Change of Light Absorption and Scattering Due to Interactions Between Nanoparticles in Black Carbon Clusters

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Ana Flavia Gomes ; Maria Luiza Ferreira Vicente ; Francisco Eduardo Gontijo Guimarães **All Authors**

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1st Ana Flavia Gomes
São Carlos Institute of Physics
University of São Paulo
São Carlos, Brasil
anaflaviagomes@ifsc.usp.br

2nd Maria Luiza Ferreira Vicente
São Carlos Institute of Physics
University of São Paulo
São Carlos, Brasil
maria.luiza.vicente@usp.br

3rd Francisco Eduardo Gontijo Guimarães
São Carlos Institute of Physics
University of São Paulo
São Carlos, Brasil
guimarae@ifsc.usp.br

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***Abstract*—Black carbon (BC) nanoparticles, formed by incomplete fossil fuel combustion, pose environmental and health risks. This study examines how dispersion and clustering in different aqueous media: Milli-Q water, alkaline solution (pH 13), and 5% coconut oil—affect their molecular electronic states. Using UV-Vis-IR spectroscopy and confocal microscopy, we found that coconut oil promotes superior dispersion (n=0.98), while the alkaline medium also improves dispersion (n=1.0). In contrast, neutral water favors agglomeration (n=0.8). Results highlight the strong influence of particle–particle interactions on BC's optical and electronic properties, with implications for environmental reactivity and pollution control strategies.**

***Index Terms*—black carbon, UV-Vis-IR, confocal microscopy, cluster.**

I. Introduction

Black carbon (BC) is produced through the incomplete combustion of fossil fuels and biomass. It consists of nanometer-scale aerosol particles that typically form fractal-like agglomerates resembling grape clusters. Once dispersed in the atmosphere, these particles can be readily inhaled, posing significant risks to human health and contributing to environmental degradation [1,2]. Due to its strong ability to absorb solar radiation, BC is also recognized as a major contributor to global warming, particularly in regions with high aerosol concentrations [3].

The optical properties of BC are closely linked to its molecular structure and the extent of particle aggregation, both of which influence its electronic characteristics, including the optical energy gap (Eg) [4]. Previous studies have demonstrated that parameters such as pH can significantly affect the size distribution and polydispersity of BC dispersions in aqueous environments [5]. However, investigations into how these environmental factors alter the electronic states and optical transitions of BC particles remain limited.

In the present study, we explore how distinct aqueous media—namely neutral water, a strongly alkaline solution (pH 13), and a 5% aqueous coconut oil solution—affect the dispersibility and optical behavior of BC nanoparticles. UV-Vis-IR spectrophotometry and confocal microscopy were employed to evaluate changes in light absorption and scattering, providing insight into the relationship between interparticle interactions, aggregation state, and the electronic structure of BC.

II. Methodology and Experiment

A. Nanoparticles in different aqueous solutions

Diesel particulate matter (DEP) was collected from bus exhaust systems in São Paulo (Brazil) using a bimetallic retainer over the course of one week in 2015. The collected material, provided by LIM-05 at the University of São Paulo School of Medicine [4], was stored in a sealed plastic container. Stock dispersions were prepared by suspending 2.7 mg of DEP in 2 mL of three distinct media: (i) Milli-Q water, (ii) alkaline aqueous solution (pH 13, NaOH), and (iii) Milli-Q water containing 5% coconut oil. Each suspension was sonicated for 40 minutes at 50°C to reduce particle agglomeration. Working samples were then diluted to achieve an optical density (OD) close to 1 at relevant wavelengths (final DEP concentration: 33.75 µg/mL).

B. UV-Vis-IR measurements

Absorption and scattering measurements were performed using a Varian Cary 50 UV-Vis and Cary Eclipse fluorometer at the Biophotonics Laboratory (IFSC–USP). Spectra were acquired in the range of 200–1100 nm using quartz cuvettes. Baseline correction was applied using solvent-only cuvettes for each medium. OD was interpreted as a combination of absorption (A), scattering (S) and transmission T, according to:

$$T = \frac{I}{I_0}, \quad OD = \ln\left(\frac{1}{T}\right) = A + S, \quad \text{where } S = C\lambda^{-n} \tag{1}$$

where n is an empirical parameter reflecting the nature of the particles and their sizes.

