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Integrated Experimental, Transport, and Risk Modeling Assessment of the Environmental Fate of $PM_{2.5}$ Bound Potentially Toxic Elements (PTEs) from Low-Temperature Thermal Wood Processing

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Abstract: Thermal modification of wood at low-level temperatures is increasingly adopted as a sustainable alternative to chemical preservation for improving dimensional stability and durability. However, thermochemical processing of biomass can emit fine particulate matter ($PM_{2.5}$) laden with potentially toxic elements (PTEs), creating significant risks to both environmental health and occupational safety. This study quantified $PM_{2.5}$-bound PTE emissions during low-temperature thermal wood processing and evaluated their atmospheric transport and health implications. A multi-phase methodology integrated gravimetric $PM_{2.5}$ sampling using PTFE filters, hotplate wet acid digestion, and determining the concentration of the PTEs using an Inductively Coupled Plasma Optical Emission Spectrometer. Ambient occupational $PM_{2.5}$ concentrations were calculated from filter mass differentials and sampled air volumes. A mechanistic Thermo–Particulate Metal Fate and Transport Model (TPM-FTM) was developed to couple thermochemical emission processes, particle–metal partitioning, atmospheric dispersion, deposition, and receptor exposure. Model performance was evaluated using statistical metrics, and uncertainty propagation was assessed through Monte Carlo simulation. Detectable concentrations of PTE-associated $PM_{2.5}$ were observed under low-temperature operational conditions, with size-resolved partitioning influencing atmospheric mobility and inhalation exposure. Occupational environments exhibited higher exposure levels compared with near-field community locations. Evaluations against established regulatory standards confirmed that exposure to these emissions poses no significant carcinogenic or non-carcinogenic health risks, with values generally falling within acceptable limits; localized emission intensities and ventilation conditions increased exposure variability. This study provides an integrated experimental–modeling framework for assessing particulate-bound metal emissions from thermally modified wood processing and offers evidence-based guidance for emission mitigation, occupational safety management, and regulatory evaluation.

Keywords: *$PM_{2.5}$; Potentially Toxic Elements (PTEs); Thermal Modification of Wood; ICP-OES; PTFE Filter Sampling; Thermochemical Emissions; Atmospheric Fate and Transport; Monte Carlo Simulation; Occupational Exposure; Environmental Risk Assessment; TPM-FTM Model.*

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I. INTRODUCTION

➢ *Overview*

This study covers the Introduction and Methodological Rationale; Research Design; Source Characterization, Analytical and Speciation, Fate and Transport Modeling, and Risk Assessment Phases; Description of the Study Area and Industrial Setting; Study Timeline; Population, Sampling Frame, and Receptors; Sampling Strategy; Gravimetric and Chemical Determination of $PM_{2.5}$; Source Characterization and Emission Measurement; Analytical Determination of Potentially Toxic Elements; Particle Size Distribution and Metal Partitioning; Meteorological Data Collection; Development of the Thermo–Particulate Metal Fate and Transport Model (TPM-FTM); Model Calibration, Validation, and Uncertainty Analysis; Exposure Pathways and Risk Metrics; Software, Data Analysis, and Statistical Methods;

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Ethical and Regulatory Considerations; Reliability, Validity, and Quality Assurance; and a Summary of the Methodological Workflow.

➢ *Introduction and Methodological Rationale*

The research methodology was designed to provide a scientifically rigorous and mechanistically integrated framework for investigating the levels of potentially toxic elements (PTEs) associated with $PM_{2.5}$ generated during low-level thermal modification of wood. The complexity of thermochemical emission processes, particulate–metal partitioning, atmospheric dispersion, and human exposure pathways necessitates a multi-phase methodological structure that links source characterization to environmental fate modeling and health risk assessment (Seinfeld & Pandis, 2016; Hinds, 1999).

The methodology is grounded in the Source–Pathway–Receptor (SPR) paradigm and environmental systems theory, which recognize that pollutant impacts cannot be fully understood without tracing contaminants from their point of origin through transport mechanisms to exposed receptors (USEPA, 2009; WHO, 2013). By integrating experimental measurements (gravimetric $PM_{2.5}$ determination, acid digestion, and ICP-OES analysis), atmospheric transport modeling (TPM-FTM), and regulatory-aligned risk assessment frameworks, the study ensures coherence between emission generation, environmental concentration fields, and exposure outcomes (Turner, 1994; Seinfeld & Pandis, 2016).

Furthermore, the adoption of standardized air sampling protocols and PTFE filter-based gravimetric analysis aligns with established particulate monitoring guidelines (USEPA, 2016; WHO, 2006). Elemental quantification was performed using a technique selected for its established multi-element capability, high sensitivity, and proven robustness when analyzing complex environmental matrices (Boss & Fredeen, 2004; Skoog et al., 2014). The application of USEPA-aligned non-carcinogenic and carcinogenic risk metrics ensures regulatory comparability health-based interpretability of exposure estimates (USEPA, 1989; USEPA, 2009).

The inclusion of model calibration, performance metrics such as RMSE and Nash–Sutcliffe Efficiency, sensitivity analysis, and Monte Carlo uncertainty propagation strengthens the predictive robustness of the Thermo–Particulate Metal Fate and Transport Model (TPM-FTM), ensuring that modeled outputs are statistically defensible and suitable for environmental decision-making (Nash & Sutcliffe, 1970; Saltelli et al., 2008; Helton & Davis, 2003).

In alignment with environmental systems theory and the source–pathway–receptor (SPR) paradigm, the methodology adopts a process-resolved, multi-scale, and risk-oriented approach that links industrial operational conditions to environmental concentration fields and human exposure outcomes. The research design integrates experimental measurements, analytical chemistry, atmospheric modeling, and environmental risk assessment tools into a unified workflow, operationalized through the proposed Thermo–Particulate Metal Fate and Transport Model (TPM-FTM). This integrative structure ensures methodological coherence between data generation, model development, validation, and interpretation, consistent with international best practices in environmental monitoring and regulatory science (USEPA, 2009; WHO, 2013; Seinfeld & Pandis, 2016).

This study adopts a comprehensive methodological approach integrating experimental procedures, analytical techniques, risk assessment models, and computational modeling tools to examine the emissions of PTEs in $PM_{2.5}$ generated during the thermal modification (TM) of wood. The methodology is structured to address three core objectives: (1) to determine the concentration of PTEs during TM, (2) to evaluate environmental and human health risks, and (3) to develop a fate and transport model for emitted pollutants. The methodological framework is explicitly derived from the theoretical and empirical foundations established in the background of the study, which emphasizes on the interdependence between thermochemical emission generation, particulate-bound metal behavior, atmospheric dispersion, and health-based risk assessment.

Overall, the methodological rationale is to establish an end-to-end analytical and modeling workflow capable of:

- Capturing thermochemical emission dynamics at the wood industrial source,
- Quantifying size-resolved particulate-bound metal concentrations,
- Simulating atmospheric transport and deposition behavior,
- Estimating occupational, community, and environmental exposure,
- Translating exposure levels into health-based risk indices.

This integrated approach advances conventional dispersion modeling by embedding thermochemical emission formation and metal speciation directly into transport and risk pathways, thereby improving mechanistic realism and policy applicability.

The methodology aims to achieve the following specific goals:

- *Quantify $PM_{2.5}$ Mass Concentrations*

Determine the concentration of fine particulate matter ($PM_{2.5}$) generated during thermal modification of wood using standardized gravimetric sampling techniques.

- *Determine PTE Concentrations in $PM_{2.5}$*

Analyze acid-digested particulate samples using ICP-OES to quantify potentially toxic elements (Pb, Cd, Zn) associated with fine particulates.

- *Characterize Source and Emission Dynamics*

Evaluate the influence of feedstock composition, thermal operating conditions, and emission characteristics on particulate-bound metal release.

- *Assess Particle–Metal Partitioning*

Investigate the distribution of metals across aerodynamic particle size fractions to inform transport behavior and inhalation exposure potential.

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- *Develop and Calibrate the TPM-FTM Model*

Construct and validate a thermochemically informed fate and transport model that integrates emission flux, atmospheric dispersion, deposition, and exposure modules.

- *Evaluate Environmental and Human Exposure Pathways*

Estimate inhalation and secondary ingestion exposures across occupational, near-field community, and environmental receptors within the SPR framework.

- *Conduct Health Risk Assessment*

Compute metrics in accordance with USEPA risk assessment guidelines.

- *Quantify Model Uncertainty and Sensitivity*

Apply sensitivity analysis and Monte Carlo simulation to assess variability and uncertainty in modeled concentration and risk estimates.

- *Ensure Analytical and Statistical Robustness*

Apply descriptive statistics, correlation analysis, multivariate analysis (PCA), and uncertainty evaluation to strengthen data interpretation and model reliability.

➢ *Study Design*

Focuses on quantitative experimental measurements with deterministic and probabilistic modeling techniques. The design is structured in four interlinked phases:

- *Source Characterization Phase:*

Quantification of the potential toxic elements (PTEs) concentrations in feedstock wood, stack emissions, and ambient particulates.

- *Analytical and Speciation Phase:*

The laboratory protocol employed ICP-OES to evaluate total metallic content and investigate phase partitioning, providing a high-resolution profile of elemental behavior in the biomass matrix.

- *Fate and Transport Modeling Phase:*

Development, calibration, and simulation of atmospheric dispersion, deposition, and environmental transfer using the TPM-FTM framework.

- *Risk Assessment Phase:*

Translation of modeled concentration fields into exposure doses and health-based risk indices using USEPA Environmental Risk Assessment (ERA) guidelines.

➢ *Description of the Study Area and Industrial Setting*

Logs and Lumber Limited (LLL), a leading timber-processing facility located within the Kumasi Metropolis of Ghana, served as the primary site for this investigation. Opposite the Asokwa Court and established in 1967, LLL is a designated Free Zone Enterprise and a cornerstone of the West African timber industry. The geographical coordinate is 6.67° N, 1.61° W. Data collection and modeling were centered at the industrial facilities of Logs and Lumber Limited (LLL) in specifically in the old boiler house (OBH) (see fig.2.0) Kumasi, Ghana. LLL's operational profile as a high-capacity timber processor makes it an ideal site for evaluating industrial emissions and material transport. The facility features a diverse production line, including plywood, veneer, and lumber, supported by a modern moulding department capable of processing 10,000 m^3 annually. Given its rigorous adherence to Chain of Custody (COC) standards and its management of thousands of hectares of natural timber concessions, the site provides a robust framework for analyzing the environmental and fate-and-transport dynamics of wood-based systems within a controlled, large-scale industrial setting. Selected based on proximity to residential or mixed-use areas and prevailing meteorological conditions conducive to particulate dispersion. This spatial characterization provides essential boundary conditions for atmospheric modeling and supports the identification of near-field and far-field receptor points, consistent with regulatory dispersion modeling practices (Turner, 1994; USEPA, 2009).

➢ *Timeline*

- Day 1– 13: Thermal processing and emissions sampling
- Day 14–28: Laboratory analysis and data processing
- The methodology was executed for close to a month.

➢ *Environmental and Occupational Receptors*

- *Receptors within the Source–Pathway–Receptor (SPR) Framework*

In accordance with the Source–Pathway–Receptor (SPR) conceptual framework, receptors in this study are defined as human and environmental entities that are plausibly exposed to potentially toxic elements (PTEs) through direct or indirect contact with particulate-bound emissions generated during thermally modified wood processing. The delineation of receptor categories is informed by proximity to emission sources, anticipated exposure pathways, and the spatial patterns of atmospheric dispersion and deposition predicted by the TPM-FTM model. This structured classification ensures that both acute and chronic exposure scenarios are systematically captured across occupational, community, and environmental domains, consistent with established environmental risk assessment practices (USEPA, 2009; WHO, 2013).

- *Occupational Receptors*

Occupational receptors comprise a defined cohort of fifteen (15) facility workers, including the boiler supervisor and operational personnel assigned to the old boiler house (OBH), thermal treatment chambers, and material handling zones. This group represents the population with the highest potential for direct inhalation exposure to freshly generated, fine and ultrafine particulate matter enriched with Potential toxic elements (PTEs), due to their proximity to emission sources and extended duration within enclosed or semi-enclosed workspaces.

Exposure characterization for this receptor group incorporates task-based time–activity patterns, ventilation conditions, and spatial variability in particulate concentrations, enabling acute and chronic inhalation doses. The occupational cohort is therefore treated as a sentinel population for evaluating the effectiveness of engineering controls, personal protective measures, and process-level

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emission mitigation strategies within the facility (WHO, 2013; USEPA, 2009).

- *Near-Field Community Receptors*

Near-field community receptors are defined as boiler-house-use zones located within a 50-meter radial buffer of the boiler tank and associated emission points. This spatial boundary is established based on preliminary dispersion modeling and regulatory guidance, which indicate that steep concentration gradients and peak deposition rates typically occur within the near-field zone of industrial point sources (Turner, 1994; USEPA, 2009).

This receptor category captures vulnerable sub-populations, including adults below 22 years, elderly, and individuals with pre-existing respiratory conditions, who may experience heightened sensitivity to particulate-bound metal exposure. Risk characterization for this group integrates continuous exposure scenarios, reflecting residential occupancy patterns and outdoor–indoor air exchange dynamics, thereby enabling the evaluation of both chronic inhalation risk and secondary ingestion pathways associated with deposited particulates in household environments.

