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RSST006 - FUNCTIONAL GROUP ANALYSIS AND ADSORPTION EFFICIENCY OF UNTREATED AND TREATED SPENT COFFEE GROUNDS IN CRYSTAL VIOLET REMOVAL

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ABSTRACT

This study investigates the potential of untreated and thermally treated spent coffee grounds (SCG) as low-cost biosorbents for the removal of crystal violet (CV) dye from aqueous solutions. Structural characterization using Fourier-transform infrared spectroscopy (FTIR) revealed functional groups such as hydroxyl, carbonyl, and aromatic groups involved in the adsorption process. Batch adsorption experiments were conducted at various SCG dosages (2–20 g/L) to determine percent removal and adsorption capacity for both untreated and treated SCG. Findings showed that untreated SCG performed slightly better than treated SCG, achieving a maximum CV of 99.7% removal and 231.0 mg/g adsorption capacity, whereas treated SCG consistently showed around 92% removal and 230.7 mg/g adsorption capacity. FTIR analysis suggested that while thermal treatment intensified certain functional groups, it may also reduce porosity and active site accessibility, negatively impacting adsorption performance. These findings highlight the promise of SCG as an eco-friendly and cost-effective adsorbent for dye-contaminated wastewater treatment.

Keywords – Spent coffee grounds, crystal violet, adsorbent, wastewater treatment, functional group characterisation

INTRODUCTION

CV is a cationic triphenylmethane synthetic dye widely used in textiles, paper, leather, printing inks, and biological staining, yet it poses serious environmental and health risks due to its toxicity and resistance to degradation (Loulidi et al., 2025). When released into water bodies, CV disrupts aquatic ecosystems and can harm human health. Traditional removal methods like coagulation, membrane filtration, and advanced oxidation are effective but expensive and energy-intensive (Homagai et al., 2022). As a result, sustainable alternatives are needed. Among emerging solutions, agro-waste-based adsorbents are gaining attention for their affordability and environmental friendliness. SCG, a major waste from global coffee consumption, is rich in cellulose, lignin, and functional groups such as hydroxyl and carboxyl that make it a promising biosorbent (Kang et al., 2022),

In Malaysia, about 31,200 tonnes of spent coffee grounds (SCG) are generated annually from coffee consumption (Omar et al., 2022), while global production reached 10 million tonnes in 2022 and is expected to rise to 12 million tonnes by 2030 (Yusufoğlu et al., 2024). Previous studies have demonstrated that SCG and its derivatives can adsorb heavy metals and synthetic dyes. However, most studies focus on treated SCG, with limited data available for raw or untreated SCG. This study evaluates the adsorption efficiency of untreated and treated SCG for CV removal, highlighting their role as an affordable and sustainable adsorbents that aligns with the United Nations Sustainable Development Goals (SDGs), particularly SDG 6 (Clean Water and Sanitation), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 12 (Responsible Consumption and Production).

OBJECTIVE

This research aims to characterize the structural and surface properties of untreated and thermally treated SCG to identify the functional groups involved in the adsorption process. It also evaluates the percent removal and adsorption capacity of CV dye using both types of SCG at various adsorbent dosages.

METHODOLOGY

SCG was collected, washed, and oven-dried at 105°C for 24 hours to remove moisture. The dried SCG was sieved through a U.S.A. Standard Sieve with a mesh size range of 850 µm to obtain a uniform particle size, and referred to as untreated SCG. A portion was thermally treated in a muffle furnace at 300°C for 2 hours (El Gheriany et al., 2020) to produce thermally treated SCG. Both forms were tested for dye adsorption performance and functional group characterization using FTIR. Spectral data were collected in the range of 4000–600 cm⁻¹ with 32 scans per sample. Batch adsorption was conducted using SCG dosages from 2–20 g/L in a 100 mg/L CV solution. The mixtures were agitated at 150 rpm for 3 hours at room temperature. After equilibrium was reached, the solutions were filtered and analyzed for residual dye concentration using a UV–Visible spectrophotometer at a maximum absorbance wavelength of 590.5 nm. Percent removal and adsorption capacity were calculated to determine adsorption performance using the equations below.

$$\text{Percent removal} = \frac{(C_i - C_e)}{C_i} \times 100\%$$

Where,

C_i is the initial dye concentration (mg/L), C_e is the equilibrium dye concentration (mg/L).

$$\text{adsorption capacity, } q_e = \frac{(C_i - C_e)V}{m}$$

Where,

C_i is the initial dye concentration (mg/L), C_e is the equilibrium dye concentration (mg/L), V is the volume of the solution (L), m is the mass of the biosorbent (g).

RESULTS AND DISCUSSION

FTIR Characterisation of Untreated and Treated SCG

Both untreated and treated SCG showed broad O-H stretching peaks at 3337 cm^{-1} and 3330 cm^{-1} , respectively. The stronger O-H peak in treated SCG suggests more hydroxyl groups due to treatment, possibly through the removal of surface impurities or decomposition of lipids and proteins (Kang et al., 2022). The C=O stretching vibrations were observed at 1744 and 1706 cm^{-1} in untreated SCG and slightly shifted to 1741 and 1702 cm^{-1} in treated SCG. This minor shift may indicate chemical rearrangement or changes in the ester or carboxylic acid groups after treatment. Both O-H and C=O groups enable hydrogen bonding with CV molecules.

