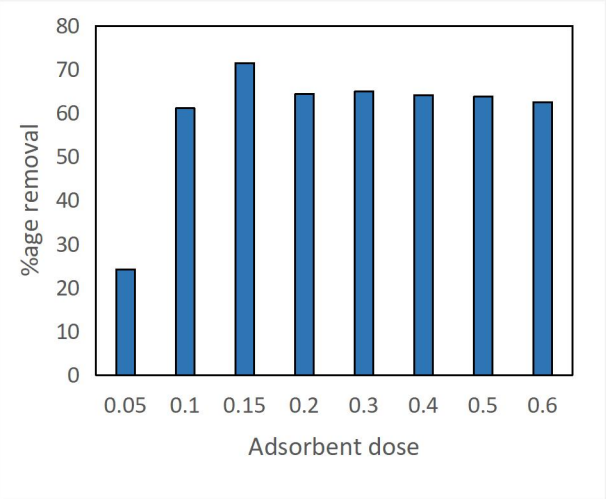


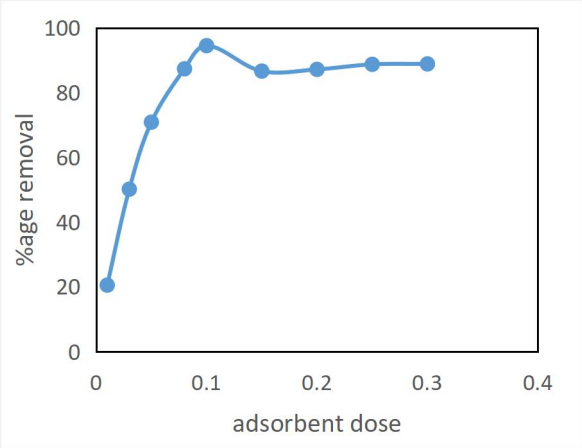
(b)

Figure 3.1: (a) Line graph of optimization of adsorbent dose of raw AI (b) Bar graph of optimization of adsorbent dose of raw AI

Table 3.2: Optimization of adsorbent dose (AI-sulfanilamide)

Initial dye concentration = 100 mg/L
Volume of dye used = 40 mL
Particle size < 100 um

Sr. no.	Absorbent dose	Initial absorbance	Final absorbance	Final concentration	%age removal
1	0.01	2.251	1.789	79.47578854	20.52421146
2	0.03	2.251	1.122	49.84451355	50.15548645
3	0.05	2.251	0.656	29.14260329	70.85739671
4	0.08	2.251	0.285	12.66103954	87.33896046
5	0.1	2.251	0.124	5.508662817	94.49133718
6	0.15	2.251	0.301	13.37183474	86.62816526
7	0.2	2.251	0.289	12.83873834	87.16126166
8	0.25	2.251	0.254	11.28387383	88.71612617
9	0.3	2.251	0.251	11.15059973	88.84940027



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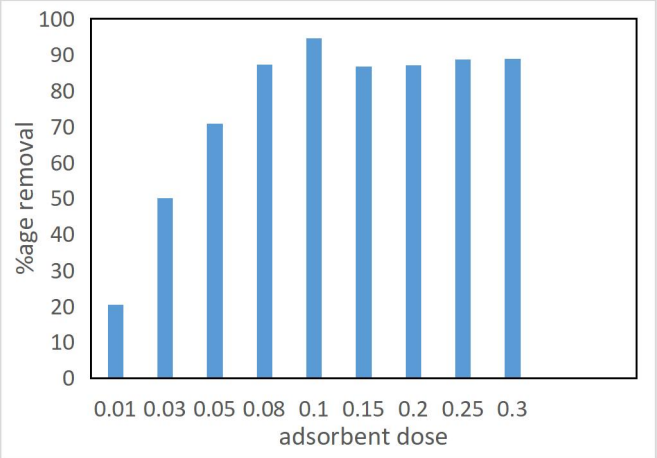


(b)

Figure 3.2 : (a) Line graph of optimization of adsorbent dose of AI-sulfanilamide(b) Bar graph of optimization of adsorbent dose of AI-sulfanilamide

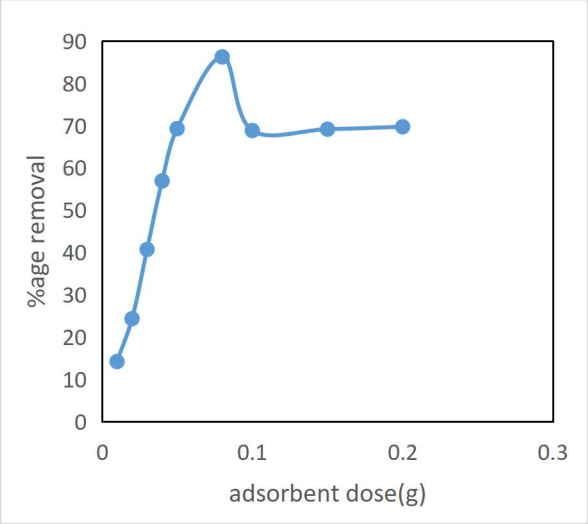
Table 3.3: Optimization of adsorbent dose (AI-malonic acid)

Initial dye concentration =100 mg/L

Volume of dye used = 40 mL

Particle size < 100 um

Sr. no.	Adsorbent dose	Initial absorbance	Final absorbance	Final concentration	%age removal
1	0.01	2.251	1.931	85.78409596	14.21590404
2	0.02	2.251	1.703	75.65526433	24.34473567
3	0.03	2.251	1.334	59.26254998	40.73745002
4	0.04	2.251	0.969	43.04753443	56.95246557
5	0.05	2.251	0.691	30.69746779	69.30253221
6	0.08	2.251	0.309	13.72723234	86.27276766
7	0.1	2.251	0.701	31.14171479	68.85828521
8	0.15	2.251	0.694	30.83074189	69.16925811
9	0.2	2.251	0.681	30.25322079	69.74677921