- *Environmental Receptors*

Environmental receptors encompass abiotic and biotic components of the local ecosystem that serve as sinks or secondary sources of PTEs following atmospheric deposition. These include:

- ✓ Soil surfaces within the ash handling and floor chamber zones, where thermally generated residues are temporarily stored before transport and field application. These soils are critical receptors for assessing metal accumulation, leaching potential, and secondary resuspension into the air column.
- ✓ Vegetation plots located approximately 100 meters from the OBH, which are positioned within the predicted zone of elevated particulate fallout. Vegetation functions as both a passive collector of airborne metals and a potential transfer medium into terrestrial food webs.
- ✓ Surface water bodies and drainage channels situated within 50 to 100 meters of the OBH, which receive runoff and wet-deposited particulates. These receptors are essential for evaluating hydrological transport, sediment-bound metal accumulation, and potential impacts on aquatic biota.

The inclusion of these environmental compartments enables a multi-media exposure assessment, capturing cross-compartmental transfer pathways such as air–soil–plant and air–water–sediment linkages. This approach aligns with integrated environmental risk assessment principles and supports the evaluation of long-term ecological impacts and cumulative contaminant loading (Alloway, 2013; WHO, 2013).

- *Rationale for Receptor Delineation*

The stratification of receptors across occupational, community, and environmental domains reflects the gradient of exposure intensity and pathway diversity inherent in industrial emission scenarios. By explicitly linking receptor locations to modeled dispersion and deposition patterns, the study ensures that risk estimates are spatially and mechanistically grounded, enhancing both the scientific validity and regulatory relevance of the findings. This receptor framework also facilitates scenario-based evaluation of mitigation measures, such as improved ventilation, relocation of ash handling areas, and vegetative buffering, by enabling comparative risk projections across receptor classes (USEPA, 2009; Turner, 1994).

II. SAMPLING STRATEGY

➢ *Sampling Materials and Procedures*

Airborne particulate sampling and occupational safety during field operations were conducted using a suite of standardized, high-integrity materials and instruments selected to ensure analytical reliability, regulatory compliance, and personnel protection. The primary sampling and safety materials included:

- Polytetrafluoroethylene (PTFE) membrane filters (PTFE/B) ($0.45\ \mu m$; diameter, $47\ mm$) for sampling of $PM_{2.5}$, selected for their chemical inertness, low metal background, high particulate retention efficiency, and compatibility with acid digestion and ICP-OES analysis.
- Medium-volume air sampler (LECKEL GmbH), operated at a nominal flowrate of $2.3\ m^3h^{-1}$, acquired from Ghana Atomic Energy Commission (GAEC), ensuring instrument traceability and standardized performance.
- Cyclone size-selective inlet ($2.3\ m^3h^{-1}$) for the aerodynamic separation of particulate fractions, enabling the isolation of respirable and inhalable particle classes relevant to exposure and fate and transport modeling.
- Heavy-duty electrical extension board (2.5 mm conductor diameter) to maintain a stable and uninterrupted power supply under industrial field conditions.
- Personal protective equipment (PPE), including respiratory gas masks, chemical splash goggles, industrial helmets, heavy-duty flexible gloves, and certified industrial safety boots, to ensure compliance with occupational health and safety standards.
- Laboratory-grade polyethylene and rubberized packaging bags, pre-cleaned and acid-rinsed, for contamination-free storage and transport of exposed and blank filters.

The selection of PTFE filters and medium-volume sampling systems aligns with international air quality monitoring protocols, which recommend inert filter media and controlled flow sampling for trace metal analysis in particulate matter (USEPA, 2009; WHO, 2013).

➢ *Sampling Protocol and Operational Parameters*

Ambient and occupational air sampling was conducted using a medium-volume gravimetric and metal-collection protocol designed to balance temporal resolution, filter loading capacity, and analytical sensitivity. A Leckel low-volume sampler was utilized at a calibrated flow rate of $2.3\ m^3h^{-1}$. To maintain volumetric accuracy, flow rates were verified against a primary flow standard both prior to and immediately following each sampling session.

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The sampling campaign followed a cyclic operational schedule synchronized with facility activity patterns:

- Total field deployment duration: 12 hours per sampling day
- Active sampling intervals: Eight (8) periods of 2 hours each
- Intermittent rest periods: 1-hour intervals between sampling cycles to prevent filter overloading, stabilize flow conditions, and accommodate machine cooling
- Effective sampling duration: Approximately 8 hours of cumulative air collection during operational hours, with 3–4 hours allocated for equipment stabilization and breaks

This intermittent sampling strategy was adopted to capture process-driven emission variability while preserving filter integrity and ensuring sufficient particulate mass for trace metal quantification.

➢ *Spatial and Temporal Sampling Design*

A stratified spatial–temporal sampling framework was implemented to ensure representativeness across emission gradients and meteorological conditions, consistent with best practices in atmospheric dispersion studies and model validation protocols (Turner, 1994; USEPA, 2009).

Sampling strata included:

- Upwind and downwind transects, established relative to prevailing wind direction to distinguish background metal concentrations from facility-attributable emissions.
- Near-field receptor locations (≤50 m), positioned within the zone of steep concentration gradients and peak particulate deposition.
- Far-field receptor locations (>100 m), selected to assess plume dilution, long-range transport, and secondary exposure potential.
- Operational period sampling, conducted during active thermal processing cycles to capture maximum emission intensity.
- Source-proximal sampling at the old boiler cylinder, where operational pressure conditions were monitored at approximately 5 bar (≈5000 mbar) to contextualize thermochemical emission behavior and support process–emission coupling within the TPM-FTM framework.

This stratification enabled the construction of spatial concentration profiles and temporal emission signatures, providing a robust empirical basis for calibrating atmospheric dispersion parameters and validating modeled concentration fields across multiple transport regimes.

III. SAMPLE PRESERVATION AND STORAGE

➢ *Preservation and Quality Control Protocol for PTFE Filter-Based $PM_{2.5}$ Sampling*

Polytetrafluoroethylene (PTFE) membrane filters were selected for $PM_{2.5}$ collection due to their chemical inertness, low hygroscopicity, minimal background metal content, and compatibility with gravimetric and elemental analysis (e.g., ICP–OES). PTFE filters are widely recommended for trace metal determination in atmospheric particulate monitoring because they exhibit low artifact formation relative to cellulose-based filters and possess high thermal and chemical stability (USEPA, 2016; Chow et al., 2005).

Sampling was conducted in the logs and lumber industrial setting at Kumasi–Asokwa using size-selective $PM_{2.5}$ inlets designed to meet aerodynamic cut-point specifications (50% efficiency at 2.5 µm). Such inlets ensure the collection of respirable fine particles consistent with regulatory definitions of $PM_{2.5}$ (WHO, 2021).

Immediately after sampling, filters were retrieved using non-metallic, acid-cleaned forceps to prevent trace metal contamination. The avoidance of metallic handling tools is a recognized contamination control measure in trace-level environmental analysis (Miller & Miller, 2018).

Each filter was placed into a pre-cleaned rubberized packaging bag and hermetically sealed to limit exposure to ambient particulates, gaseous contaminants, and moisture. Secondary wrapping in aluminum foil provided additional protection against photochemical reactions and electrostatic interference. Photo-oxidation and electrostatic effects can alter particle composition or redistribute deposited particulates across the filter surface, potentially compromising analytical integrity (Chow et al., 2005).

Comprehensive labeling, including sample ID, location, date/time, flow rate, and operator initials, ensured traceability within a documented chain-of-custody framework, consistent with environmental monitoring quality systems (USEPA, 2016).

➢ *Transport and Environmental Stabilization*

Preserved filters were transported in a rigid, insulated container to maintain structural integrity and minimize mechanical disturbance. Protection from direct sunlight and elevated temperature is critical because semi-volatile particulate components may volatilize under thermal stress, leading to mass loss (Seinfeld & Pandis, 2016).

Desiccant sachets were included to control humidity and prevent condensation. Hygroscopic growth and phase changes in aerosol components, particularly ammonium nitrate and certain organic species, are highly sensitive to relative humidity (Seinfeld & Pandis, 2016). Condensation can redistribute dissolved metals across the filter surface, thereby affecting both gravimetric and elemental results.

Transport time did not exceed 12 hours, minimizing holding time before laboratory conditioning. Short holding periods are recommended to reduce chemical transformation of reactive particulate constituents (USEPA, 2016).

➢ *Laboratory Receipt and Pre-Digestion Storage*

Upon laboratory receipt, samples were logged into a registry and verified against chain-of-custody documentation. Documentation integrity is essential for defensibility and regulatory compliance (ISO 17025:2017).

Filters were stored at 4 °C in a designated metal-free storage environment to suppress volatilization of semi-volatile

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species and minimize contamination risk. Low-temperature storage slows chemical reactions and phase transitions in particle-bound constituents (Seinfeld & Pandis, 2016). Restricted access further reduced cross-contamination risk, consistent with trace-level analytical quality assurance practices.

➢ *Gravimetric Determination of $PM_{2.5}$ and the Characteristics of PTFE Filter*

Gravimetric analysis is the reference method for $PM_{2.5}$ determination and forms the basis of regulatory air quality standards worldwide (USEPA, 2016; WHO, 2021). The method relies on accurate mass difference measurement between pre- and post-sampling filter weights under controlled environmental conditions (20 –23 °C; 30–40% RH recommended).

The mass of $PM_{2.5}$ (see equation 3.1) was calculated as:

$$Mass\ of\ the\ PM_{2.5} fine\ particles\ = M_{post\ PTFE\ filter} - M_{pre\ PTFE\ filter} \tag{3.1}$$

This calculation assumes that mass change is solely due to particulate deposition. However, filter artifacts may introduce bias. Therefore, in practice, this assumption may be influenced by filter artifacts, which can be either positive or negative, leading to apparent mass gains or losses that are not exclusively due to $PM_{2.5}$ loading.

PTFE filters are preferred because they exhibit:

- Low moisture uptake
- Minimal organic carbon adsorption compared to quartz filters
- Chemical resistance during acid digestion for trace metal analysis

These properties enhance suitability for combined gravimetic–ICP analysis workflows (Chow et al., 2005).

- *Positive Artifact (Apparent Mass Gain)*

Positive artifacts occur when gaseous semi-volatile compounds adsorb or condense onto the filter surface, artificially increasing measured mass. Semi-volatile organic compounds (SVOCs), nitric acid vapor, and other acidic gases may partition onto filter substrates depending on temperature and humidity conditions (Seinfeld & Pandis, 2016).

Although PTFE filters are relatively inert, adsorption of gaseous species can still occur under favorable thermodynamic conditions, particularly at low temperatures or high relative humidity. Such uptake leads to systematic overestimation of $PM_{2.5}$ mass (Chow et al., 2005).

Field blanks and controlled conditioning procedures are standard QA/QC tools used to quantify and correct for positive artifacts (USEPA, 2016).

- *Negative Artifact (Apparent Mass Loss)*

Negative artifacts arise from volatilization of semi-volatile particulate components during or after sampling. Ammonium nitrate (NH_4NO_3) and certain organic fractions are particularly prone to dissociation and evaporation when exposed to changes in temperature and pressure (Seinfeld & Pandis, 2016).

Thermodynamically, ammonium nitrate equilibrium:

$$NH_4NO_{3\,(s)} \rightleftharpoons NH_{3\,(g)} + HNO_{3\,(g)}$$

is strongly temperature dependent, making $PM_{2.5}$ mass sensitive to environmental transitions between field and laboratory conditions. Negative artifacts can lead to underestimation of $PM_{2.5}$ mass and, in extreme cases, negative net mass differences. Controlled equilibration and standardized weighing conditions mitigate this risk (USEPA, 2016).

Conversely, a negative artifact is observed when the post-sampling mass of the PTFE filter is equal to or lower than the pre-sampling mass, resulting in an apparent reduction in filter mass. This observation is primarily attributed to the volatilization of semi-volatile particulate components, which transition from the solid to liquid phase into the gas phase under elevated temperatures, particularly ammonium nitrate ($NH_4NO_{3\,(s)}$) and certain organic compounds from the filter during or after sampling (Chow et al., 2005; US EPA, 2016). Semi-volatile species are thermodynamically unstable and may dissociate or evaporate when environmental conditions shift, especially during transport and equilibration before weighing (Tsai & Perng, 1998; Solomon et al., 2014). Variations in temperature, pressure, and relative humidity between the sampling site and the weighing laboratory can exacerbate this loss, promoting the decomposition of ammonium nitrate into gaseous ammonia ($NH_{3\,(g)}$) and nitric acid ($HNO_{3\,(g)}$), thereby reducing the retained particulate mass (Hering & Cass, 1999; Chow et al., 2005).

Negative artifacts may consequently partial loss of semi-volatile components from the filter surface before gravimetric weighing results in negative bias in $PM_{2.5}$ mass measurements (US EPA, 2016; EN 12341, 2014). In extreme cases, this process can produce anomalously low or even negative net $PM_{2.5}$ values after blank correction, underscoring the necessity for stringent environmental control during filter conditioning, handling, and weighing (Chow et al., 2006).

