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Elemental Analysis of Particulate Matter at Relief Market, Egbu, Imo State

[1]Chisom Ugonna Obi, [2]James James Robert and [1]Theodore Chidiezie Chineke

[1]Department of Physics, Imo State University, Owerri
[2]Department of Physics, Faculty of Natural and Applied Sciences, Ignatius Ajuru University of Education, Port-Harcourt

*Corresponding Author's Email: chisomobi7@gmail.com

ABSTRACT
Ionizing radiation induces complex physicochemical interactions in biological systems through ultrafast ionization, excitation, and radical-generation processes that damage cellular biomolecules. Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) have emerged as important computational approaches for investigating these radiation-induced mechanisms at the molecular level. This review analyzes published studies from 2015–2025 involving DFT-based simulations of radiation interactions with water, DNA, proteins, and lipids, with emphasis on computational predictions validated against experimental spectroscopy and radiochemical data. Literature was selected from major scientific databases including Scopus, Web of Science, and PubMed using keywords related to radiation chemistry, biomolecular damage, and quantum chemical modeling. Comparative findings show that DFT effectively predicts bond dissociation energies, charge-transfer mechanisms, radical formation pathways, and oxidative damage processes associated with water radiolysis, DNA strand breaks, protein oxidation, and lipid peroxidation. The review also highlights recent advances such as hybrid QM/MM techniques, fragment-based DFT, and machine-learning-assisted simulations that improve the modeling of large biomolecular systems. However, limitations including high computational cost, restricted system size, and challenges in accurately reproducing dynamic cellular environments remain significant. Overall, DFT-based approaches continue to enhance mechanistic understanding in radiation biology and support applications in radiotherapy optimization, radioprotection, and predictive health-risk assessment.

Keywords:
Particulate matter,
Elemental composition,
Air quality.

INTRODUCTION

Particulate matter in ambient air contains a complex mixture of elements originating from both natural and anthropogenic sources. Elements such as aluminum, calcium, iron, zinc, and lead are frequently used as indicators of construction activities, vehicular emissions, mechanical abrasion, and resuspended soil dust. Particulate matter (PM) is a major environmental pollutant that poses a pressing global concern and significant threats to both ecosystems and human health. One remarkable contributor to this problem is particulate matter (PM), which includes tiny solid or liquid particles suspended in the air. These particles vary in size, composition, and origin. Particulate matter comes in two major sizes, namely;

i. PM_{10}, which is particulate matter smaller than 10 micrometers in diameter, and
ii. $PM_{2.5}$ (or fine particles) is particulate matter smaller than 2,5 micrometers in diameter. The size of the particle is linked to the its potential to cause health issues.

The accessibility of every human being to clean air is a fundamental human right. Recognizing this fact, World Health Organization (WHO, 1987) published air quality guidelines containing health risk assessments of major air contaminants. Rapid industrialization and urbanization during this time led to increase in anthropogenic emissions from both fossil fuel and biomass combustion (Chowdhury et al. 2001). The United States Environmental Protection Agency (USEPA, 2017) defines particulate matter or particle pollution as a complex mixture of extremely small particles and liquid droplets that get into air. PM can consist of both primary particles and those formed because of secondary processes. This diverse nature of PM makes its characterization and analysis essential for understanding and mitigating environmental pollution. Studies also shown that 9 out of every 10 people worldwide breathe unhealthy air (WHO, 2018).

Obi & Chineke (2025), assessed the particulate matter concentration at four selected locations in Egbu. However, they did not analyze the elemental composition of the PM. The rapid urbanization in Egbu calls for thorough research on the elemental constitute in PM within the environs. From the particulate matter analysis carried out by Robert et al. (2018), in a construction site at Rivers state, Nigeria. The result shown the presence of heavy metals such as Zinc, copper and selenium at higher concentration, hence posing significant health threat to those within and inside the construction site.