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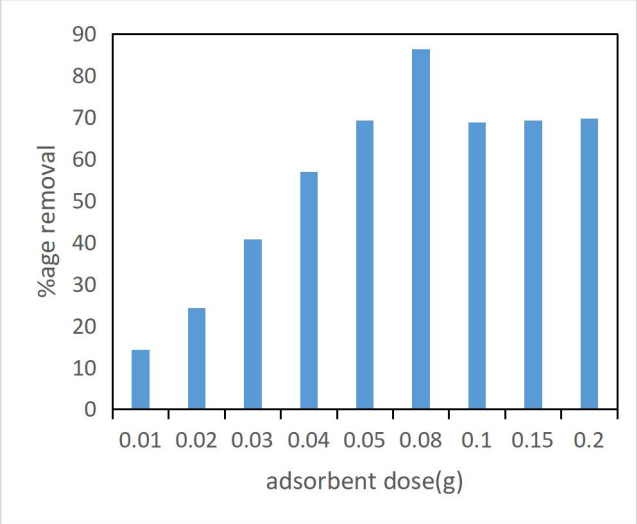


(b)

Figure 3.3: (a) Line graph of optimization of adsorbent dose of AI-malonic acid(b) Bar graph of optimization of adsorbent dose of AI-malonic acid

With increase in adsorbent dose, active sites towards dye molecule becomes limited due to aggregation of adsorbent molecules and hence, reduction in %age removal efficiency of dye occurs. The curves in graphs clearly depicts this relationship

3.2 Comparative analysis of optimized adsorbent dose

Table 3.4: Comparative study of optimized adsorbent dose

Sr. no.	optimized Adsorbent dose(g)	%age removal
1	Raw AI(0.15g)	71.43491781
2	AI-sulfanilamide(0.1g)	94.49133718
3	AI-malonic acid(0.08g)	86.27276766

3.3 Effect of contact time

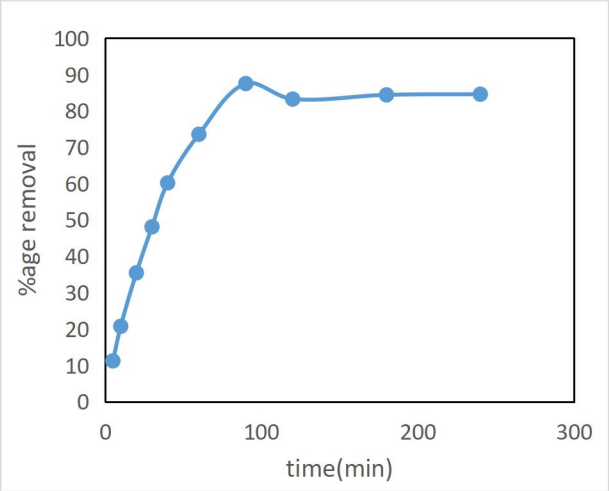
The adsorption of CV was rapid during the initial stages, with significant removal occurring within the first 60–90 minutes depending on the adsorbent. For raw AI, equilibrium was reached at 90 minutes, whereas AI-sulfanilamide and AI-malonic acid achieved equilibrium at 60 minutes [19]. The faster equilibrium for modified adsorbents can be attributed to the increased surface functionality and enhanced binding affinity introduced by the modifying agents, which reduced the diffusion path length of dye molecules into the pores [20].

Table 3.5: Optimization of time factor of raw neem (AI)

Amount of adsorbent = 0.15 g
Initial dye concentration = 100 mg/L
Particle size < 100 um

Sr. no.	Time(min)	Initial absorbance	Final absorbance	Final concentration	%age removal
1	5	2.251	2	88.76055087	11.23944913
2	10	2.251	1.784	79.25366504	20.74633496
3	20	2.251	1.453	64.54908929	35.45091071
4	30	2.251	1.168	51.88804976	48.11195024
5	40	2.251	0.896	39.80453132	60.19546868
6	60	2.251	0.595	26.43269658	73.56730342

7	90	2.251	0.281	12.48334074	87.51665926
8	120	2.251	0.377	16.74811195	83.25188805
9	180	2.251	0.351	15.59306975	84.40693025
10	240	2.251	0.347	15.41537095	84.58462905



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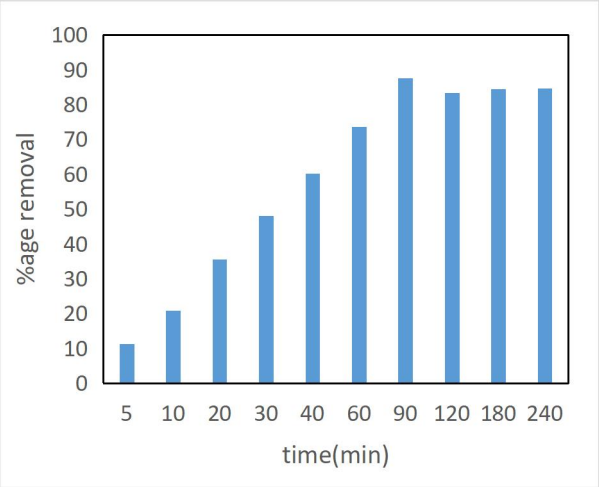


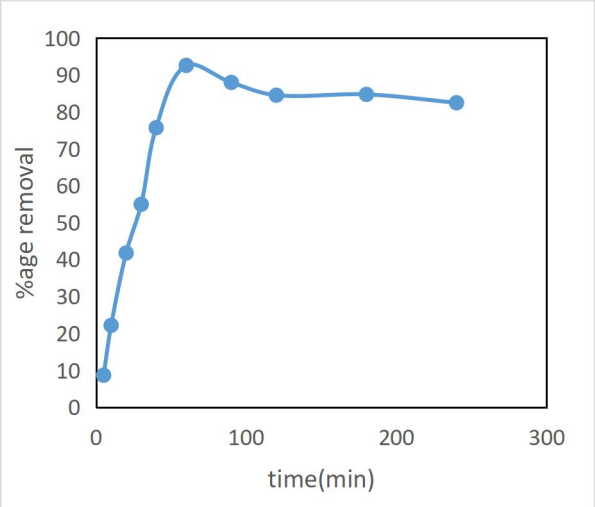
(b)

Figure 3.5:(a) Line graph of optimization of contact time of raw AI (b) Bar graph of optimization of contact time of raw AI