The occurrence of both positive artifacts (e.g., adsorption of water vapor or organic vapors) and negative artifacts highlights the critical importance of comprehensive QA/QC in gravimetric $PM_{2.5}$ analysis (Chow et al., 2005; Solomon et al., 2014). Standardized conditioning protocols typically 23 °C, 40 % relative humidity for at least 24h recommended to ensure mass stability before weighing (US EPA, 2016; EN 12341, 2014). In this study, the use of PTFE filters, controlled conditioning environments, field and laboratory blanks, and a high-precision microbalance (±1 µg sensitivity) was intended to minimize such artifacts. Nonetheless, any observed increase or decrease in filter mass beyond acceptable QA/QC limits was interpreted within the framework of potential sampling artifacts rather than as a direct representation of true ambient $PM_{2.5}$ concentrations.

By explicitly acknowledging the influence of sampling artifacts, the gravimetric results are interpreted with an appropriate level of analytical caution and statistical confidence. This approach strengthens the scientific credibility of the findings and ensures that conclusions regarding particulate pollution levels are supported by established methodological standards and defensible analytical reasoning (US EPA, 2016; Solomon et al., 2014).

IV. CONCENTRATION DETERMINATION OF $PM_{2.5}$

➢ *Concentration Determination of $PM_{2.5}$ Particles in relation to the of PTFE Filter*

$PM_{2.5}$ concentrations in ambient air were determined gravimetrically, calculating the mass of particulate matter captured on PTFE filters relative to the total volume of air sampled. This procedure aligns with internationally recognized reference methods for fine particulate monitoring, specifically adhering to the US EPA Federal Reference Methods (FRM) (40 CFR Part 50, Appendix L).

Gravimetric filter-based measurement remains the regulatory gold standard for $PM_{2.5}$ quantification because it directly measures particle mass under controlled temperature and humidity conditions, thereby minimizing systematic bias (USEPA, 2016; WHO, 2021).

➢ *Volume of Air Sampled*

The volume of air drawn by the sampler, denoted as (V_a), cumulative sample volume was determined by integrating the sampler's calibrated flow rate over the total exposure period. This volume, recorded in cubic meters (m³), represents the total air mass subjected to gravimetric filtration and subsequent elemental analysis, as shown in Equation (3):

Volume of air drawn by the sampler unto the filter paper

(PTFE) $(V_a) = Q \times t$ (4.1)

Where:

Q = the average volumetric flow rate of the sampler (m³/h), and

t = the total sampling time (h).

Accurate flow rate calibration is critical because errors in Q propagate directly into concentration calculations. Flow calibration was performed using traceable calibration devices consistent with air monitoring best practices (USEPA, 2016).

Maintaining stable flow ensures isokinetic sampling and minimizes particle loss due to turbulence or inlet inefficiency (Hinds, 1999).

➢ *Mass of $PM_{2.5}$ Collected on the PTFE Filter*

The mass of $PM_{2.5}$ collected on the PTFE filter paper, $m_{PM_{2.5}}$ (see equation 3.1), was obtained from gravimetric analysis as a results of determining the difference between the post-sampling and pre-sampling filter masses. This mass represents the total $PM_{2.5}$ captured from the sampled air volume.

In equation 3.1, this mass difference method assumes that the observed change reflects true particulate deposition. However, as established in atmospheric sampling literature, filter artifacts such as volatilization losses or gaseous adsorption may introduce bias (Chow et al., 2005; Seinfeld & Pandis, 2016). PTFE filters are preferred for combined gravimetric and elemental analysis due to their chemical inertness, low hygroscopicity, and compatibility with acid digestion for trace metal determination (USEPA, 2016).

➢ *Concentration of $PM_{2.5}$ in Ambient Air*

The ambient air concentration of $PM_{2.5}$, denoted as C_a, was calculated by normalizing the collected $PM_{2.5}$ mass to the volume of air sampled, as given in Equation (4):

Concentration of air ($PM_{2.5}$) drawn unto the filter paper

(PTFE) (($C_a) = \frac{c_{PM2.5}}{V_a}$ (4.2)

Where:

C_a = the concentration of $PM_{2.5}$ in ambient air (µg/dm³),
$m_{PM_{2.5}}$ = the mass of $PM_{2.5}$ collected on the PTFE filter (mg), and
V_a = the total volume of air drawn through the sampler (m³).

This calculation assumes uniform particle collection efficiency across the $PM_{2.5}$ size fraction and negligible particle loss within the sampling system. Size-selective inlets designed for a 2.5 µm aerodynamic cut-point ensure compliance with regulatory $PM_{2.5}$ definitions (WHO, 2021).

The calculated $PM_{2.5}$ concentration represents the average ambient particulate concentration over the sampling period. Any deviation in measured concentration may be influenced by sampling artifacts, including volatilization losses, adsorption of gaseous species, or flow rate variability. Consequently, accurate determination of both $m_{PM_{2.5}}$ and $V_a$is critical for reliable estimation of ambient $PM_{2.5}$ levels (Hinds, 1999).

- *Unit Conversion*

For reporting consistency:

$$1\ \mu g L^{-1} = 1000\ \mu g m^{-3}$$

Standardization of units facilitates comparison with regulatory thresholds and published literature.

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V. ACID DIGESTION PROCEDURE

A. Acid Digestion Procedure for $PM_{2.5}$ Samples Collected on PTFE Filters (Hotplate (Open-Vessel) Wet Acid Digestion of PTFE Filters for Trace Metal Analysis

The determination of particulate-bound potentially toxic elements (PTEs) was preceded by acid digestion of $PM_{2.5}$ samples collected on polytetrafluoroethylene (PTFE) membrane filters. Acid digestion is widely recognized as a prerequisite step for converting particulate-bound metals into a measurable aqueous phase prior to spectrometric analysis (USEPA, 1996; ISO 11466, 1995). A wet acid digestion method using concentrated nitric acid (HNO_3) was employed to solubilize metal constituents embedded within the particulate matrix and to generate clear aqueous extracts suitable for instrumental analysis, consistent with established environmental sample preparation protocols (Skoog et al., 2018; Welz & Sperling, 1999).

Prior to digestion, all glassware were rigorously acid-cleaned by soaking in 10 % ($^{v}/_{v}$) nitric acid, followed by thorough rinsing with deionized water and air-drying in a contamination-free environment. Acid washing of laboratory ware is a standard contamination control practice in trace metal analysis, significantly reducing background contributions and memory effects (APHA, 2017; Taylor, 1987). The use of high-resistivity deionized water further minimizes ionic contamination and ensures analytical integrity during ultra-trace determinations (Harris, 2016).

Each PTFE filter was carefully transferred using acid-washed plastic forceps into a clean 50 mL borosilicate glass beaker to avoid extraneous metal contamination. PTFE is preferred for $PM_{2.5}$ sampling due to its chemical inertness, low metal background, and high thermal stability (Chow, Watson, & Lowenthal, 2005). 10 mL nitric acid (concentrated) was added to the beaker. Nitric acid is commonly used in environmental digestion procedures because of its strong oxidizing properties and effectiveness in dissolving most environmentally relevant metals without introducing interfering species (USEPA Method 3050B; Skoog et al., 2018). The sample was allowed to stand for several minutes to permit complete pre-wetting of the filter matrix and initial dissolution of readily soluble metal fractions, a step that enhances digestion efficiency and moderates exothermic reactions during heating (Welz & Sperling, 1999).

The beaker was subsequently placed on a temperature-controlled hotplate and heated gently at approximately 95 °C under reflux conditions or within a covered digestion basin to prevent sample loss due to splattering. Controlled heating below the boiling point of nitric acid is recommended in open-vessel digestion to ensure progressive oxidation of organic matter while minimizing volatilization losses of semi-volatile metal species (USEPA Method 3050B; ISO 11466, 1995). The digestion was maintained for approximately 3 hours, during which the acid solution gradually decomposed the particulate matrix and liberated metal constituents into solution. Vigorous boiling was avoided to reduce analyte loss and maintain controlled reaction kinetics, consistent with good laboratory practice in wet digestion procedures (APHA, 2017).

Following digestion, the beaker was taken from the hotplate and allowed to cool naturally for approximately 20 minutes. Controlled cooling ensures thermal equilibration, reduces the risk of pressure-related splashing, and prevents volumetric inaccuracies during subsequent quantitative transfer (Harris, 2016).

The digested extract was quickly transferred into a 50 mL volumetric flask. To ensure complete recovery of dissolved metals, the digestion beaker was rinsed three times with 5 mL aliquots of ultrapure water, and each rinse was added to the volumetric flask. Quantitative transfer and multiple rinsing steps are essential components of gravimetric and volumetric analytical protocols to minimize systematic error and ensure mass balance integrity (Skoog et al., 2018; Taylor, 1987). The combined solution was then diluted to the calibration mark with ultrapure water and homogenized by gentle inversion.

The resulting digestate served as the analytical matrix for elemental quantification via Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES). This technique was selected for its established multi-element capabilities, high sensitivity, and proven robustness in characterizing trace metals within complex environmental matrices (Boss & Fredeen, 2004; Welz & Sperling, 1999). Procedural blanks were prepared using identical digestion steps without filters to assess background contamination and to support quality assurance and quality control (QA/QC), in accordance with standard environmental analytical guidelines (USEPA, 1996; APHA, 2017).

Overall, this digestion protocol ensured effective solubilization of particulate-bound metals while maintaining compatibility with downstream spectrometric analysis and quantitative risk assessment modeling. Immediate sealing of containers minimized atmospheric contamination and evaporative losses, thereby preserving analyte stability and supporting defensible environmental data generation consistent with regulatory monitoring frameworks (USEPA, 2007; Eurachem, 2014).

B. Concentration of Fine ($PM_{2.5}$) Particles in Solution after Acid Digestion of PTFE Filters

Following the gravimetric determination of $PM_{2.5}$ mass (equation 5.1), the PTFE filters containing the collected fine particulate matter were subjected to acid digestion to transfer the particulate-bound constituents into an aqueous phase suitable for instrumental analysis. Post-digestion, the resulting extract was quantitatively transferred and diluted to a fixed volume with deionized water. This standardization ensured matrix consistency and reproducibility, optimizing the samples for subsequent ICP-OES analysis.

The volume of deionized water used for dilution of the acid-digested sample is denoted as (V_{dw}) and was measured in milliliters (mL). For concentration calculations, all volumes were converted to liters (L) using the standard conversion:

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$$1\ mL = 1\ \times 10^{-3}\ L = 1000\frac{\mu g}{L} = 1\ ppb$$

These units align with trace metal reporting conventions in environmental monitoring (Skoog et al., 2018).

➢ *Mass of $PM_{2.5}$ in the Acid Digested Sample*

The mass of $PM_{2.5}$ collected on the PTFE filter paper, denoted as $m_{PM_{2.5}}$, mass was determined gravimetrically by calculating the net difference between the post-sampling filter weight. This methodology aligns with internationally recognized reference standards for $PM_{2.5}$ determination, specifically adhering to the gravimetric protocols established by the U.S. Environmental Protection Agency (USEPA, 40 CFR Part 50) and the European standard EN 12341, which define filter-based mass measurement as the primary reference technique for ambient particulate monitoring.

Before weighing, filters were conditioned under controlled temperature (23 °C) and relative humidity (40 %) conditions for at least 24 hours to achieve hygroscopic equilibrium and minimize moisture-induced mass variability. Conditioning and equilibration are critical because $PM_{2.5}$ particles and filter media can adsorb or desorb water depending on ambient humidity, potentially introducing systematic bias into mass determination (Chow et al., 2005; USEPA, 2016). Gravimetric measurements were performed using a calibrated microbalance with a sensitivity of at least ±1 µg, consistent with trace-level particulate monitoring requirements (ISO 15767; EN 12341). The net particulate mass was therefore calculated using equation 3.1.

Where $M_{post\ PTFE\ filter}$ is the conditioned post-sampling filter mass and $M_{pre\ PTFE\ filter}$ is the conditioned pre-sampling filter mass. This differential measurement approach minimizes systematic instrument bias and accounts for intrinsic filter mass variability, thereby improving analytical accuracy and repeatability (Hinds, 1999; Harris, 2016).

PTFE membrane filters are widely used in fine particulate sampling due to their low hygroscopicity, chemical inertness, minimal background metal content, and compatibility with both gravimetric and elemental analysis (Chow et al., 2005). Their dimensional and thermal stability ensure that the measured mass difference predominantly reflects collected particulate matter rather than filter degradation or chemical alteration during sampling.

The gravimetrically determined mass represents the total $PM_{2.5}$ fraction captured from the sampled air volume and is assumed to be quantitatively transferred into solution following complete acid digestion. Under controlled wet acid digestion conditions using concentrated nitric acid, PTFE filters remain chemically inert while particulate-bound constituents are solubilized into the aqueous phase, enabling mass conservation between the solid and liquid analytical stages (USEPA Method 3050B; Skoog et al., 2018). The assumption of quantitative transfer is further supported by rigorous rinsing and volumetric recovery steps designed to prevent analyte loss and maintain mass balance integrity (Taylor, 1987).