Egbu, located in Imo State, Nigeria, is experiencing gradual urbanization accompanied by increased commercial activities, traffic density, road construction, and domestic energy use. These activities are potential sources of particulate matter emissions. However, despite the growing anthropogenic pressures in the area, there is a lack of comprehensive and reliable data on elemental analysis in particulate matter in Egbu.While larger cities like Lagos and Port Harcourt have received some air quality attention, Egbu and its environs remain understudied, leaving a gap in understanding the extent of air pollution and associated elemental contaminants in this area. Without localized data, it is difficult for policymakers, environmental agencies, and public health officials to assess the risks posed by airborne particles, identify major emission sources, or develop effective mitigation strategies.

Elemental composition of Particulate matter (PM) can be determined by means of various spectroscopic techniques such as Atomic Absorption Spectrometry (AAS), Inductively Coupled Plasma Mass Spectrometry (ICP-MS), Laser-Induced Breakdown Spectroscopy (LIBS), X-ray Fluorescence (XRF), Neutron Activation Analysis (NAA) etc. Atomic Absorption Spectrometry (AAS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) are majorly used as standardized techniques for PM characterization (M. Ogrizek et. al., 2022). According to Bozic & Dunja (2022), some of the most common techniques used in the laboratories today are X-ray fluorescence (XRF), Absorption Atomic Spectroscopy (AAS), and Inductively Coupled Plasma (ICP) techniques: ICP-optical emission spectroscopy (ICP-OES) and ICP-mass spectrometry (ICP-MS).

This paper therefore examines the elemental composition of ambient air in relief market, Egbu, Imo State, Nigeria. For this study, AAS was used for the analysis due to its high sensitivity, selectivity, and cost-effectiveness.

MATERIALS AND METHODS

The Study Area

Egbu is a town in Owerri North Local Government Area of Imo state in southern Nigeria, located on the Otamiri River near the city of Owerri. It has a geographical location of Latitude 5.48333° or 5° 29′ north and Longitude 7.06667° or 7° 4′ east. Relief market, Egbu was used for this study.

Sample collection

The method of sample collection was direct deposition method under gravity using plastic funnel with Whatman filter paper of diameter 0.125m. The plastic funnel with the Whatman filter paper was mounted in the market and left for a period of 1 week (12th December – 19th December, 2025) to collect the sample by direct deposition under gravity.

Then the sample was taken to the laboratory for spectroscopic analysis using atomic absorption spectrometer. This analysis identified the distinct elements (Pb, Fe, Cu, Mg, Zn) present in the sample and their concentration values.

Principles of AAS and Sample analysis

Atomic Absorption Spectroscopy (AAS) was employed in the analysis of the particulate matter samples collected due its high sensitivity to trace elements and cost-effectiveness. The instrument used for such analysis is called atomic absorption spectrophotometer. According to TutorVista.com (2017), AAS is a technique for measuring the concentration of various elements in the sample through their absorption of light. As an analytical technique, it uses electromagnetic wavelengths, coming from a light source. Distinct elements will absorb these wavelengths differently. It provides a picture of the concentration of a specific element in the material, or liquid being tested.

AAS can also be used to determine the concentration of metal atoms/ions in a sample. Metals make up around 75% of the earth's chemical elements. In some cases, metal content in a material is desirable, but metals can also be contaminants (poisons) – because metal occurs naturally and essential to life but can be poisons when accumulated. The basic principles of AAS can be expressed as follows;

Firstly, all atoms or ions can absorb light at specific, unique wavelengths. When the quartz fiber filter (sample), is exposed to light of different wavelengths. The amount of light absorbed at this wavelength is directly proportional to the concentration of the absorbing ions or atoms. The electrons within an atom exist at various energy levels. When the atom is exposed to its own unique wavelength, it can absorb the energy (photons) and electrons move from a ground state to excited states. The radiant energy absorbed by the electrons is directly related to the transition that occurs during this process. Furthermore, since the electronic structure of every element is unique, the radiation absorbed represents a unique property of each individual element present in the sample and it can be measured. Atomic absorption spectrometer uses these basic principles and applies them in practical quantitative analysis. A typical atomic absorption spectrometer consists of four main components: the light source, the atomization system, the monochromator and the detection system (Figure 1).