Table 3.6: Optimization of contact time of AI-sulfanilamide

Adsorbent dose = 0.1 g
Initial dye concentration =100 mg/L
Dye volume used =40 mL
Particle size < 100 um

Sr. no.	Time(min)	Initial absorbance	Final absorbance	Final concentration	%age removal
1	5	2.251	2.056	91.33718347	8.662816526
2	10	2.251	1.752	77.83207463	22.16792537
3	20	2.251	1.311	58.24078187	41.75921813
4	30	2.251	1.014	45.04664594	54.95335406
5	40	2.251	0.547	24.30031097	75.69968903
6	60	2.251	0.167	7.418924922	92.58107508
7	90	2.251	0.271	12.03909374	87.96090626
8	120	2.251	0.349	15.50422035	84.49577965
9	180	2.251	0.344	15.28209685	84.71790315
10	240	2.251	0.395	17.54775655	82.45224345



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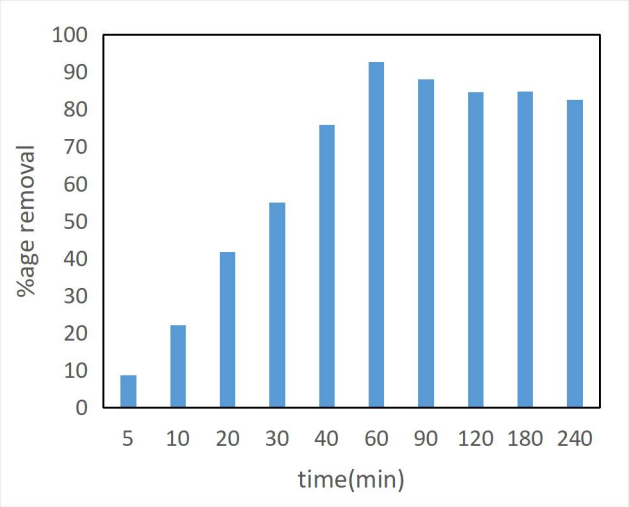


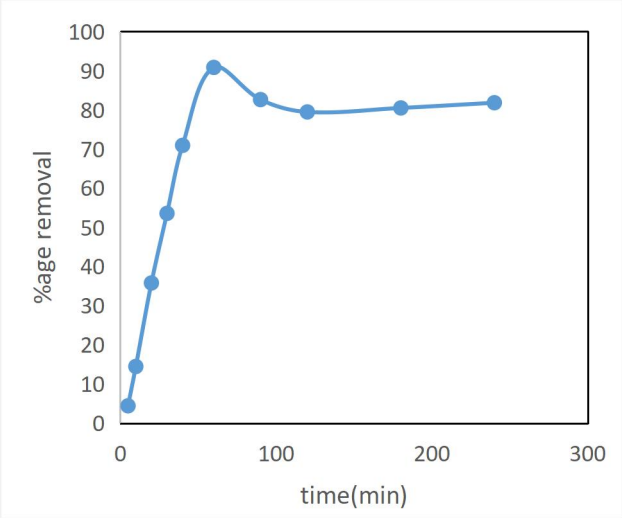
(b)

Figure 3.6: (a) Line graph of optimization of contact time of AI-sulfanilamide(b) Bar graph for optimization of contact time of AI-sulfanilamide

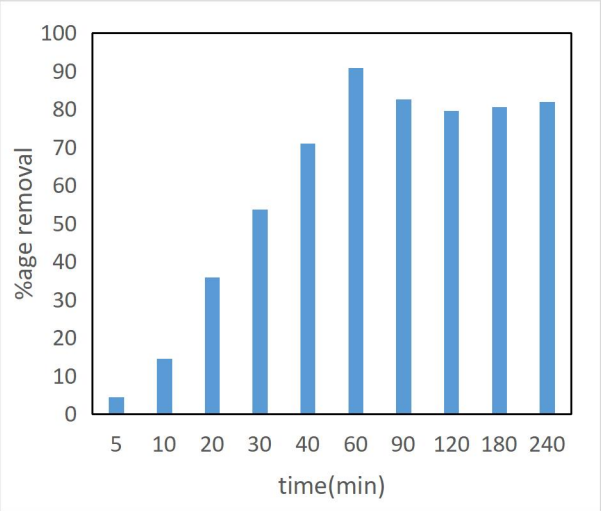
Table 3.7: Optimization of time contact of AI-malonic acid

Adsorbent dose = 0.08 g
Initial dye concentration = 100 mg/L
Dye volume used = 40 mL
Particle size<100um

Sr. no.	Time	Initial absorbance	Final absorbance	Final concentration	%age removal
1	5	2.251	2.151	95.55752999	4.442470013
2	10	2.251	1.925	85.51754776	14.48245224
3	20	2.251	1.445	64.19369169	35.80630831
4	30	2.251	1.045	46.42381164	53.57618836
5	40	2.251	0.654	29.05375389	70.94624611
6	60	2.251	0.206	9.151488227	90.84851177
7	90	2.251	0.391	17.37005775	82.62994225
8	120	2.251	0.462	20.52421146	79.47578854
9	180	2.251	0.439	19.50244336	80.49755664
10	240	2.251	0.409	18.16970235	81.83029765



(a)



(b)

Figure 3.7: (a) Line graph of optimization of contact time of AI-malonic acid(b) Bar graph of optimization of contact time of AI-malonic acid

3.4 Comparative analysis of optimized contact time

Table 3.8: Comparative study of optimized contact time

Sr. no.	optimized time(min)	%age removal
1	Raw AI(90 min)	87.51665926
2	AI-sulfanilamide(60 min)	92.58107508
3	AI-malonic acid(60 min)	90.84851177