From a metrological perspective, the gravimetric determination of $m_{PM_{2.5}}$ constitutes the foundational quantitative parameter linking atmospheric particulate sampling to subsequent chemical characterization, exposure modeling, and risk assessment. Any uncertainty associated with balance precision, filter handling, conditioning variability, or static charge effects directly propagates into calculated ambient concentrations and derived exposure metrics. Therefore, strict adherence to standardized gravimetric protocols ensures traceability, reproducibility, and regulatory defensibility of $PM_{2.5}$ mass measurements (USEPA, 2016; Eurachem, 2014).

In summary, the gravimetric mass difference method provides a scientifically robust and internationally validated basis for determining $m_{PM_{2.5}}$ representing the total fine particulate burden collected on the PTFE filter and subsequently transferred into solution for elemental analysis and environmental health assessment.

➢ *Concentration of $PM_{2.5}$ in the Digested Solution*

The concentration of $PM_{2.5}$ in the digested solution (C_{FS})was calculated using Equation (5.1) ;

$$C_{FS} = \frac{m_{PM_{2.5}}}{V_{dw}} \tag{5.1}$$

Where:

C_{FS} is the concentration of $PM_{2.5}$ in the digested solution (mg/L),
$PM_{2.5}$ is the mass of $PM_{2.5}$ collected on the filter (mg), and
V_{dw} is the final volume of the digested solution (L).

This calculation assumes quantitative transfer of particulate matter from the PTFE filter into the aqueous phase during digestion, an assumption supported by the chemical inertness, thermal stability, and low metal background characteristics of polytetrafluoroethylene (PTFE) membranes (Chow et al., 2005; Hinds, 1999). PTFE is resistant to concentrated mineral acids, including nitric acid, and does not readily leach or adsorb trace metals under controlled digestion conditions, thereby minimizing analyte loss or contamination (Skoog et al., 2018). The application of strong oxidizing acids such as HNO_3 promotes effective solubilization of particulate-bound metals and supports near-quantitative recovery when appropriate heating and rinsing protocols are followed (USEPA Method 3050B; ISO 11466). Under these controlled conditions, the assumption of complete analyte transfer from the solid filter matrix to the liquid digest is consistent with established environmental digestion procedures (Eurachem, 2014).

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For ease of interpretation and alignment with environmental and instrumental reporting standards, the calculated concentrations were converted using the following relationships:

$$1\frac{mg}{L} = 1000\frac{\mu g}{L} = 1\ ppb$$

In dilute aqueous solutions, particularly in environmental for sample digest matrices with densities approximating 1 kg/L, mg/L is numerically equivalent to ppm and µg/L to ppb, facilitating standardized trace-level reporting (Skoog et al., 2018; Harris, 2016). These units are widely adopted in trace metal analysis, regulatory monitoring, and instrumental calibration frameworks, ensuring comparability with detection limits, guideline thresholds, and published literature (WHO, 2017; USEPA, 2016).

The determination of $PM_{2.5}$ concentration in the digested solution therefore provides a critical analytical bridge between gravimetric particulate mass measurement and subsequent chemical characterization (e.g., trace metals or ionic species). Because concentration is directly dependent on both measured mass and final dilution volume, accurate volumetric measurement using calibrated glassware, strict unit conversion, and meticulous handling of PTFE filters are essential to minimize propagated uncertainty (Eurachem, 2014). Errors in volume determination, incomplete transfer, or contamination can systematically bias elemental concentration estimates and, consequently, affect downstream exposure modeling and health risk assessment calculations (Taylor, 1987).

By integrating quantitative digestion efficiency, standardized unit conversion, and rigorous volumetric control, the calculated solution concentrations reliably reflect the particulate burden captured during sampling and maintain analytical traceability within internationally recognized environmental monitoring frameworks.

C. Post-Digestion Storage and Backup Preservation

Following digestion, the resulting solutions were maintained in a refrigerated environment at 4 °C to preserve chemical stability prior to instrumental quantification. Refrigerated storage slows redox reactions and precipitation processes in metal-containing solutions (Miller & Miller, 2018). To support analytical reliability and auditability, aliquots of each digested sample were retained as backup samples, providing a reserve for:

- Re-analysis in the event of instrument malfunction or anomalous results
- Inter-laboratory comparison or external quality assurance checks
- Verification of calibration and recovery performance over time

These retained samples formed part of the study's internal quality control (QC) system, ensuring reproducibility and long-term data integrity. Consistent with ISO 17025 quality management principles established by the International Organization for Standardization.

D. Quality Control and Contamination Prevention Measures

The quality assurance framework included:

- Field and laboratory blanks to quantify background contamination
- Acid-cleaned, metal-free containers
- Powder-free nitrile gloves to prevent trace contamination

These procedures align with best practices for environmental trace metal analysis (USEPA, 2016; ISO 17025).

The multi-layer preservation and contamination control strategy safeguarded both the physical integrity of $PM_{2.5}$ samples and the chemical stability of particle-bound Pb, Cd, and Zn.

Retention of backup digests strengthened reproducibility, auditability, and regulatory defensibility of analytical outputs critical for subsequent atmospheric modeling, exposure estimation, and risk assessment.

The retention of backup digested samples further strengthens the study's quality control architecture by enabling verification, reproducibility testing, and audit trails, consistent with best practices in environmental monitoring and regulatory science.

E. Instrumentation

- *Instrumental Working Principles of Inductively Coupled Plasma–Optical Emission Spectrometer (ICP-OES)*

As illustrated in Fig. 3.0, the analytical process proceeds through sequential and highly controlled physicochemical stages: (1) sample introduction and aerosol generation, (2) plasma-based atomization and excitation, and (3) wavelength dispersion and optical detection (Hou & Jones, 2000; Becker, 2007). The robustness of these stages underpins the technique's wide acceptance in environmental metal analysis, particularly for trace quantification of Pb, Cd, Zn, and other potentially toxic elements in air, water, and soil matrices (Montaser, 1998; Thomas et al., 2012).

Figure 3.0 is a multi-element analytical technique widely used for the quantitative determination of trace and major elements in environmental samples (ambient air samples). In this study, ICP-OES was employed to determine the concentrations of potentially toxic elements (PTEs) associated with $PM_{2.5}$ collected from air particulates (ambient air particulates) generated during low-level thermal modification of wood.

The high-temperature atomic emission technique is recognized as a gold standard for multi-element analysis in environmental, industrial, and biological matrices. The method is founded on well-established principles of atomic excitation and optical emission spectroscopy, offering high sensitivity, wide dynamic range, and excellent analytical precision (Skoog et al., 2018; Welz & Sperling, 1999).

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- *Sample Introduction and Aerosol Formation*

As shown in Fig. 3.0 (Stage 1–2), the acid-digested $PM_{2.5}$ (ambient air) extract is aspirated into a nebulizer, where it is converted into a fine aerosol by argon gas flow. The aerosol then enters the spray chamber, which removes large droplets through inertial separation, allowing only fine droplets to pass into the plasma torch. This size selection is essential for:

- ✓ Stable plasma loading
- ✓ Reduced matrix effects
- ✓ Improved signal precision

Efficient aerosol transport enhances analytical repeatability and minimizes transport-related signal fluctuation (Boss & Fredeen, 2004). The use of argon as a carrier gas ensures chemical inertness and prevents unwanted secondary reactions before plasma introduction.

- *Plasma Generation, Desolvation, Atomization, and Excitation*

In Fig. 3.0 (Quartz Torch Region), argon gas flows through concentric quartz tubes positioned within a radiofrequency (RF) induction coil. When RF energy (typically 27–40 MHz) is applied, an oscillating electromagnetic field ionizes the argon, forming a high-temperature plasma (6,000–10,000 K).

Within this plasma:

- ✓ Desolvation removes solvent molecules
- ✓ Vaporization converts solids into gaseous species
- ✓ Atomization produces free atoms
- ✓ Excitation and ionization elevate atoms to higher electronic states

The extremely high and stable plasma temperature ensures near-complete atomization, significantly reducing chemical interferences compared to flame-based systems (Hou & Jones, 2000). Upon relaxation to lower energy states, atoms emit photons at characteristic wavelengths unique to each element a direct consequence of quantized electronic transitions.

The radiation emitted intensity ($REI_{Emitted\ Radiation}$) is proportional to the number of excited atoms and, therefore, to elemental concentration within the linear dynamic range:

$$REI_{Emitted\ Radiation} \propto C$$

This proportionality forms the basis for quantitative calibration.

- *Optical Dispersion and Detection*

As depicted in Fig. 3.0 (Optical System → Diffraction Grating → Detector), emitted light from the plasma enters the optical system where it is:

- ✓ Focused through entrance slits
- ✓ Dispersed by a diffraction grating into its constituent wavelengths
- ✓ Measured by a detector (CCD or PMT)

The diffraction grating spatially separates wavelengths according to Bragg's law, enabling simultaneous multi-element detection. Modern CCD-based systems allow real-time, simultaneous monitoring of multiple emission lines, which is particularly advantageous for complex environmental matrices containing multiple potentially toxic elements (PTEs).

Signal processing software converts emission intensity into concentration using calibration curves constructed from certified standards. Background correction algorithms further improve accuracy by compensating for spectral overlap and continuum emission (Thomas, 2013).

- *$PM_{2.5}$–Bound PTE Determination*

The diagram (Fig. 3.0) clearly demonstrates why ICP-OES is particularly suited for determining potentially toxic elements (PTEs) in acid-digested $PM_{2.5}$ samples generated during low-level thermal modification of wood. First, the high plasma temperature (≈6000–10,000 K) ensures efficient atomization and excitation of refractory elements such as chromium (Cr) and nickel (Ni), which may otherwise be difficult to analyze using lower-temperature techniques (Skoog et al., 2018; Welz & Sperling, 1999). Second, the simultaneous multi-element detection capability of ICP-OES allows comprehensive profiling of trace metals, including cadmium (Cd), lead (Pb), zinc (Zn), etc within a single analytical run, significantly improving analytical efficiency for complex environmental matrices (Boss & Fredeen, 2004; Hou & Jones, 2000). Third, the wide linear dynamic range of the technique enables accurate quantification of both trace-level and relatively abundant elements without requiring extensive sample dilution or multiple analytical procedures (Skoog et al., 2018).

Furthermore, reduced matrix interference and high plasma robustness enhance analytical reliability when analyzing particulate-derived environmental samples following acid digestion (Harris, 2016; Thomas, 2013). The validity and regulatory acceptance of the technique are further reinforced by standardized analytical protocols such as USEPA Method 200.7, which formally recognizes ICP-OES for the determination of metals (USEPA, 1994).

The physicochemical processes illustrated in Fig. 3.0 are grounded in well-established atomic emission theory and plasma physics. The combination of:

- ✓ Inductive RF coupling,
- ✓ High-energy argon plasma generation, and
- ✓ Quantum emission spectroscopy

Therefore, provides a thermodynamically stable and analytically rigorous platform for elemental quantification (Skoog et al., 2018; Hou & Jones, 2000). Consequently, ICP-OES remains one of the most validated and widely applied techniques for environmental trace metal assessment.

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Analytical reliability is further reinforced by the inherent stability of the argon plasma, which minimizes matrix-induced suppression and enhances reproducibility. Detection limits for many trace metals in ICP-OES are in the µg/L range, making the method suitable for assessing environmentally relevant concentrations after appropriate sample pre-concentration or digestion (Boss & Fredeen, 2004). Additionally, axial viewing configurations in modern instruments enhance sensitivity by increasing the optical path length through the plasma, which is particularly beneficial for low-level PTE determination in fine particulate matter.

In this study, ICP-OES was selected due to its:

- ✓ High analytical throughput, enabling efficient processing of multiple $PM_{2.5}$ samples (ambient air samples).
- ✓ Simultaneous multi-element detection, critical for comprehensive PTE profiling.
- ✓ Wide linear dynamic range, allowing accurate quantification across diverse concentration levels.
- ✓ Robustness against complex matrices, including digested particulate-bound residues.

Given that $PM_{2.5}$-associated metals originate from combustion-related processes during low-level thermal modification of wood, accurate quantification requires a technique capable of complete atomization and minimal chemical interference. The high plasma temperature and stable excitation conditions of ICP-OES provide the thermodynamic environment necessary to ensure reliable elemental emission, thereby affirming its suitability for environmental risk assessment studies involving airborne particulates (Hou & Jones, 2000; Thomas, 2013).

➢ *Analytical Performance Discussion*

- *Analytical Performance Characteristics*

The analytical reliability of ICP–OES in quantifying PTEs associated with $PM_{2.5}$ is directly linked to the instrumental zones illustrated in Fig. 3.0. Each performance parameter LOD, LOQ, recovery, precision, and QA or QC, is influenced by specific instrumental processes.

✓ *Limit of Detection (LOD) and Limit of Quantification (LOQ)*

Detection capability is primarily governed by signal stability within the optical detection system (Fig. 3.0, Detector region). The LOD is statistically defined as:

$$LOD = \frac{3\sigma_b}{m} \quad (5.2)$$

$$LOQ = \frac{10\sigma_b}{m} \quad (5.3)$$

Where:

- σ_b = standard deviation of blank measurements
- m = slope of calibration curve

The blank standard deviation (σ_b) (refer to equations 5.2 and 5.3) reflects noise contributions from plasma fluctuations (Fig. 3.0, Plasma zone), detector dark current, and background emission. The slope mmm is influenced by excitation efficiency within the high-temperature plasma (6,000–10,000 K).