i. Hollow Cathode Lamp: it is the radiation source that produces a narrow-band, intense light specifically characteristic of the element being analyzed.
ii. Flame: it is the atomizer that converts the liquid sample into free ground-state atoms.
iii. Monochromator: it selects the specific wavelength of light absorbed by the analyte and rejects stray light/background emission from the flame.
iv. Detector (detection system): Measures the intensity of the light transmitted through the sample. The reduction in light intensity is proportional to the concentration of analyte atoms in the atomizer.

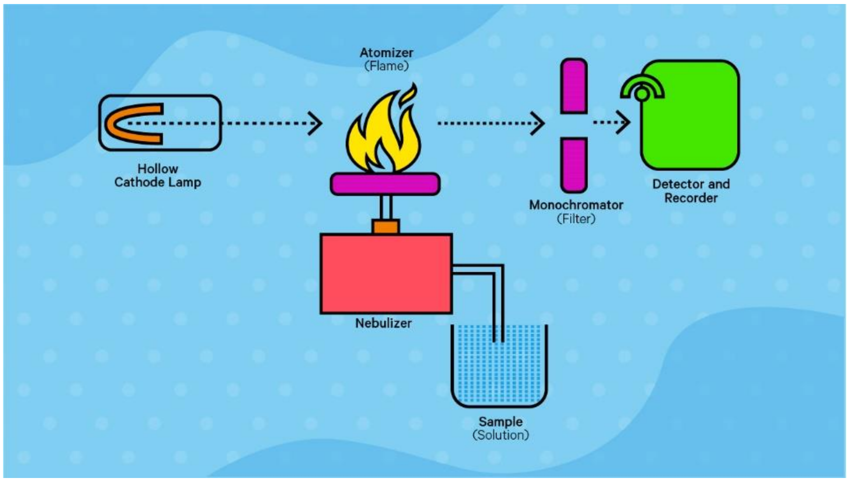

Figure 1: Schematic diagram of a typical atomic absorption spectrometer

Figure 2 below shows agilent Technologies Network Atomic absorption spectrometer SN-PGAA 500 used for the analysis. The quartz fiber filter containing the collected particulate matter from the market was carefully handled to avoid contamination. The filter was placed in a flask and treated with concentrated Nitric Acid and heated to dissolve the PM. The resulting solution was filtered to remove remaining filter paper fibers and then diluted to a precise volume (50mL) using deionized water.

The prepared liquid sample was extracted into the SN-PGAA 500 AAS instrument, where it was converted into a fine mist. The mist passed through a flame (atomization) and the high heat broke the liquid droplets and reduced the metal ions to free atoms. A hollow-cathode lamp (HCL) specific to the target metal emits light, which is directed through the atomic vapor. The free atoms absorb this light. A detector measured the intensity of the absorbed light. According to Beer's law, absorbance is directly proportional to the concentration of the metal in a sample.

A standard calibration curve was generated using known concentrations of the target metal (Pb, Zn, Fe, Mg) to determine the unknown concentration in the digested filter sample. The measured concentration in the liquid was converted to the concentration per unit volume of air (g/m^3) based on the air sampling flow rate. A blank filter paper was processed through the entire digestion and filtration procedure to account for any trace metal contaminants.

Figure 2: Agilent Technologies Network Atomic absorption spectrometer SN-PGAA 500

RESULTS AND DISCUSSION

This section presents the mass of particulate matter collected from the market; the distinct elements present in the sample and their concentration values. The mass of filter paper before it was mounted in the market for sample collection 0.8g, the mass increased to 0.96 after the sample was collected over a one-week period. Therefore, the mass of the sample collected is 0.16g.