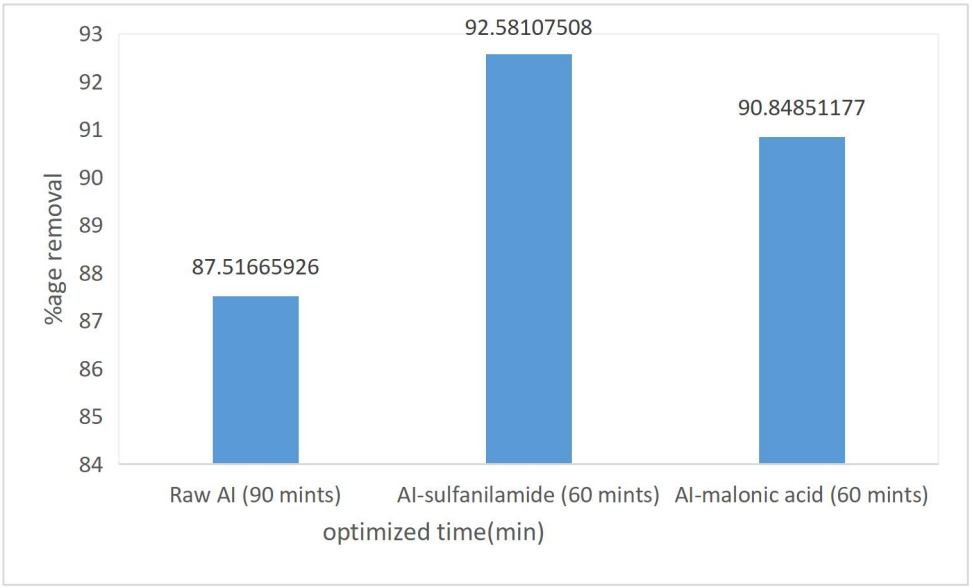


Figure 3.8 : *Comparative study of optimized contact time*

From (**figures 3.7 – 3.8**), it was clear that optimized contact time for raw neem (AI) was 90 minutes, for neem leaves (AI) modified with sulfanilamide, the optimized contact time was 60 minutes and for AI leaves modified with malonic acid optimized time was 60 minutes. (**Figure 3.8**) clearly indicates the comparison of %age removal of CV dye at the

optimized time of each adsorbent. So after modification of biomass, its adsorption capacity increases and modification of neem leaves biomass with sulfanilamide showed greatest %age removal efficiency. It means that after modification, active sites of adsorbent increases which interacts with dye molecules more strongly and hence the %age removal efficiency of dye by the adsorbent increases.

3.5 Effect of Initial Dye Concentration

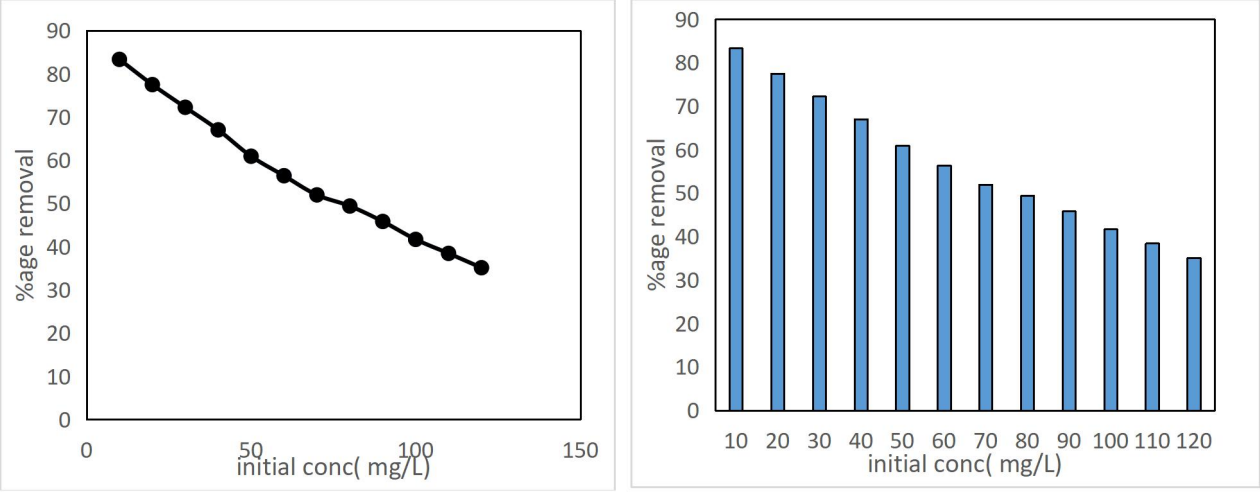
An increase in initial CV concentration from 10 to 50 mg/L resulted in a decrease in percentage removal for all adsorbents. This is due to the saturation of active sites at higher dye concentrations, causing reduced removal efficiency despite a higher absolute amount of dye adsorbed [21]. At lower concentrations, the ratio of available binding sites to dye molecules is higher, leading to more effective adsorption. The trend aligns with other studies on cationic dye removal using plant-based biosorbents [22].

Table 3.9: Optimization of initial dye concentration of raw neem (AI)

Adsorbent dose = 0.15 g
Contact time = 90 min
Dye volume used = 40 mL

Sr. no.	Initial concentration	Initial absorbance	Final absorbance	Final concentration	%age removal
1	10	0.306	0.051	1.666666667	83.33333333
2	20	0.702	0.158	4.501424501	77.49287749
3	30	0.825	0.229	8.327272727	72.24242424
4	40	0.937	0.309	13.19103522	67.02241195
5	50	1.113	0.435	19.54177898	60.91644205
6	60	1.342	0.585	26.15499255	56.40834575
7	70	1.551	0.745	33.62346873	51.96647324
8	80	1.802	0.912	40.48834628	49.38956715
9	90	2.034	1.102	48.76106195	45.82104228
10	100	2.251	1.313	58.32963127	41.67036873
11	110	2.399	1.477	67.72405169	38.43268028
12	120	2.711	1.759	77.86056806	35.11619329

Particle size < 100 um



(a) (b)

Figure 3.9: (a) Line graph of optimization of initial dye concentration of raw AI (b) Bar graph of optimization of initial dye concentration of raw AI