C. Confocal microscopy measurements

Fluorescence confocal imaging was performed using a Zeiss LSM 780 inverted microscope equipped with a Ti:sapphire femtosecond pulsed laser (100 fs, 80 MHz, 690–1050 nm), located at the Multiuser Laboratory of the São Carlos Institute of Physics (USP). Two-photon excitation was used to assess nanoparticle dispersion, aggregation states, and photophysical properties in each medium. With a lateral resolution of 200 nm, the system enabled detailed visualization of aggregates, although single nanoparticle resolution was limited.

III. Results and Discussion

A. UV-Vis-IR measurements

Figure 1 summarizes the principal spectroscopic characteristics of stable diesel exhaust particle (DEP) suspensions in three different aqueous media: pure water at neutral pH (pH=7; light green circles), alkaline solution (pH=13; pink circles), and Milli-Q water containing 5% coconut oil (violet circles), covering the spectral range from 250 to 1100 nm. Figure 1a presents the optical density (OD) on a linear scale, while Figure 1b displays the same data on a log–log scale to emphasize both the linear behavior associated with scattering and the subtle spectral features of the OD.

In all three cases, the OD exhibits a smooth increase toward shorter wavelengths, characteristic of light losses primarily attributed to scattering. For this reason, only OD values below 2 were considered in this analysis, as higher values typically result in significant measurement uncertainty in colloidal suspensions of absorbing particles such as DEP. Assuming that scattering dominates over absorption in the near-infrared region (800–1100nm)—consistent with the weak absorption expected from polycyclic aromatic hydrocarbon (PAH) aggregates that constitute DEP—the wavelength dependence of the scattering component S(λ) can be determined.

To quantify the scattering behavior of DEP in each medium, a power-law function S(λ) proportional to λ^{-n} was fitted to the OD spectra in the near-infrared region (800–1100 nm), where absorption is minimal. The exponents obtained were n = 0.98 for the coconut oil suspension (violet dashed line), n = 1.0 for the alkaline solution (pink dashed line), and n = 0.8 for the neutral aqueous suspension (light green dashed line). These values are significantly lower than the Rayleigh prediction (n = 4), indicating that BC clusters do not act as isolated spherical particles but as fractal aggregates with broader size distributions, in qualitative agreement with Mie scattering models. Lower n values correspond to better dispersion and smaller effective particle sizes, consistent with the enhanced disaggregation promoted by coconut oil. Similar behaviors have been reported for carbonaceous nanoparticles in other stabilization media [6]. The absorption components (colored solid line in Figure 1) were then obtained by subtracting the scattering contribution from the total OD curves. The sample containing only Milli-Q water and DEP (Sample 1) exhibited the lowest optical density (OD) among the three conditions. This behavior is consistent with the hydrophobic nature of diesel exhaust particles in aqueous media, which promotes particle agglomeration and reduces their effective interaction with light via absorption and scattering mechanisms [7].

In contrast, a substantial increase in OD was observed for the sample prepared in alkaline solution, indicative of