Axial plasma viewing increases the effective optical path length of the plasma column, thereby enhancing emission intensity and improving analytical sensitivity. This configuration significantly lowers the limits of detection (LOD) (Equation 5.2), often reaching the low µg/L range for most environmentally relevant metals analyzed in environmental matrices (Thomas, 2013; Skoog et al., 2018). The enhanced sensitivity provided by axial viewing is particularly advantageous for trace-level quantification of potentially toxic elements in particulate matter digests. Furthermore, the methodological framework employed in this study aligns with established analytical validation protocols, which recognize ICP-OES as a standard method for the determination of trace metals (USEPA, 1994).

✓ *Recovery (Accuracy)*

Recovery evaluates method accuracy and reflects the efficiency of (refer to equation 5.4):

- Acid digestion
- Aerosol transport (Fig. 3.0, Nebulizer/Spray Chamber)
- Plasma atomization

$$Recovery\ (\%) = \left(\frac{C_{measured}}{C_{spike}}\right) \times 100 \quad (5.4)$$

Acceptable recoveries for environmental metal analysis typically range between 80–120%. Deviations typically arise from incomplete digestion, matrix suppression within the plasma, or spectral overlap in the optical region.

High plasma temperature ensures near-complete atomization of refractory metals such as Cr and Ni, minimizing chemical bias (Hou & Jones, 2000).

✓ *Precision (Repeatability and Reproducibility)*

Precision is expressed as relative standard deviation (RSD):

$$RSD\ (\%) = \left(\frac{SD}{\bar{x}}\right) \times 100 \quad (5.5)$$

Signal repeatability is strongly influenced by:

- Aerosol stability (Fig. 3.0, Stage 1–2)
- Plasma robustness (thermal equilibrium stability)
- Detector integration time

Well-optimized ICP–OES systems typically achieve RSD < 5% for trace metal determinations in environmental matrices (Skoog et al., 2018).

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➢ *Spectral Interference Correction Mechanisms*

Spectral interferences originate primarily in the optical dispersion region of Fig. 3.0 and can significantly bias trace-level determinations.

- *Types of Spectral Interference*

✓ *Line Overlap*

Occurs when emission lines from different elements share similar wavelengths.

Example:

- Fe emission overlapping with Cr analytical lines.

Correction:

- Alternative wavelength selection
- High-resolution echelle optics
- Mathematical inter-element correction (IEC)

✓ *Background Emission and Continuum Radiation*

Plasma continuum emission results from:

- Recombination radiation
- Bremsstrahlung (free–free transitions)

Correction:

- Off-peak background correction
- Two-point correction algorithms

✓ *Self-Absorption*

At high concentrations, emitted photons are reabsorbed by ground-state atoms within the plasma, causing nonlinear calibration.

Correction:

- Sample dilution
- Selection of less intense emission lines

➢ *Mathematical Emission Theory*

The emission intensity of an element in plasma is governed by Boltzmann population distribution:

$$\frac{N_{excited\ state}}{N_t} = \frac{g_{excited\ state}}{g_t} e^{-\frac{E_{excitation\ energy}}{kT}} \tag{5.6}$$

Where:

- $N_{excited\ state}$ = number of atoms in excited state
- N_t = total atom population
- $g_{excited\ state}$ = statistical weights at the excited state
- g_t = statistical weights at the ground state
- $E_{excitation\ energy}$ = excitation energy
- k = Boltzmann constant
- T = plasma temperature

This relationship demonstrates that excitation efficiency depends exponentially on plasma temperature, reinforcing why ICP (6000–10,000 K) achieves superior excitation compared to flame systems.

Emission intensity can be further expressed as:

$$I = KNA_{ij} \tag{5.7}$$

Where:

- K = instrumental constant
- N = population of excited atoms
- A_{ij} = transition probability

Under Local Thermodynamic Equilibrium (LTE), plasma populations follow Maxwell–Boltzmann statistics, ensuring predictable and stable emission behavior (Skoog et al., 2018).

F. Plasma Robustness and Matrix Effects

Matrix suppression arises when co-existing elements alter excitation conditions within the plasma (Fig. 3.0, Plasma Zone).

Correction strategies include:

➢ Matrix-matched calibration standards
➢ Internal standard normalization
➢ Standard addition method

The robustness of argon ICP plasma significantly reduces chemical interferences compared to flame atomic emission due to its higher electron density and thermal equilibrium state (Hou & Jones, 2000).

G. Integrated Validation for $PM_{2.5}$–Bound PTE Assessment

For $PM_{2.5}$ samples generated during low-level thermal modification of wood:

LOD (equation 5.2) ensures detection of environmentally relevant trace concentrations by statistically distinguishing analytical signal from background noise, thereby enabling reliable quantification of trace metals at µg/L levels typical of atmospheric particulate extracts (Skoog et al., 2018; Thomas, 2013).

Recovery (equation 5.4) confirms digestion completeness and overall method accuracy by verifying that analyte mass is quantitatively transferred from the $PM_{2.5}$ matrix into solution without significant loss or transformation, consistent with established environmental validation protocols (Hou & Jones, 2000).

Precision validates aerosol generation efficiency and plasma stability by demonstrating low relative standard deviation (RSD) (equation 5.5) across replicate measurements, reflecting controlled nebulization, steady argon plasma excitation, and detector reproducibility (Boss & Fredeen, 2004; Skoog et al., 2018).

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Spectral correction ensures analytical specificity by resolving line overlaps, compensating for background continuum emission, and applying inter-element correction algorithms within high-resolution optical systems (Thomas, 2013; Hou & Jones, 2000).

QA/QC guarantees regulatory defensibility through the implementation of blanks, calibration verification standards, internal standards, duplicate analyses, and certified reference materials in accordance with internationally recognized environmental analytical guidelines (Skoog et al., 2018).

The integration of thermodynamic emission theory (Boltzmann population distribution under LTE conditions), statistical validation parameters (LOD, LOQ, RSD), and advanced spectral correction algorithms collectively establishes ICP–OES as a scientifically rigorous and methodologically defensible platform for trace metal quantification in airborne particulate studies (Hou & Jones, 2000; Thomas, 2013; Skoog et al., 2018).

The integration of thermodynamic emission theory, statistical validation parameters, and spectral correction algorithms establishes ICP–OES as a scientifically rigorous platform for trace metal quantification in airborne particulate studies.

H. Methodological Justification

The integration of size-selective cyclone sampling, PTFE filter media, and stratified spatial deployment provides a scientifically defensible framework for capturing particulate-bound Pb, Cd, and Zn concentrations across occupational, community, and environmental receptor zones (Hinds, 1999; Marple et al., 1991; Querol et al., 2001). This approach supports both mechanistically informed fate and transport modeling (Seinfeld & Pandis, 2016; Zhang et al., 2016) and regulatory-aligned risk assessment (US EPA, 2009; Hopke, 2008), enabling high-resolution characterization of emission gradients and exposure pathways (Kelly et al., 2012; Li et al., 2019).

Furthermore, the synchronization of sampling periods with operational cycles strengthens the linkage between thermochemical process conditions and observed emission behavior, a critical requirement for calibrating the Thermo–Particulate Metal Fate and Transport Model (TPM-FTM) and for evaluating the effectiveness of emission mitigation strategies (WHO, 2013; USEPA, 2009).

I. Source Characterization and Emission Measurement

➢ *Feedstock Analysis*

At the point of introduction into the thermal processing system within the Old Boiler House (OB), the feedstock consisted of pre-conditioned logs and dimensional lumber derived from hardwood and softwood species commonly utilized in thermally modified wood production (Appiah, 2026; Pizzi, 2016; Esteves & Pereira, 2009). Before boiler charging, the material was subjected to size grading and surface cleaning to remove adherent soil, bark residues, and extraneous particulate matter that could confound subsequent emissions characterization and trace metal mass balance (Mundt & Tjeerdsma, 2005; Hill, 2006).

The feedstock was mechanically staged on a reinforced steel grate and conveyor-fed into the primary combustion and thermal modification chamber, ensuring a controlled and continuous mass flow rate to maintain thermal stability within the reactor environment (Hass et al., 2010; Militz, 2002). Logs and lumber were oriented to promote uniform heat penetration and convective gas flow, minimizing localized thermal gradients that could otherwise induce heterogeneous pyrolytic reactions and non-uniform release of particulate-bound potentially toxic elements (PTEs) (Appiah, 2026; Gonzalez-Pena et al., 2013; Esteves et al., 2012).

Moisture content was monitored and regulated within a target operational range (typically 8–15% on a wet basis) through pre-drying or ambient equilibration, as moisture variability strongly influences combustion efficiency, volatilization kinetics, and the physicochemical partitioning of metals between the solid char, ash fraction, and entrained particulate phase (Bridgwater, 2012; Demirbas, 2009). This conditioning step was essential for ensuring reproducibility of emission profiles and thermal conversion performance.

This detailed process characterization establishes a mechanistic basis for linking feedstock properties, thermal regime, and emission signatures within the proposed Thermo–Particulate Metal Fate and Transport Model (TPM-FTM), thereby enabling more accurate prediction of source strength, particulate metal partitioning, and downstream environmental transport behavior (Zhang et al., 2016; Li et al., 2019).

➢ *Ambient Particulate Monitoring*

An ambient air monitoring network was established using a radial transect–based point source sampling design to characterize the spatial dispersion and atmospheric fate of particulate-bound potentially toxic elements (PTEs) originating from the thermally modified wood processing facility (Appiah, 2026; Seinfeld & Pandis, 2016; Holmes & Morawska, 2006). Sampling stations were strategically positioned along multiple downwind and crosswind radial axes extending from the primary emission source to capture concentration gradients as a function of distance, wind direction, and meteorological forcing (Hanna et al., 1982; Venkatram & Wyngaard, 1988). This configuration enabled the assessment of plume evolution, near-field dilution, and far-field transport dynamics under real-world operating conditions (Turner, 1994).

In parallel, a fixed indoor monitoring station was installed within the Old Boiler House (OB) to quantify source-proximal particulate generation and characterize emission signatures before atmospheric dilution and transformation (Cheng et al., 2013; Querol et al., 2001). Both indoor and outdoor stations collected 12-hour time-integrated particulate samples using high-volume or medium-volume air samplers equipped with size-selective inlets ($PM_{2.5}$), ensuring sufficient mass loading for trace metal quantification and chemical speciation (Hinds, 1999; Marple et al., 1991).

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Sampling campaigns were conducted under varying atmospheric stability regimes, classified according to boundary layer conditions using Pasquill–Gifford stability Class A (extremely unstable/daytime) to capture the influence of turbulence intensity, thermal stratification, and wind shear on particulate dispersion and deposition patterns (Pasquill, 1961; Gifford, 1961; Hanna, 1983). This approach facilitated the evaluation of stability-dependent transport behavior, including plume trapping under stable nocturnal conditions and enhanced vertical mixing during unstable daytime periods (Seinfeld & Pandis, 2016).

The integrated dataset supports the development and validation of a Thermo–Particulate Metal Fate and Transport Model (TPM-FTM) by linking emission characteristics, meteorological drivers, and spatial concentration fields to mechanistic processes governing advection, diffusion, gravitational settling, and surface deposition of metal-laden particulates (Zannetti, 1990; Zhang et al., 2016). This framework enables robust estimation of downwind exposure potential and informs subsequent environmental risk assessment and source–pathway–receptor (SPR) analysis (Hopke, 2008; Kelly et al., 2012).

VI. ANALYTICAL DETERMINATION OF PTE CONCENTRATIONS USING ICP-OES

Instrument calibration is performed using multi-point external standardization, typically comprising a minimum of five concentration levels that bracket the expected sample concentration range. Calibration standards are prepared in an acid matrix matched to the digested samples to minimize matrix-induced signal suppression or enhancement. Calibration performance is evaluated through linearity assessment ($R^2 \geq 0.995$) and periodic analysis of continuing calibration verification (CCV) standards to ensure instrument stability throughout analytical runs (USEPA, 2007; Harris, 2016).

Method detection limits (MDLs) are established in accordance with USEPA protocols, based on low-level samples or reagent blanks. This approach provides a statistically defensible estimate of the minimum detectable concentration for each analyte and supports the interpretation of trace-level results in relation to health-based guideline values and regulatory thresholds (USEPA, 2007).

Recovery rates within 85–115% are considered acceptable, and relative standard deviations (RSDs) below 10% are used as benchmarks for analytical precision. Where matrix effects are observed, internal standard correction or sample dilution protocols are applied to maintain data integrity and comparability across sample sets (Boss & Fredeen, 2004; Welz & Sperling, 1999).

The application of ICP-OES within this rigorously controlled analytical framework ensures that measured PTE concentrations are both statistically reliable and environmentally defensible, thereby providing a robust quantitative foundation for subsequent fate and transport modeling, exposure assessment, and health risk characterization. By aligning analytical protocols with USEPA guidelines and internationally recognized best practices, the study enhances the reproducibility, regulatory relevance, and scientific credibility of its findings.