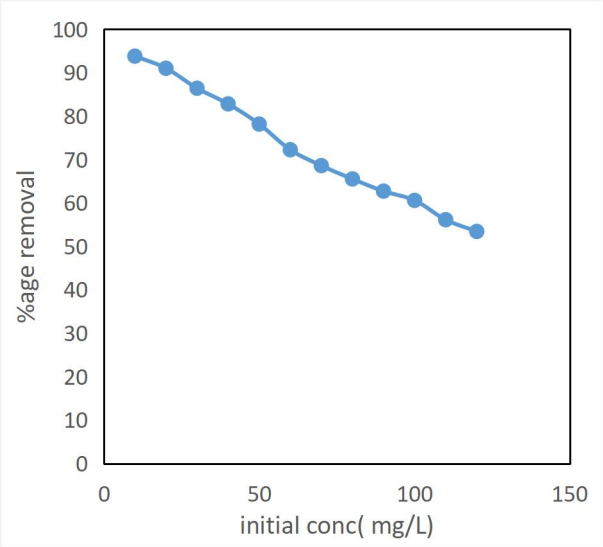
Table 3.10: ptimization of initial dye concentration of AI-sulfanilamide

Adsorbent dose = 0.1 g

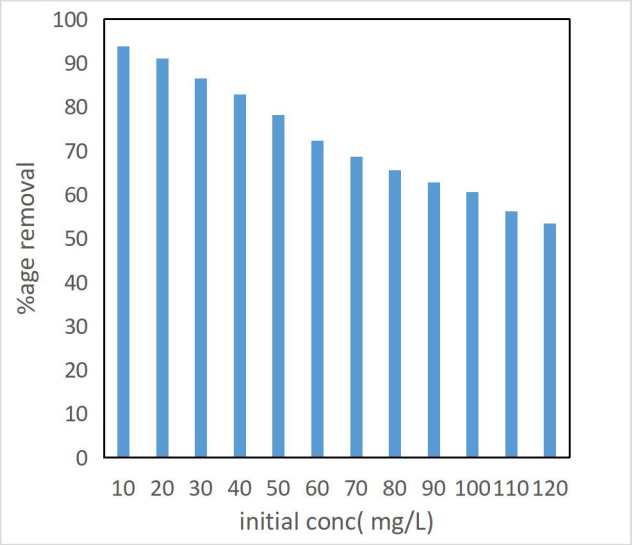
Time of contact = 40 min

Particle size < 100 um

Sr. no.	Initial concentration	Initial absorbance(nm)	Final absorbance	Final concentration	%age removal
1	10	0.307	0.019	0.618892508	93.81107492
2	20	0.702	0.063	1.794871795	91.02564103
3	30	0.825	0.112	4.072727273	86.42424242
4	40	0.937	0.161	6.872998933	82.81750267
5	50	1.113	0.243	10.91644205	78.1671159
6	60	1.352	0.375	16.64201183	72.26331361
7	70	1.551	0.487	21.97936815	68.60090264
8	80	1.802	0.621	27.56936737	65.53829079
9	90	2.034	0.758	33.53982301	62.73352999
10	100	2.251	0.887	39.40470902	60.59529098
11	110	2.399	1.052	48.23676532	56.14839516
12	120	2.711	1.262	55.86130579	53.44891184



(a)



(b)

Figure 3.10 : *(a) Line graph of optimization of initial dye concentration of AI-sulfanilamide (b) Bar graph of optimization of initial dye concentration of AI-sulfanilamide*

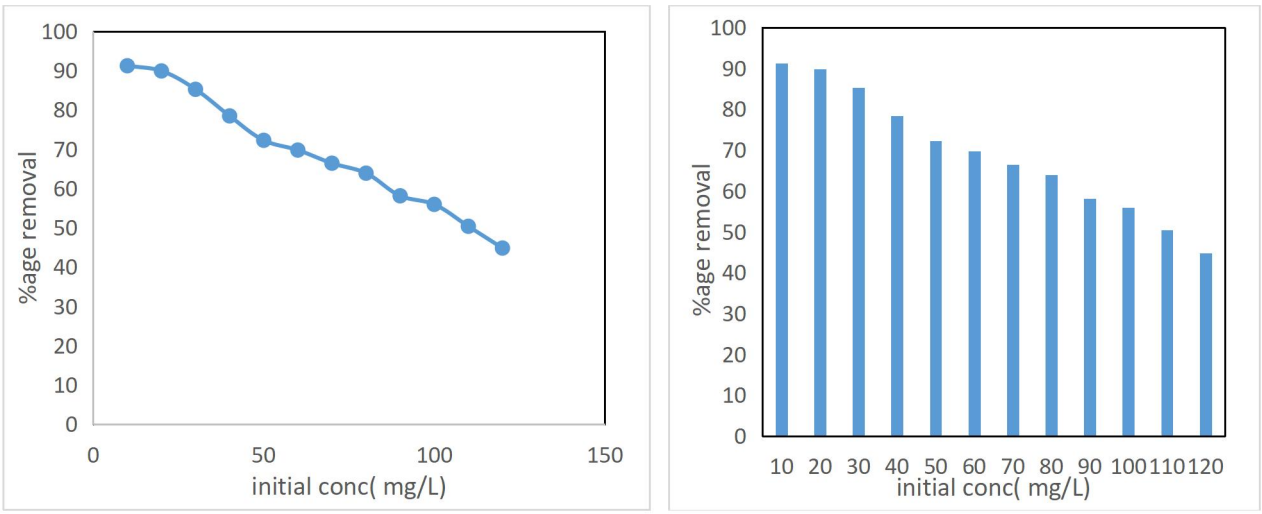
Table 3.12: Optimization of initial dye concentration of AI-malonic acid

Adsorbent dose = 0.08 g

Contact time = 60 min

Sr. no.	Initial concentration	Initial absorbance(nm)	Final absorbance(nm)	Final concentration	%age removal
1	10	0.307	0.027	0.879478827	91.20521173
2	20	0.702	0.071	2.022792023	89.88603989
3	30	0.825	0.122	4.436363636	85.21212121
4	40	0.937	0.202	8.623265742	78.44183565
5	50	1.113	0.309	13.88140162	72.23719677
6	60	1.352	0.409	18.15088757	69.74852071
7	70	1.551	0.521	23.51386202	66.40876854
8	80	1.802	0.651	28.90122087	63.87347392
9	90	2.034	0.852	37.69911504	58.1120944
10	100	2.251	0.992	44.06930253	55.93069747
11	110	2.399	1.191	54.61025427	50.3543143

12	120	2.711	1.496	66.21910734	44.81741055



(a) (b)