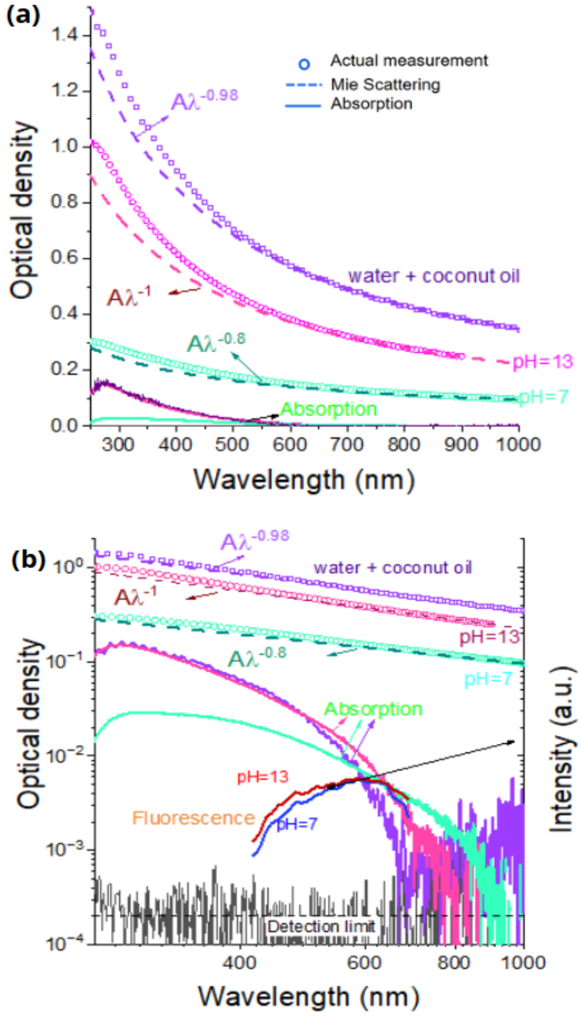

Fig. 1. Optical density (OD) spectra of diesel exhaust particle (DEP) suspensions in three aqueous environments: Milli-Q water (pH=7, light green circles), alkaline solution (pH=13, pink circles), and Milli-Q water containing 5% coconut oil (violet circles). (a) OD plotted on a linear scale. (b) Same data plotted on a log–log scale, highlighting the scattering-dominated regime at longer wavelengths. Dashed lines in (b) represent linear fits according to the power-law scattering model, including fluorescence contributions and detection limits. Source: Authors.

improved particle dispersion. This enhancement is attributed to the deprotonation of surface functional groups on black carbon under basic conditions, which leads to an increase in surface negative charge and electrostatic repulsion between particles, thereby favoring their separation and stabilization in suspension [8].

The sample prepared in Milli-Q water containing 5% coconut oil (Sample 3) presented a distinct spectral profile across the entire measured range, with significantly higher OD values compared to the other samples. This behavior is attributed to the amphiphilic properties of coconut oil constituents, which act as natural surfactants and facilitate the disaggregation of particle clusters. The resulting suspension contains a higher number of individualized nanoparticles with increased surface area available for light interaction, leading to enhanced optical signals [9].

These findings are in line with previous studies [9], which demonstrate that changes in the dispersing medium—particularly the inclusion of surfactants or polymers—can significantly alter the morphology and optical behavior of PBC aggregates. In the present work, both the alkaline solution and the medium containing coconut oil effectively promoted the disaggregation of DEP clusters, as evidenced by increased OD values and notable modifications in the absorption spectral profile. These spectral changes likely reflect a reorganization of the electronic states of the nanoparticles due to reduced interparticle interactions [9].

Remarkably, the absorption spectra of DEP dispersed in both the alkaline solution and the coconut oil medium are nearly superimposable, indicating the formation of more uniform nanoparticle populations. This spectral similarity suggests a comparable degree of particle disaggregation and stabilization in both environments. Furthermore, the relatively low absorption values observed across all samples—despite the pronounced optical density—highlight the dominant role of scattering in the overall light attenuation process, underscoring the high efficiency of scattering losses in these suspensions.

It is important to emphasize that the baseline of the absorption spectrum (black continuous line), as shown in Figure 1b, closely aligns with the instrumental noise level for wavelengths beyond 750nm. This observation supports the hypothesis that the absorption contribution from suspended soot nanoparticles is negligible in this spectral region, thereby validating both the application of a power-law for the scattering component and the method employed for scattering subtraction. These findings are further corroborated by the fluorescence emission spectra of DEP in both pure water and pH 13 solutions (Figure 1), where the emission intensity decreases at the same rate as the absorption in the 620–700 nm range. This spectral behavior reinforces the interpretation that light attenuation in these samples is dominated by scattering, with minimal absorption contribution at longer wavelengths.