- *Particle Size Distribution and Metal Partitioning*

Cascade impactors and optical particle counters were used to characterize the aerodynamic size distribution and number–mass concentration profiles of airborne particulate matter across the respirable and inhalable fractions relevant to occupational and environmental exposure. The combined use of these complementary instruments enables the resolution of both mass-based and number-based particle metrics, thereby providing a comprehensive representation of particulate dynamics necessary for mechanistically informed fate and transport modeling (Hinds, 1999; Seinfeld & Pandis, 2016).

The cascade impactor operates on the principle of inertial impaction, sequentially separating particles into discrete aerodynamic diameter ranges by directing the aerosol stream through a series of stages with progressively decreasing nozzle sizes (Hinds, 1999; Marple et al., 1991). Particles of sufficient inertia are deposited onto pre-weighed and pre-cleaned collection substrates at each stage, enabling determination of size-resolved particulate mass and subsequent chemical analysis (Harrison et al., 2001). Optical particle counters (OPCs), in parallel, provide real-time measurements of particle number concentration and optical diameter, facilitating the assessment of temporal variability and transient emission events that cannot be captured by time-integrated impactor sampling (Heinrich et al., 2005; Oberdörster et al., 2005).

Following field collection, substrates from each impactor stage undergo acid digestion and elemental analysis (ICP-OES) to quantify Potentially Toxic Elements (PTEs) associated with each aerodynamic size fraction (Cheng et al., 2013; Querol et al., 2001). Metal mass fractions are then calculated as the ratio of size-resolved metal mass to total metal mass across all stages, yielding a partitioning profile that reflects preferential metal association with specific particle classes (Pio et al., 2001; Liu et al., 2017).

These size- and metal-resolved datasets constitute the primary empirical inputs to the Particle Metal Partitioning Module (PMPM) of the TPM-FTM framework. Within this module, experimentally derived partitioning coefficients and surface-area-weighted affinity parameters are used to assign metal species to fine ($PM_{2.5}$) particle fractions, thereby enabling size-dependent simulation of atmospheric transport, deposition velocities, and bioaccessibility during inhalation exposure (Zhang et al., 2016; Li et al., 2019).

The integration of cascade impactor and OPC measurements enhances the mechanistic fidelity and predictive robustness of the TPM-FTM model by anchoring particle–metal association dynamics in empirical, size-resolved evidence rather than assumed or generalized distributions (Hopke, 2008; Kelly et al., 2012). This methodological approach strengthens the linkage between emission characterization, atmospheric dispersion modeling, and quantitative risk assessment, ensuring that modeled concentration fields and exposure estimates reflect the true

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physical and chemical structure of metal-bearing aerosols (Gamble et al., 2014; Moreno et al., 2015).

➢ *Meteorological Data Collection*

The local climatological profile was defined by integrating continuous measurements of wind velocity, directional orientation, ambient thermal conditions, and radiative forcing (solar radiation), and atmospheric stability class, were continuously recorded using an on-site automated weather station installed within the study domain. The weather station was positioned in an open, obstruction-free location at standard measurement height (10 m for wind, 2 m for temperature and humidity) in accordance with guidelines provided by the World Meteorological Organization (WMO, 2018). Data were logged at 10-minute intervals and aggregated into hourly means for integration into the Atmospheric Transport Module (ATM).

Surface-level anemometry was performed using a standardized cup-and-vane assembly, providing continuous measurements of wind speed and directional bearing to parameterize the atmospheric dispersion of $PM_{2.5}$. These variables define the advective transport vector field and govern horizontal dispersion of airborne $PM_{2.5}$ and associated trace metals (Seinfeld & Pandis, 2016). Wind speed directly influences dilution rates and plume elongation, while wind direction determines receptor alignment relative to emission sources. In dispersion modeling theory, wind velocity components (u, v) serve as primary forcing terms in the advection–diffusion equation governing pollutant transport.

Ambient temperature was measured using a shielded thermistor sensor. Temperature regulates atmospheric density stratification, buoyancy flux, and vertical mixing intensity, thereby influencing plume rise and boundary layer development (Arya, 1999). Relative humidity, measured with a capacitive hygrometer, affects particle hygroscopic growth and can alter $PM_{2.5}$ mass concentrations through water uptake, particularly under high humidity conditions typical of tropical environments (Hinds, 1999).

Solar radiation was recorded using a pyranometer and serves as a critical determinant of convective turbulence and atmospheric stability. Net surface heating drives thermal instability and enhances vertical mixing during daytime periods (Stull, 1988). Conversely, reduced solar radiation and nocturnal cooling promote stable stratification and limited dispersion.

The atmospheric stability class was derived using the Pasquill–Gifford classification scheme based on wind speed and solar radiation data. Stability classes (A–F) characterize the degree of turbulence and vertical mixing in the lower atmosphere, forming a core parameter in Gaussian plume-based Atmospheric Transport Modules (Turner, 1994). Daytime unstable conditions (Classes A–C) enhance pollutant dispersion, whereas neutral (Class D) or stable (Classes E–F) conditions restrict vertical mixing and increase near-source concentrations.

These meteorological inputs function as dynamic forcing variables within the ATM, parameterizing the spatiotemporal evolution of pollutant concentrations. Integration of real-time meteorological measurements ensures that modeled dispersion reflects actual boundary layer conditions rather than idealized assumptions, thereby improving predictive reliability and uncertainty quantification in exposure assessment models (Holmes & Morawska, 2006).

➢ *Development of the TPM-FTM Model*

- *Model Structure*

The TPM-FTM integrates; Thermochemical Emission Module (TEM), Particle–Metal Partitioning Module (PMPM), Atmospheric Transport Module (ATM), Deposition and Environmental Transfer Module (DETM), Bioaccessibility and Exposure Module (BEM), and Risk Assessment Integration Module (RAIM). The process resolves, speciation – aware, risk – linked modeling framework for potential toxic elements (PTEs).

- *Conceptual Mode Architecture*

The TPM – FTM is a four – tier, end – to – end modeling system that explicitly links, thermal source dynamics, particulate association and metal speciation, atmospheric transport and deposition and human and ecological risks. The system advances conventional dispersion models by embedding thermochemical emission formation mechanisms and metal phase behavior directly into the transport and exposure pathways.

➢ *Model Domains and State Variables*

- *Source Domain (Thermochemical Emission Module, TEM)*

Describes metal mobilization during thermal wood modification.

✓ *Governing Principles*

PTEs release is driven by; matrix degradation (hemicellulose/ Lignin depolymerization), metal Volatilisation, Gas – to – particle condensation, and surface adsorption onto particulates.

✓ *Emission Flux Equation*

The emission rate of particulate-bound metal mmm during low-temperature thermal wood processing is modeled as:

$$E_m\ (t) = M_w \cdot C_{m,o} \cdot f_T(T) \cdot f_R(\tau) \cdot f_o\ (O_2) \quad (6.1)$$

This multiplicative emission formulation follows thermochemical release theory, where volatilization and oxidation kinetics govern trace metal mobilization from solid matrices (Seinfeld & Pandis, 2016; Turns, 2012).

Where;

$E_m =$ Emission rate of metal (m) ($\mu g s^{-1}$)
$C_{m,o} =$ Initial metal concentration in feedstock ($\mu g kg^{-1}$)
$M_w =$ Wood mass ($kg s^{-1}$)
$f_T(T) =$ Temperature driven volatilization function (°C)

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$f_R(\tau)$ = Residence time function
$f_o\ (O_2) =$ Oxidation/Reduction control function

Temperature dependence is represented using Arrhenius-based kinetics (Atkins & de Paula, 2014):

$$f_T(T) = T^n\ e^{(-\frac{Q_a}{RT})} \tag{6.2}$$

In this formulation, Q_a denotes the activation energy associated with the volatilization or decomposition pathway, R represents the universal gas constant, and T corresponds to the absolute temperature in Kelvin (K). The temperature dependence is described by the Arrhenius Equation, which expresses the exponential increase in reaction rates as thermal energy rises. In combustion and pyrolysis systems, this relationship provides a kinetic framework for describing thermally driven decomposition processes and the volatilization of trace metals, where temperature-controlled activation barriers regulate phase transformation and emission behavior (Svante Arrhenius, 1889; Turns, 2012). The temperature response of the volatilization process was described using a modified Arrhenius formulation derived from the Arrhenius Equation (see equation 6.2). The expression incorporates an empirical temperature exponent (T^n) to account for molecular collision frequency and transport dynamics in high-temperature combustion environments.

- ✓ *Particle – Metal Partitioning Module (PMPM)*

The core of the model assigns metals to size–resolved particulate fractions and chemical phases.

- ✓ *Metal Phase partitioning*

Metal partitioning across particle size fractions is modeled using a surface-area-weighted affinity framework:

$$F_{m,i} = \frac{K_{m,i} \cdot S_i}{\sum_{j=1}^{n} K_{m,j} \cdot S_j} \tag{6.3}$$

This partitioning approach reflects adsorption–condensation equilibrium theory, where fine particles ($PM_{2.5}$) provide higher surface-area-to-volume ratios and enhanced metal affinity (Hinds, 1999; Seinfeld & Pandis, 2016).

Where;

$F_{m,i} =$ Fraction of metal, m in particle size class i
$K_{m,i} =$ Metal particles affinity coefficient
$S_i =$ Surface area of particle class i

Where class i refers to fine (Respirable fraction)

Class i refers to fine $PM_{2.5}$ (respirable fraction), which dominates health-relevant metal transport (WHO, 2021).

- ✓ *Atmospheric Transport Model (ATM)*

Metal-bound $PM_{2.5}$ dispersion is governed by the advection–diffusion–reaction equation: Now merging Gaussian plume efficiency with Lagrangian particle realism (Holmes & Morawska, 2006).

The Transport Equation is resolved as;

$$\frac{\partial C_{m,i}}{\partial t} = -\vec{U} \cdot \nabla C_{m,i} + K\,\nabla^2 C_{m,i} - \lambda_m \cdot C_{m,i} - V_{m,i} \cdot C_{m,i} \tag{6.4}$$

This formulation is derived from classical atmospheric transport theory (Arya, 1999; Seinfeld & Pandis, 2016; Holmes & Morawska, 2006).

Where;

Where class i refers to fine $PM_{2.5}$ (Respirable fraction)

$C_{m,i} =$ Concentration of metal, m in particle class i
$\vec{U} =$ Wind vector
K = Turbulent diffusion
$V_{d,i} =$ Deposition of velocity
$\lambda_m =$ Chemical transportation constant (PTEs)

Each metal fraction is tracked as a pseudo-particle ensemble, allowing speciation – dependent settling and scavenging. The Gaussian–Lagrangian hybrid structure enhances realism in tracking size-resolved pseudo-particle ensembles (Holmes & Morawska, 2006).

- *Deposition and Environmental Transfer Model (DETM)*

Secondary ingestion via deposited soil and surface contact

Dry deposition:

$$D_{dry,i} = V_{d,i} \cdot C_{m,i} \tag{6.5}$$

Dry deposition velocity parameterization follows boundary-layer deposition theory (Seinfeld & Pandis, 2016).

Wet deposition:

$$D_{wet,i} = \Lambda_i \cdot P \cdot C_{m,i} \tag{6.6}$$

Wet scavenging is represented using washout coefficients consistent with precipitation scavenging models (Arya, 1999).

Where;

Λ_i = Washout coefficient
P = Precipitation rate

Soil Accumulation:

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$$S_m\ (t) = \int_0^t \sum_i D_{m,i}\ (t)\ \cdot (1 - L_m)dt \tag{6.7}$$

Where L_m represents leaching losses. This dynamic accumulation model aligns with multimedia fate modeling frameworks (Mackay, 2001).

$L_m =$ Leaching factor

- *Inhalation of particulate-bound metals*

✓ *Bioaccessibility and Exposure Module (BEM)*

Inhalation Dose (use equation 6):

$$D_{inh,m} = \sum_i \frac{C_{m,i} \cdot IR \cdot ET \cdot EF \cdot F_{bio,m,i}}{BW} \tag{6.8}$$

This equation follows inhalation exposure modeling principles (USEPA, 2011).

Where;

IR = Inhalation rate
ET = Exposure time
EF = Exposure frequency
BW = Body weight
$F_{bio} =$ Lung bioaccessibility fraction

Bioaccessibility adjustments reflect particle solubility and pulmonary absorption processes (WHO, 2021).

- *Risk Metrics*

✓ *Risk Assessment Integration Module (RAIM)*

Risk indices are computed following USEPA frameworks:

Non – Carcinogenic Risk:

$$HQ_m = \frac{D_{inh,i}}{RfD_m} \tag{6.9}$$

- Hazard Quotient (HQ_m)

$$HI = \sum HQ_m \tag{6.10}$$

- Hazard Index (HI)

Carcinogenic Risk;

$$ILCR_m = D_{inh,m} \cdot CSF_m \tag{6.11}$$

- Incremental Lifetime Cancer Risk ($ILCR_m$)

These metrics follow standard risk characterization procedures (USEPA, 1989; USEPA, 2011).