Figure 3.11: (a) Line graph of optimization of initial dye concentration of AI-malonic acid (b) Bar graph of optimization of initial dye concentration of AI-malonic acid

3.3.1 Comparative analysis of initial dye concentration

Table 3.13: Comparative study of initial dye concentration

Sr. no.	Initial concentration(mg/L)	%age removal
1	raw AI(100 mg/L)	41.67036873
2	AI-sulfanilamide(100 mg/L)	60.58529098
3	AI-malonic acid(100 mg/L)	55.93069747

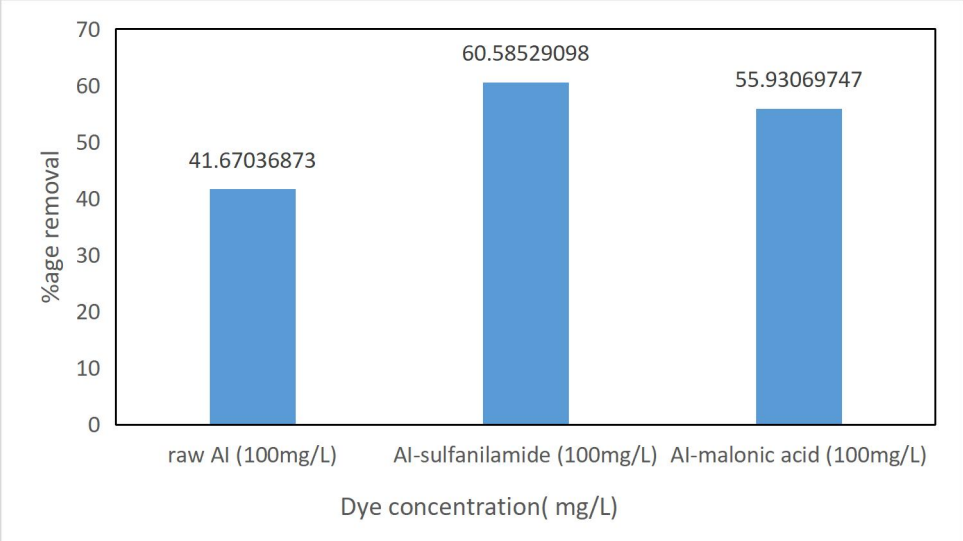


Figure 3.12: Comparative study of initial dye concentration

(Figures 29- 31) shows that by increasing initial dye concentration of solution from 10 to 120, the adsorption rate decreases as adsorptive capacity of adsorbent remains same as there is same adsorbent dose in each solution and by increasing solution's

concentration, the competition between dye molecule increases to get adsorbed on active sites provided by the adsorbent. Therefore, overall %age removal goes on decreasing by increasing initial dye concentration. Suppose we compare the results at 100 mg/L, (**figure 3.12)** clearly indicates the comparison of %age removal of all the adsorbents and AI modified with sulfanilamide showed best results.

3.6 Effect of pH

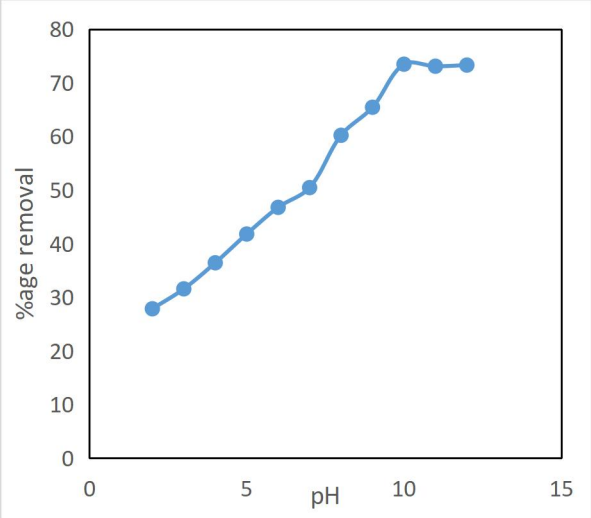
Solution pH had a significant influence on CV adsorption. Maximum removal occurred under alkaline conditions (pH 8–10) for all adsorbents, with AI-sulfanilamide showing the highest efficiency (~97%) [23]. The improved performance at higher pH is due to increased deprotonation of functional groups on the adsorbent surface, enhancing electrostatic attraction between the negatively charged sites and the positively charged CV molecules [24]. In acidic media, protonation of surface groups reduces the binding affinity for cationic dyes, leading to lower removal rates.

Table 3.14: Optimization of pH of raw neem (AI)

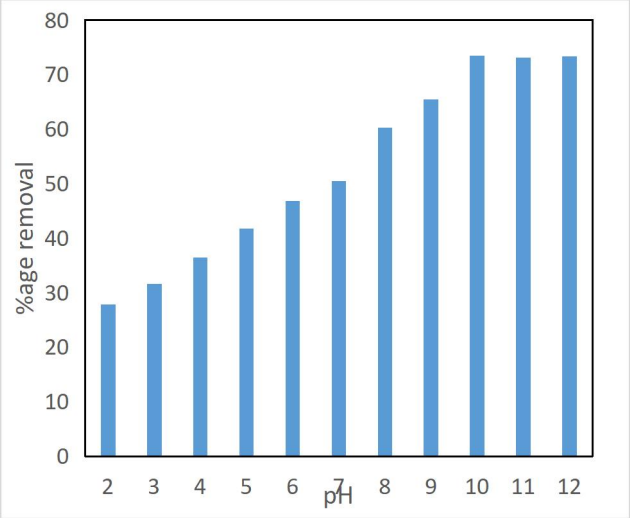
Adsorbent dose = 0.15 g
Contact time = 90 min

Sr. no.	pH	Initial absorbance(nm)	Final absorbance(nm)	Final concentration	%age removal
1	2	2.261	1.631	72.13622291	27.86377709
2	3	2.131	1.458	68.41858282	31.58141718
3	4	2.091	1.329	63.55810617	36.44189383
4	5	2.105	1.225	58.19477435	41.80522565
5	6	2.095	1.115	53.22195704	46.77804296
6	7	2.045	1.013	49.53545232	50.46454768
7	8	2.456	0.977	39.78013029	60.21986971
8	9	1.835	0.634	34.55040872	65.44959128
9	10	1.723	0.457	26.52350551	73.47649449
10	11	1.606	0.432	26.89912827	73.10087173
11	12	0.993	0.265	26.68680765	73.31319235