B. Confocal Microscopy Measurements

Figure 2 presents confocal microscopy images of diesel exhaust particles (DEP) dispersed in aqueous media at pH 7 (Figure 2a) and pH 13 (Figure 2b). These images provide qualitative insight into the particle–particle interactions that occur when a droplet of each suspension is deposited onto a glass substrate. At neutral pH (Figure 2a), the formation of large black carbon (BC) agglomerates is evident, consistent with the hydrophobic nature of DEP in water, which promotes aggregation. In contrast, at pH 13 (Figure 2b), no significant clustering is observed, indicating a high degree of dispersion in the alkaline medium.

The differences observed in the spectral profiles (Figures 2a and 2b) reflect the influence of molecular aggregation on the optical properties of the system. In particular, changes in the shape and intensity of the emission curves indicate that particle aggregation significantly alters the electronic states of the nanoparticles, thereby modifying their optical absorption characteristics, as previously demonstrated.

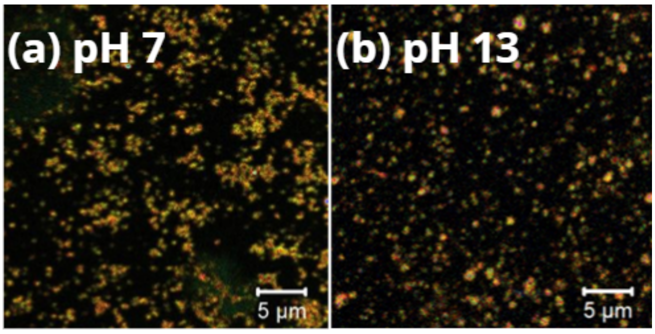

Fig. 2. (a) At pH 7, the nanoparticles form clusters ranging from 200 nm to 2 µm in diameter. (b) At pH 13, the nanoparticles show dispersion into individual nanoparticles, and the size of the nanoparticles is limited by the 200 nm lateral resolution of the confocal microscope. Source: authors.

IV. Conclusion

This study demonstrated that the optical and structural properties of Black Carbon (BC) nanoparticles are significantly influenced by their dispersion in different aqueous media. UV-Vis-IR spectroscopy and confocal microscopy revealed enhanced nanoparticle dispersion in alkaline and surfactant-containing solutions, while neutral pH favored agglomeration. These findings underscore the role of interparticle interactions in modulating BC's electronic states, with relevant environmental and toxicological implications, as well as potential strategies for controlling BC behavior in aqueous systems.

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References

[1] Schmidt, M. W., et al. (2001). Global Biogeochemical Cycles, 15(1), 163–167.
[2] Bove, H. et al. (2019). Nature Communications, 10(1), 1–7. https://doi.org/10.1038/s41467-019 11654-3.
[3] Kelesidis, S.E. Pratsinis. Proc. Combust. Inst., 37 (2019), pp. 1177-1184.
[4] Ridaoui, H., Jada, A., Vidal, L., Donnet, J. B. (2006). Colloids and Surfaces A: Physicochemical and Engineering Aspects, 278(1–3), 149–156.
[5] Frias, D. P. et al. (2020). Scientific Reports, 10(1), 1–10.
[6] Bohren and Huffman. Absorption and Scattering of Light by Small Particles, Wiley, 2008.
[7] Lian, F., Xing, B. (2017). Environmental Science Technology, 51(23), 13517–13532. https://doi.org/10.1021/acs.est.7b02528
[8] Crotti, A. E. M., Vessecchi, R., Lopes, J. L. C., Lopes, N. P. (2006). Química Nova, 29(2), 287–292.
[9] Growney, D. J., Mykhaylyk, O. O., Middlemiss, L., Fielding, L. A., Derry, M. J., Aragrag, N., Lamb, G. D., Armes, S. P. (2015). Langmuir, 31(37), 10358–10369. https://doi.org/10.1021/acs.langmuir.5b02017.