The C=C aromatic peak also shifted from 1653 to 1604 cm^{-1} , possibly due to changes in the lignin structure or interaction with electron-withdrawing groups introduced during treatment. The presence of C=C in CSG might facilitate π - π interactions with the aromatic rings of CV (Loulidi et al., 2025). The C-O stretching peak shifted from 1022 cm^{-1} in untreated SCG to 1063 cm^{-1} in the treated SCG. This is likely due to polysaccharide degradation and increased surface exposure of C-O-C linkages in cellulose or lignin (Jóźwiak et al., 2021). These changes suggest more active sites were available for dye adsorption. Additionally, a minor shift in the C-N group from 1154 cm^{-1} to 1161 cm^{-1} could be attributed to oxidation or hydrolysis of amine groups (Zuluaga et al., 2024). These nitrogen-containing groups can attract the positively charged CV through electrostatic or hydrogen bonding interactions.

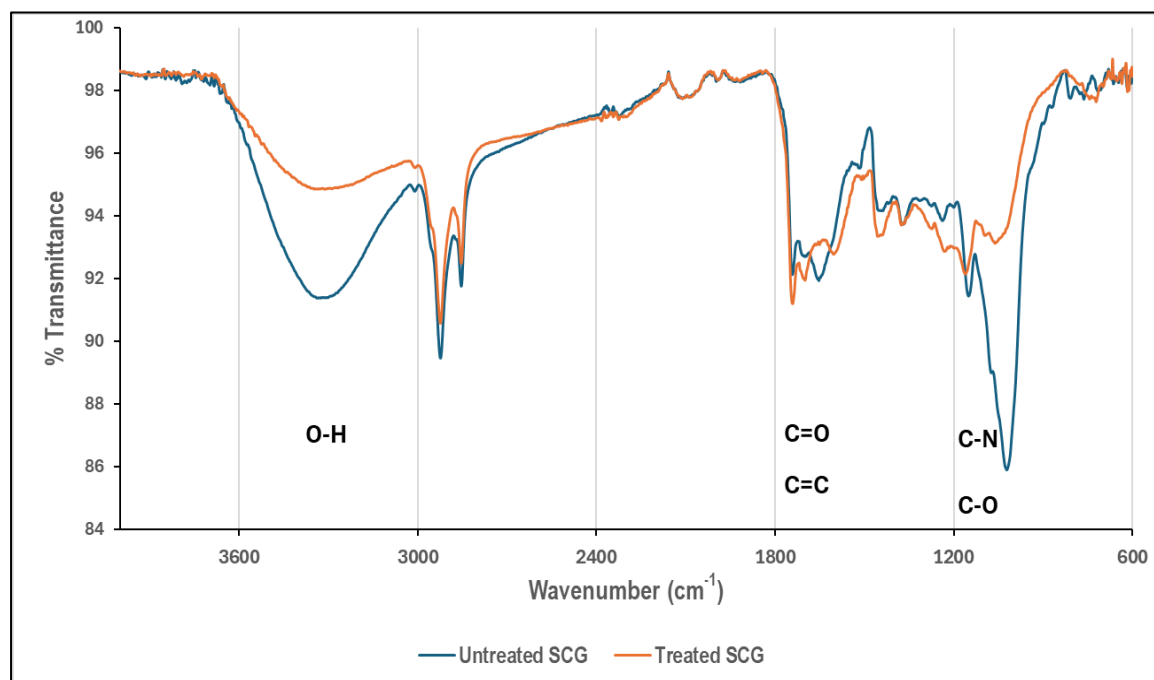


Figure 1: FTIR spectra for untreated and treated SCG

Adsorption Efficiency

At a low adsorbent dosage of 2 g/L , both untreated and treated SCG demonstrated high percent removal above 92% , with adsorption capacities of 231.0 mg/g and 230.7 mg/g , respectively. As the dosage increased, untreated SCG reached a maximum percent removal of 99.7% at 0.8 g , while its adsorption capacity dropped to 24.9 mg/g . In contrast,

treated SCG maintained a nearly constant percent removal of around 92%, regardless of dosage, and showed a similar decrease in adsorption capacity to 23.1 mg/g. Table 1 presents a detailed comparison between untreated and treated SCG.

Table 1: Percent removal and adsorption capacity of CV by untreated and thermally treated SCG at varying dosages

Dosage (g/L)	Untreated SCG		Thermally treated SCG	
	Removal (%)	Adsorption capacity (mg/g)	Removal (%)	Adsorption capacity (mg/g)
2	92.4	231.0	92.3	230.7
4	92.5	115.7	92.2	115.2
8	96.5	60.3	92.4	57.7
12	99.3	41.4	92.1	38.4
16	99.8	31.2	92.4	28.9
20	99.7	24.9	92.4	23.1

The high adsorption capacity at low dosages can be attributed to the abundance of available active sites relative to the number of dye molecules. As dosage increases, the relative number of active sites exceeds the dye concentration, resulting in site underutilization and a drop in adsorption capacity (mg/g), despite higher overall percent removal (Homagai et al., 2022). Despite treatment intensifying certain functional groups like O-H, it did not improve overall adsorption. This could be due to the breakdown of larger structures such as lignin or hemicellulose, leading to a more compact and less porous structure, which limits dye access to binding sites (El Gheriany et al., 2020).

CONCLUSION

Both untreated and treated SCG exhibit strong potential as biosorbents for CV dye. However, untreated SCG demonstrated better performance, particularly in terms of removal efficiency at higher adsorbent masses. FTIR analysis confirmed the presence of functional groups responsible for effective dye interactions, but also revealed that excessive treatment may diminish surface accessibility. Therefore, raw SCG may offer a more cost-effective and structurally favorable option for practical wastewater dye removal applications.

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