Initial dye concentration = 100 mg/L



(a)



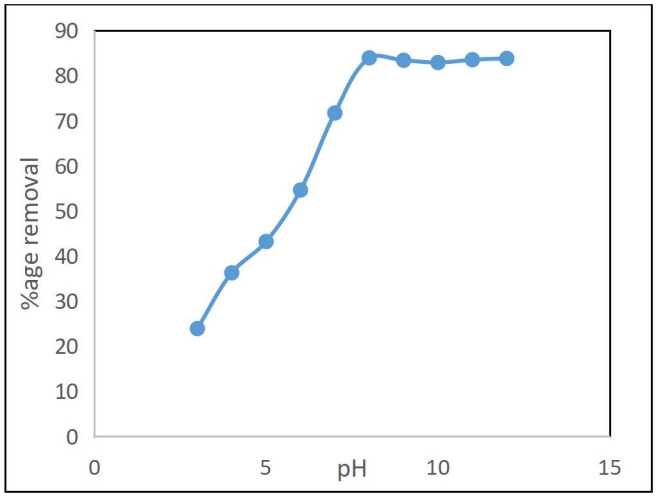
(b)

Figure 3.13: (a) Line graph for optimization of pH of raw AI (b) Bar graph for optimization of pH of raw AI

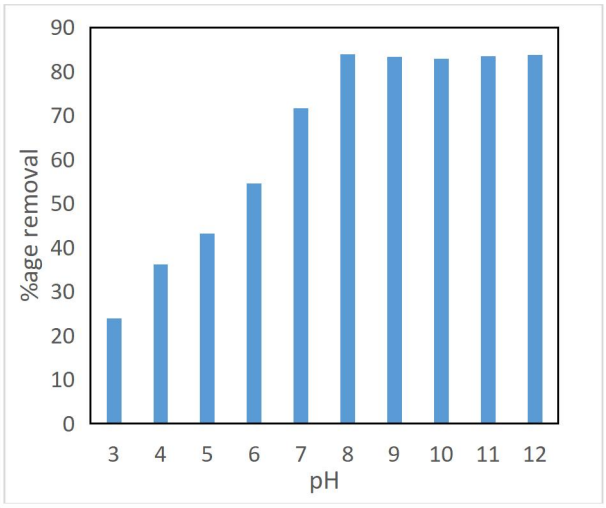
Table 3.15: Optimization of pH of AI-sulfanilamide

Adsorbent dose = 0.1g
Contact time = 40 min
Initial dye concentration = 100 mg/L
Particle size<100um

Sr. no.	pH	Initial absorbance(nm)	Final absorbance(nm)	Final concentration	%age removal
1	3	2.131	1.622	76.11450023	23.88549977
2	4	2.091	1.333	63.7494022	36.2505978
3	5	2.105	1.196	56.81710214	43.18289786
4	6	2.095	0.951	45.39379475	54.60620525
5	7	2.045	0.579	28.31295844	71.68704156
6	8	2.456	0.395	16.08306189	83.91693811
7	9	1.835	0.305	16.62125341	83.37874659
8	10	1.723	0.295	17.12130006	82.87869994
9	11	1.606	0.265	16.50062267	83.49937733
10	12	0.993	0.161	16.21349446	83.78650554



(a)



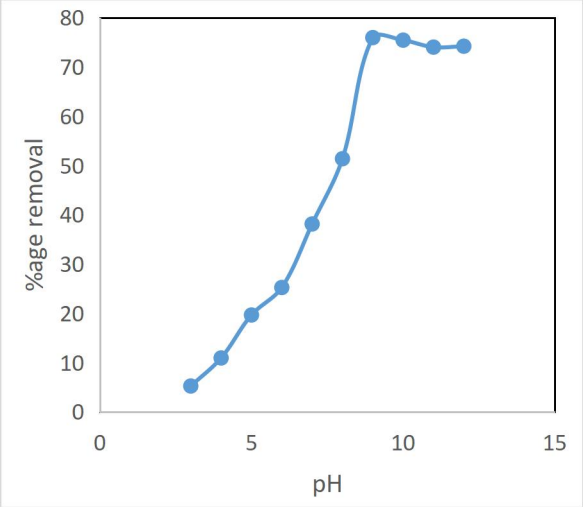
(b)

Figure 3.14 23: (a) Line graph for optimization of pH of AI-sulfanilamide (b) Bar graph for optimization of pH of AI-sulfanilamide

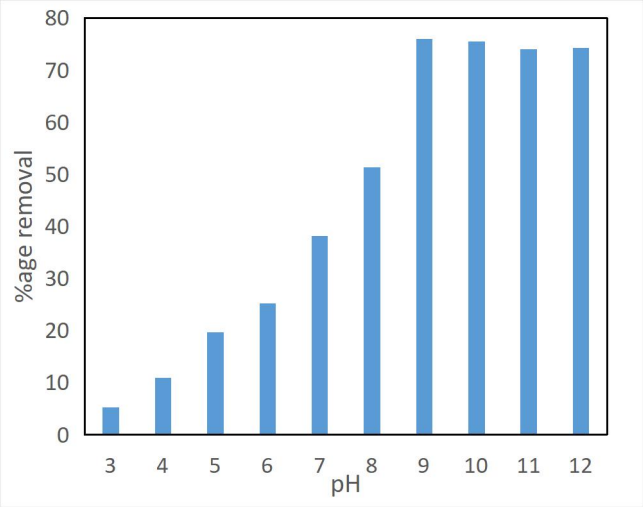
Table 3.16: Optimization of pH of AI-malonic acid

Adsorbent dose = 0.08 g
Time contact = 60 min
Initial dye concentration = 100 mg/L