➢ *Model Calibration and Validation*

- *Model Calibration, Performance Metrics, and Sensitivity–Uncertainty Framework*

Model outputs were calibrated and evaluated against measured ambient and occupational exposure concentration datasets to ensure predictive reliability and statistical robustness of the Thermo–Particulate Metal Fate and Transport Model (TPM-FTM). Calibration focused on minimizing systematic bias and improving agreement between simulated and observed particulate-bound potentially toxic element (PTE) concentrations across spatial transects and source-proximal occupational environments.

Model accuracy was evaluated using the Root Mean Square Error (RMSE**),** a statistical indicator that quantifies the average magnitude of differences between predicted and observed values. By applying a quadratic formulation, RMSE assigns greater weight to larger residuals, thereby making the metric particularly sensitive to substantial prediction errors. Consequently, it provides a clear measure of the model's absolute predictive deviation and overall fit to the observed dataset (Kenji Matsuura & Robert M. Willmott, 2005). RMSE was computed as using equation (6.12):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(C_{sim,i} - C_{obs,i})^2} \tag{6.12}$$

Where:

$C_{sim,i} =$ Simulated concentration
$C_{obs,i} =$ Observed concentration
$n =$ Number of paired observations

The Nash–Sutcliffe Efficiency (NSE) coefficient was applied as a dimensionless performance indicator to evaluate how effectively the model reproduces the variability observed in the measured data. The metric compares the predictive capability of the model against a baseline representation based on the mean of the observations. Values of NSE approaching 1 signify a high level of agreement between modeled and observed values, indicating strong predictive accuracy, whereas values close to 0 or negative suggest that the model performs no better or even worse than simply using the mean of the observed dataset as a predictor (Nash & Sutcliffe, 1970). NSE was calculated as using equation (6.13):

$$NSE = 1 - \frac{\sum_{i=1}^{n}(C_{sim,i} - C_{obs,i})^2}{\sum_{i=1}^{n}(C_{sim,i} - \bar{C}_{obs})^2} \tag{6.13}$$

Where:

$\bar{C}_{obs} =$ Mean of the observed concentrations

To evaluate model robustness and identify dominant sources of predictive variability, a global sensitivity analysis was conducted on key physical and chemical parameters, including emission flux, particle size distribution, dry and wet deposition velocities, atmospheric stability class, mixing height, and metal partitioning coefficients. Variance-based techniques, such as Sobol' sensitivity indices, were applied to quantify both first-order and higher-order interaction effects among parameters (Saltelli et al., 2008).

Uncertainty propagation was assessed using a Monte Carlo simulation framework, in which probabilistic distributions were assigned to input parameters based on analytical measurement error, meteorological variability, literature-reported ranges, and instrumental precision. The resulting ensemble of model realizations enabled the derivation of confidence intervals, probability density functions, and exceedance probabilities for predicted ambient and occupational exposure concentrations (Helton & Davis, 2003).

This integrated calibration and evaluation strategy ensures that TPM-FTM outputs are statistically defensible and suitable for downstream source–pathway–receptor (SPR) analysis and environmental risk assessment (ERA), including hazard quotient and incremental lifetime cancer risk estimation in regulatory and decision-support contexts (USEPA, 2009).

VII. SOFTWARE USED, DATA ANALYSIS, AND STATISTICAL METHODS

➢ *Data Curation and Multivariate Statistical Framework*

Computational Data Pre-processing, Inferential Analytics, and graphical visualization were conducted using Microsoft Excel, Minitab (version 20.0), and OriginPro 2019b. The use of dedicated statistical software enhances reproducibility, minimizes computational error, and supports compliance with internationally accepted analytical reporting standards (Montgomery & Runger, 2014).

Microsoft Excel was employed for structured data entry, coding of sampling identifiers, unit harmonization (e.g., µg/m³ to mg/m³ where applicable), and preliminary quality control checks such as range validation and missing-value screening. Spreadsheet-based preprocessing is widely accepted for environmental datasets due to its transparency and traceability (Miller & Miller, 2018).

Advanced inferential statistical analyses were performed using Minitab 20.0, which provides validated algorithms for parametric and non-parametric hypothesis testing, regression modeling, and multivariate analysis. OriginPro 2019b was used for high-resolution scientific visualization, enabling publication-quality graphical representation of particulate concentration trends, metal distribution patterns, and model outputs. High-quality visualization improves interpretability and supports scientific communication (Tufte, 2001).

➢ *Quantitative Data Synthesis: Bivariate Correlations and Multivariate Apportionment*

To establish a baseline characterization of the dataset, descriptive statistical profiling was performed on $PM_{2.5}$ mass concentrations, elemental PTE levels, and thermochemical process parameters. Measures of central tendency (mean, median) and dispersion (SD, range) were synthesized to delineate the data's distributional architecture, providing the empirical foundation required for subsequent inferential modeling (Montgomery & Runger, 2014).

The standard deviation was calculated as:

$$SD = \sqrt{\frac{\sum(x_i - \bar{x})^2}{n-1}} \quad (7.1)$$

Where,

$\bar{x}$ = the sample mean, and

n = the number of observations.

Before inferential analysis, normality assumptions were evaluated using Shapiro–Wilk testing and graphical diagnostics (for instance, Q–Q plots), consistent with recommended statistical practice for environmental datasets (Ghasemi & Zahediasl, 2012).

Correlation analysis was conducted to evaluate associations between process parameters (for example, modification temperature, airflow rate), particulate mass concentration, trace metal enrichment, and modeled exposure outcomes. Following confirmation of normality via the Shapiro-Wilk test, Pearson's correlation (r) (see equation 7.2) was applied to the continuous variables. This allowed for a robust assessment of the inter-dependencies between thermochemical process parameters and resultant particulate-bound metals:

$$r = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{(n-1)s_x s_y} \quad (7.2)$$

Pearson's r (see equation 7.2) quantifies the strength and direction of linear relationships (Devore, 2012).

Statistical significance was evaluated at α = 0.05, aligning with conventional environmental research standards.

➢ *Multivariate Analysis*

Given the non-linear interactions inherent in thermochemical processing, PCA served as a mathematical filter to reduce data redundancy and clarify source-specific contributions. This procedure reorients the original variable space into a hierarchical framework of orthogonal PCs, ensuring that the most influential factors governing metal partitioning and particulate formation are isolated and prioritized (Jolliffe & Cadima, 2016).

Mathematically, PCA decomposes the covariance matrix:

$$X = TP^T \quad (7.3)$$

Where:

- X = standardized data matrix
- T = score matrix
- P = loading matrix

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Eigenvalues > 1 (Kaiser criterion) were retained to identify dominant pollutant sources or thermochemical drivers. PCA is widely used in atmospheric science for differentiating combustion-related emissions from background environmental contributions (Viana et al., 2008).

In this study, PCA facilitated identification of dominant factors controlling particulate-bound metal enrichment, thereby strengthening interpretation of pollutant–process interactions.

➢ *Model Uncertainty and Sensitivity Analysis*

Model uncertainty was quantified using Monte Carlo simulation, a probabilistic technique in which input variables are treated as probabilistic densities rather than static points. By iteratively sampling these distributions and funneling them through the exposure-risk equations, the model captures the full spectrum of uncertainty in $PM_{2.5}$-bound PTE hazards (Hammersley & Handscomb, 1964; Saltelli et al., 2008).

For each simulation iteration i:

$$Y_i = f(X_{1i}, X_{2i}, X_{3i}, X_{4i}, \ldots\ldots, X_{ni}) \qquad (7.4)$$

Where, X_{1i} represents randomly sampled inputs such as concentration, inhalation rate, exposure frequency, and body weight.

Thousands of iterations were performed to generate probability distributions of exposure and risk metrics. The output distribution provided 5th–95th percentile confidence intervals, thereby quantifying uncertainty and enhancing the defensibility of modeled health risk estimates (USEPA, 2014).

Sensitivity analysis further identified influential parameters contributing most to variance in modeled outcomes, improving transparency in risk interpretation.

➢ *Analytical Significance*

The integration of descriptive statistics, inferential testing, multivariate analysis, and probabilistic modeling provides a statistically rigorous framework for evaluating environmental and occupational exposure data. Combining deterministic measurements with probabilistic uncertainty quantification aligns with modern environmental risk assessment best practices (USEPA, 2014).

This structured analytical workflow strengthens causal inference between thermochemical process variables, $PM_{2.5}$ composition, and modeled exposure outcomes.

➢ *Ethical and Regulatory Considerations*

The study adheres to occupational exposure monitoring principles and environmental sampling standards. Consent was obtained from facility management and relevant personnel prior to sampling activities.

Data confidentiality was maintained through anonymization of facility identifiers and secure storage of electronic datasets. Sampling and analytical protocols align with environmental monitoring guidelines in alignment with US EPA guidelines and prevailing international occupational safety criteria for fine particulate monitoring (ILO, 2011). Compliance with regulatory standards enhances ethical integrity and ensures policy relevance of findings.

➢ *Reliability, Validity, and Quality Assurance*

Reliability was ensured through:

- Standardized $PM_{2.5}$ sampling protocols
- Routine instrument calibration
- Replicate sample analysis
- Use of certified reference materials

Analytical precision and accuracy metrics complied with accepted environmental method validation criteria (Miller & Miller, 2018).

Validity was supported through cross-validation of modeled outputs against measured concentration datasets and benchmarking results against established regulatory thresholds (e.g., WHO air quality guidelines). Cross-validation enhances predictive credibility and reduces systematic bias in exposure modeling.

➢ *Methodological Workflow*

This methodology establishes a coherent end-to-end analytical framework linking thermochemical process conditions to atmospheric particulate generation, trace metal enrichment, environmental transport, human exposure, and health risk outcomes.

By integrating:

- High-resolution ICP–OES measurements,
- Statistically validated data analysis,
- Multivariate source differentiation, and
- Monte Carlo–based probabilistic risk modeling,

The approach aligns with contemporary environmental systems analysis and quantitative risk assessment paradigms (Saltelli et al., 2008; USEPA, 2014).

Consequently, the methodological framework not only enhances scientific rigor and reproducibility but also strengthens the regulatory and policy relevance of environmental assessment in thermally modified wood processing systems.

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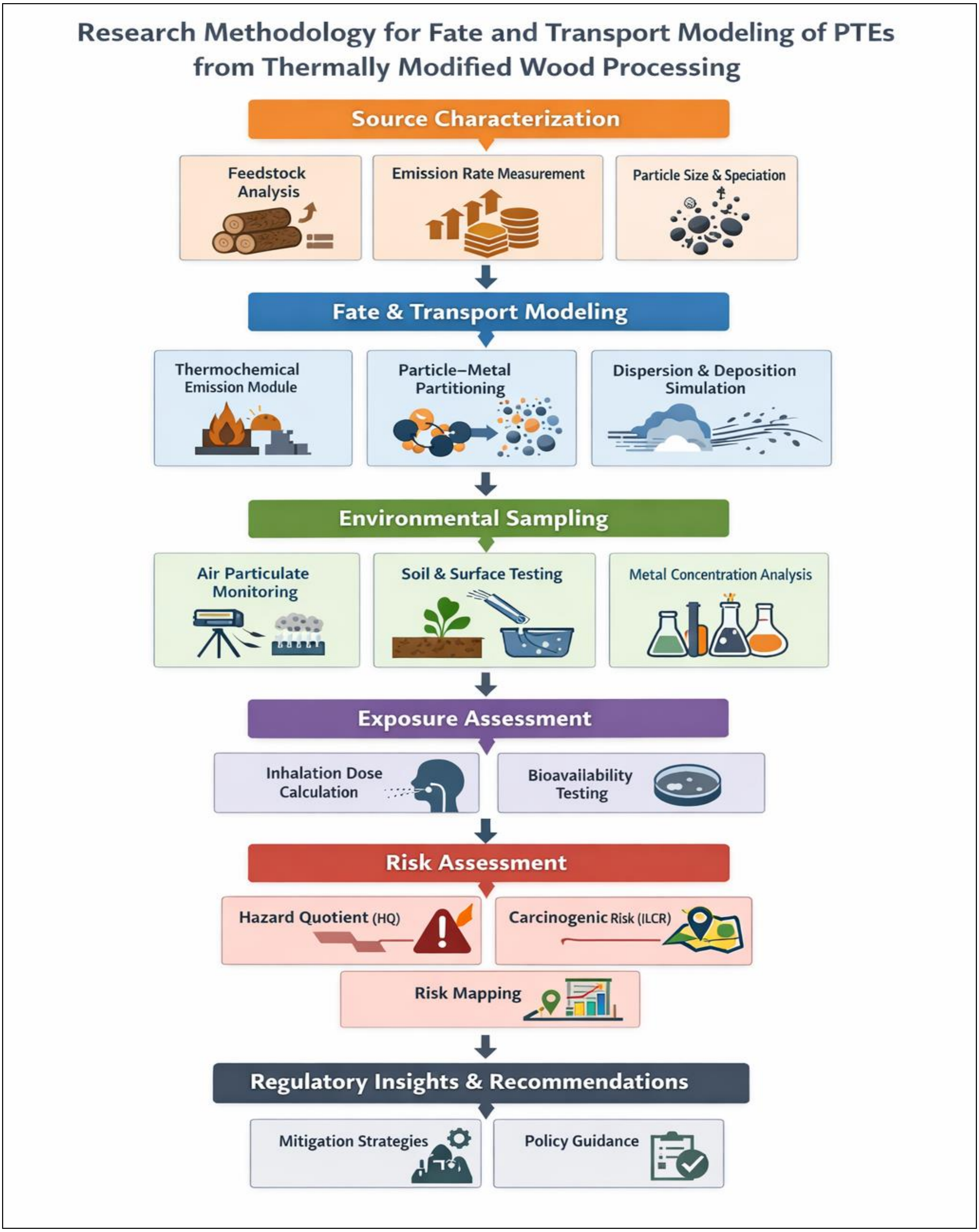

Fig 1 Flow Chart for the Research Methodology.