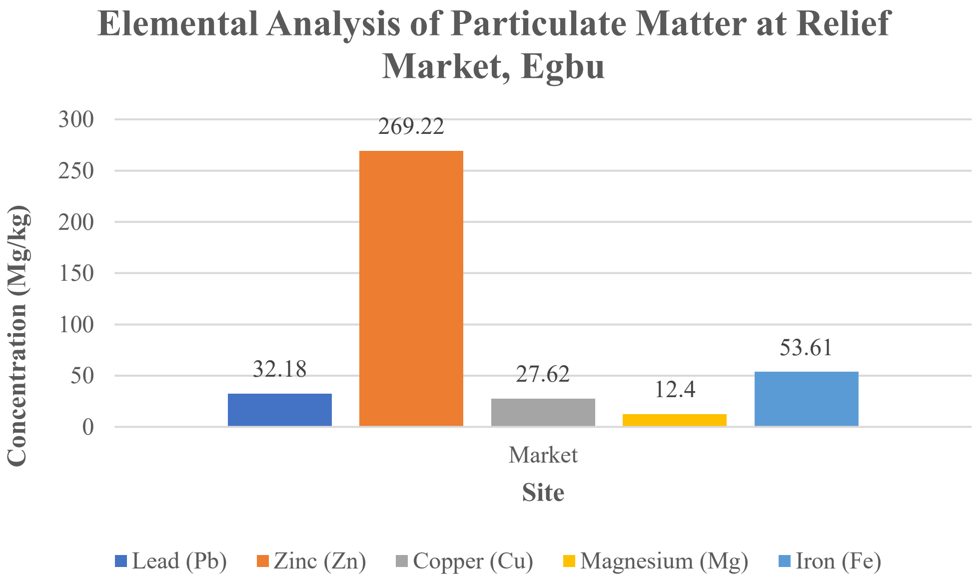

Figure 3: Elemental composition of Particulate matter at Relief market, Egbu

Figure 3 illustrates the elemental composition of particulate matter at Relief Market, Egbu, showing the concentrations of lead (Pb), zinc (Zn), copper (Cu), magnesium (Mg), and iron (Fe). Zinc recorded the highest concentration at 269.22 Mg/kg, indicating that it is the dominant element in the particulate matter. This elevated level of zinc may be associated with anthropogenic activities commonly observed in market environments, such as vehicular emissions, abrasion of galvanized materials, waste burning, and the handling of metal-containing goods.

Iron had the second-highest concentration with a value of 53.61 Mg/kg. This suggests a strong influence of soil and road dust resuspension, as well as possible contributions from construction activities, corrosion of metallic structures, and frequent movement of vehicles within and around the market area. The presence of iron is typical in busy commercial locations where human and mechanical activities are intense.

Lead showed a moderate concentration of 32.18 Mg/kg. Although its level is lower than that of zinc and iron, the presence of lead is of significant environmental and public health concern due to its toxicity, even at relatively low concentrations. Potential sources of lead in the market environment include vehicular emissions, discarded batteries, old paints, and improper waste disposal practices.

Copper was present at a concentration of 27.62 Mg/kg, which may be linked to the use and wear of electrical components, metal tools, and mechanical parts from vehicles and generators frequently operated in the market. Magnesium recorded the lowest concentration at 12.4 Mg/kg, indicating minimal contribution from crustal materials or limited anthropogenic input compared to the other elements.

CONCLUSION

The observed distribution of elements suggests that particulate matter pollution at Relief Market, Egbu is largely influenced by human activities related to traffic, trading, and waste management. The dominance of zinc and iron reflects intense commercial and mechanical operations, while the detectable level of lead highlights the need for environmental monitoring and appropriate control measures to reduce potential health risks to traders and the general public. A good number of studies have shown that some of these elements present from the analysis constitute serious health problems to man when they are inhaled or ingested, hence the need for safety measures to be put in place in order to protect traders in the market and individuals living within the environment from their harmful effects. Efforts are ongoing to extend the work to nearby locations.

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