Sr. no.	pH	Initial absorbance(nm)	Final absorbance	Final concentration(mg/L)	%age removal
1	3	2.131	2.019	94.74425153	5.255748475
2	4	2.091	1.862	89.04830225	10.95169775
3	5	2.105	1.691	80.33254157	19.66745843
4	6	2.095	1.566	74.74940334	25.25059666
5	7	2.045	1.265	61.85819071	38.14180929
6	8	2.456	1.194	48.61563518	51.38436482
7	9	1.835	0.441	24.03269755	75.96730245
8	10	1.723	0.423	24.55020313	75.44979687
9	11	1.606	0.417	25.96513076	74.03486924
10	12	0.993	0.256	25.78046324	74.21953676



(a)



(b)

Figure 3.15: (a) Line graph for optimization of pH of AI-malonic acid (b) Bar graph for optimization of pH of AI-malonic acid

3.7 Comparison of Raw and Modified Adsorbents

Both chemical modifications substantially improved the adsorption performance compared to raw AI.[25] Sulfanilamide-modified AI exhibited the highest overall efficiency, which can be attributed to the introduction of additional amine groups that enhance electrostatic interactions and hydrogen bonding with CV molecules[26]. Malonic acid modification also improved adsorption capacity, likely due to the introduction of additional carboxylic groups that provided new binding sites [27].

3.8 Comparative analysis of optimized pH

Table 3.17: Comparison of optimization of pH

Sr. no.	Optimized pH	%age removal
1	Raw AI(pH =10)	73.47649449

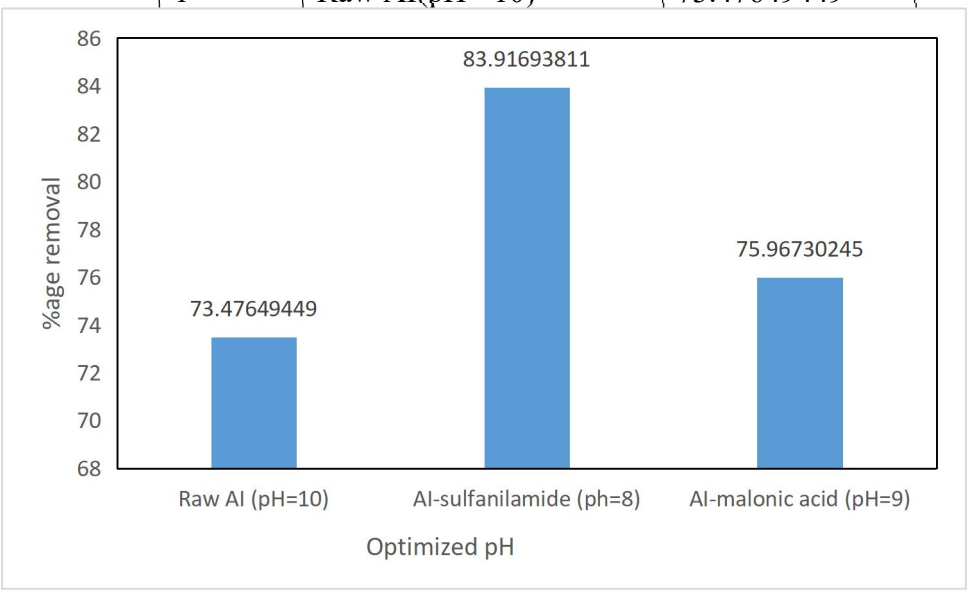


Figure 3.16: *Comparative study of optimization of pH*

From (**figures 3.14- 3.16**), it was clear that optimized pH for raw neem (AI) was 10, for neem leaves (AI) modified with sulfanilamide, the optimized pH was 8 and for AI leaves modified with malonic acid optimized pH was 9. (**Figure 3.16)** clearly indicates the comparison of %age removal of CV dye at the optimized pH of each adsorbent. So after modification of biomass, its adsorption capacity increases and modification of neem leaves biomass with sulfanilamide showed best %age removal efficiency. It means that after modification, active sites of adsorbent increases which interacts with dye molecules more strongly.

3.9 Adsorption Mechanism

The adsorption process is likely governed by a combination of electrostatic attraction, hydrogen bonding, and π–π interactions between the aromatic rings of CV and the functional groups on the adsorbent surface[28]. The improved performance of modified adsorbents confirms that surface functionalization enhances the number and type of active sites available for interaction with dye molecules[29].

Overall, the results indicate that neem biomass especially when chemically modified is an effective, low-cost, and sustainable adsorbent for CV removal from aqueous media. These findings support the potential application of such bio-based adsorbents in industrial wastewater treatment, particularly in textile effluent management[30].

Conclusion

Neem leaf powder (NLP), a readily available and abundant natural resource across Pakistan, was selected in this study due to its high efficiency in removing dyes from aqueous solutions. As a bioadsorbent, NLP offers a simple, rapid, and economical method for eliminating dyes commonly used in the textile industry. To further enhance its adsorption efficiency, neem biomass was chemically modified using an organic acid (malonic acid) and sulfanilamide, enabling improved removal of crystal violet (CV) dye from aqueous media. The adsorption performance of both raw and modified neem biomass was evaluated under varying experimental parameters, including adsorbent dosage, contact time, initial dye concentration, and solution pH.

The results revealed that contact time was directly related to adsorption until the available active sites on the adsorbent surface became saturated; beyond this point, further increases in contact time had no significant effect. The optimal contact times were found to be 90 minutes for raw neem (AI), 40 minutes for AI-sulfanilamide, and 60 minutes for AI-malonic acid. Regarding adsorbent dosage, the optimum amounts were 0.15 g for both raw AI and AI-sulfanilamide, and 0.08 g for AI-malonic acid, indicating the high efficiency of neem biomass, as small quantities were sufficient to achieve substantial dye removal. However, increasing the adsorbent dose beyond the optimum led to a decline in adsorption efficiency, likely due to particle aggregation that blocked active sites.

In terms of dye concentration, higher initial CV concentrations resulted in greater adsorption capacity, as more dye molecules were available for interaction with the adsorbent surface. pH also played a critical role in adsorption behavior: at low pH, the removal efficiency decreased due to electrostatic repulsion between the positively charged CV molecules and protonated adsorbent surface sites. As the pH increased, the adsorption rate improved because deprotonation reduced repulsion, allowing stronger electrostatic attraction between the cationic dye and the negatively charged biomass surface.

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