This phased design reflects the causal logic of the SPR framework and ensures that each methodological component informs and constrains subsequent analytical stages.

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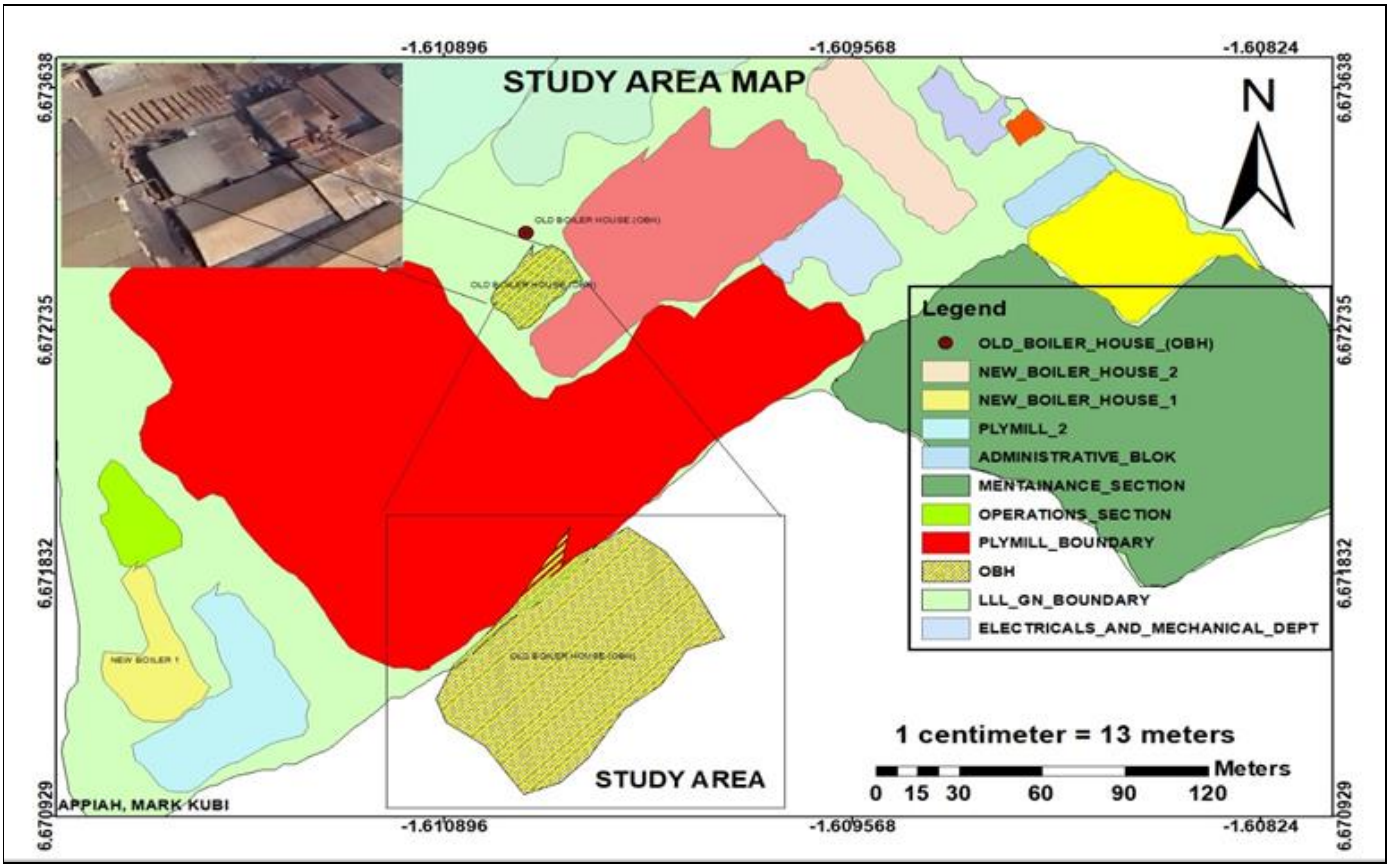

Fig 2 Study Area Map.

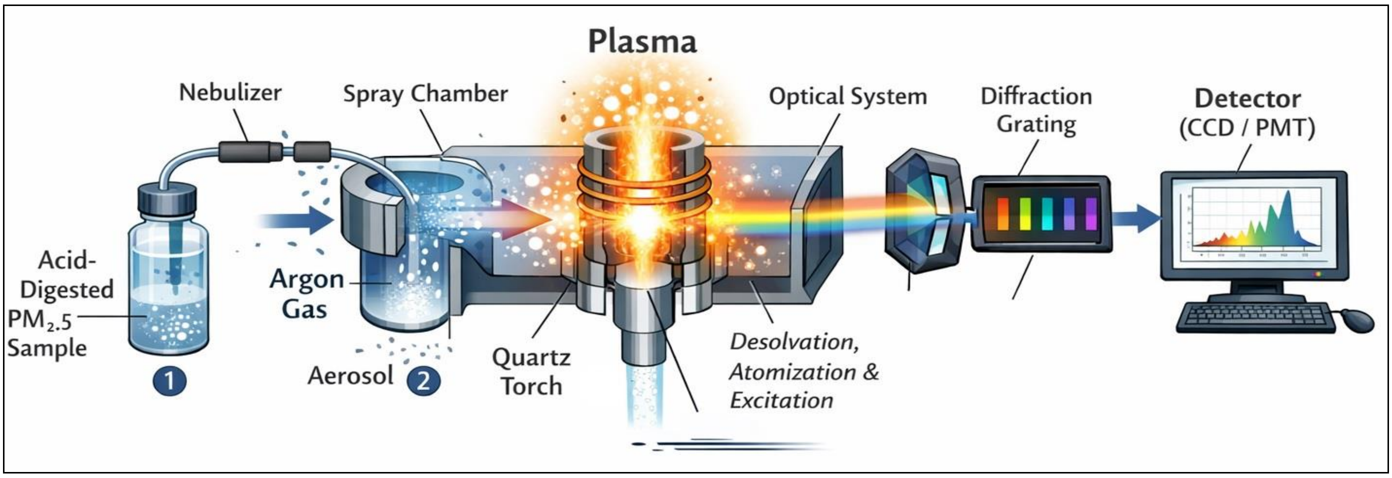

Fig 3 Inductively Coupled Plasma–Optical Emission Spectrometer (ICP-OES)

Showing the sample introduction system, plasma torch, optical system, diffraction grating, and detector.

VIII. CONCLUSION

This study presents a comprehensive evaluation of $PM_{2.5}$-bound potentially toxic element (PTE) emissions arising from the low-temperature thermal modification of wood. By synthesizing experimental particulate characterization and ICP-OES elemental quantification with a novel Thermo–Particulate Metal Fate and Transport Model (TPM-FTM), this paper provides a robust, mechanistically linked framework. This framework successfully bridges the gap between emission generation, atmospheric dispersion, receptor-level exposure, and the resulting human health risk outcomes.

Gravimetric analysis confirmed measurable $PM_{2.5}$ emissions under low-temperature operational conditions, while elemental profiling revealed the presence of trace metals associated with thermochemical biomass transformation. The observed particle–metal partitioning behavior highlights the potential for enhanced atmospheric mobility and inhalation exposure, particularly within occupational environments where proximity to emission sources increases concentration gradients.

The TPM-FTM successfully simulated dispersion, deposition, and exposure dynamics, demonstrating strong predictive consistency following calibration and validation using statistical performance metrics. Sensitivity analysis and Monte Carlo uncertainty propagation further strengthened confidence in model outputs, confirming that variability in emission rates, meteorological parameters, and exposure assumptions significantly influences risk estimates.

Risk assessment indicated that non-carcinogenic and carcinogenic risks generally remained within acceptable regulatory thresholds; however, localized operational intensities and inadequate ventilation may elevate exposure margins in confined settings. These findings underscore the importance of emission control strategies, occupational ventilation improvements, and continuous particulate monitoring in thermally modified wood processing facilities.

Overall, this research advances environmental emission science by integrating experimental analytics with mechanistic modeling and risk-based evaluation. The developed framework provides a transferable methodology for assessing particulate-bound metal emissions from biomass thermal processes and supports evidence-based regulatory and occupational health decision-making.

METHODOLOGICAL CONTRIBUTION

The overarching objective of the methodology is not merely measurement, but the development of a mechanistically linked, risk-informed environmental assessment framework that bridges industrial thermochemical processes with environmental transport and human health outcomes. This structured approach ensures that conclusions drawn regarding PTE emissions from thermally modified wood processing are scientifically defensible, reproducible, and aligned with regulatory environmental health standards.

LIMITATIONS AND FUTURE RESEARCH

This study provides an integrated experimental and modeling assessment of PTE-bound $PM_{2.5}$ emissions from low-temperature thermal modification of wood; however, certain limitations should be acknowledged. First, particulate sampling was based primarily on filter-integrated measurements, which probably will not fully capture short-term emission transient peak events. Second, elemental analysis focused on total metal concentrations without detailed chemical speciation, limiting interpretation of bioavailability and toxicity differentials among oxidation states. Third, the TPM-FTM simulations were parameterized using site-specific operational and meteorological inputs, which may constrain broader regional generalization. In addition, health risk estimates were derived from established regulatory exposure assumptions that may not reflect individual behavioral variability or cumulative multi-pathway exposure dynamics.

Future research should incorporate real-time particle sizing and chemical characterization techniques to improve temporal resolution and capture dynamic emission profiles. Advanced metal speciation analyses and in vitro bioaccessibility testing are recommended to refine toxicological relevance and dose–response assumptions. Expanding the modeling framework to regional-scale dispersion systems and coupling it with secondary aerosol chemistry modules would enhance predictive robustness. Further evaluation of engineering controls, ventilation efficiency, and emission mitigation strategies within thermal processing facilities is also warranted. Collectively, these advancements would strengthen mechanistic understanding, improve exposure quantification, and support more comprehensive environmental and occupational health risk evaluations.

Figure Labels: Use 8 point Times New Roman for Figure labels. Use words rather than symbols or abbreviations when writing Figure axis labels to avoid confusing the reader. As an example, write the quantity "Magnetization," or "Magnetization, M," not just "M." If including units in the label, present them within parentheses. Do not label axes only with units. In the example, write "Magnetization (A/m)" or "Magnetization (A (m(1)," not just "A/m." Do not label axes with a ratio of quantities and units. For example, write "Temperature (K)," not "Temperature/K."

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- *Author's Declaration*

I, Appiah, Mark Kubi, hereby declare that this research methodology titled: "Integrated Experimental and Modeling Assessment of Potentially Toxic Element–Bound $PM_{2.5}$ Emissions from Low-Temperature Thermal Wood Processing" is the result of my own original research methodology work conducted under approved academic supervision.

All sources of information, data, figures, and scholarly materials used in this study have been duly acknowledged and cited in accordance with accepted Journal standards. The experimental design, data collection, analytical procedures, modeling framework (TPM-FTM), statistical analyses, and risk assessment interpretations presented in this study were carried out by me.

I accept full responsibility and affirm that it represents my independent scholarly contribution to the field of environmental emission assessment and health risk evaluation.

- *Author Contributions*

Mark Kubi Appiah conceptualized and designed the study, including the development of the thermochemical environmental assessment framework linking wood thermal modification processes to $PM_{2.5}$ generation, trace metal characterization, and exposure modeling. He conducted field

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sampling, laboratory experimentation (gravimetric analysis, acid digestion, and ICP–OES measurements).

He worked on data processing, statistical analysis (descriptive statistics, correlation analysis, PCA), and Monte Carlo–based uncertainty and sensitivity modeling. He also developed the mathematical formulations for particulate concentration determination, emission characterization, and exposure–risk integration.

The author drafted the original manuscript, prepared all figures and tables, conducted literature synthesis, and interpreted the results within regulatory and environmental health contexts.

➢ *Conflict of Interest Declaration*

The author declares that there are no known financial, personal, institutional, or professional relationships that could be perceived as influencing the research methodology presented in this study titled: "Integrated Experimental and Modeling Assessment of Potentially Toxic Element–Bound $PM_{2.5}$ Emissions from Low-Temperature Thermal Wood Processing". The research was conducted independently and objectively. No external funding sources, commercial entities, or affiliated organizations had any role in the study design, data collection, analysis, interpretation of results, manuscript preparation. The author affirms that there are no competing interests that could have appeared to influence the outcomes or conclusions of this research.

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