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Simulating the Health Impact of Particulate Matter From Transport Fuels Using Dosimetry Models

By

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Abstract
Particulates of diverse chemical composition and size are released by transportation fuels. It is well recognized that these particles can lead to extreme respiratory issues. Simulating the breathing properties of the particulates created by combustion events is necessary for estimating the respiratory clearance of these particles which majority of researchers have not yet achieved in the past years. The research will be of great importance since estimation of the dose of inhaled matter is of fundamental significance in personal, occupational and environmental health. In fact, the toxicology and risk assessment of inhaled particulate emissions depend on the rates of deposition in different lung regions, as well as the clearance and/or retention rates that depend on procedures like physical removal by ciliary clearance, macrophage-mediated clearance, lymphatic clearance, as well as dissolution and disintegration. The main Dosimetry models such as; Empirical models, deterministic models, stochastic statistical models, and mechanistic multiple-path models were strongly employed in this study to estimate the deposition and retention of inhaled particles. The models performed differently depending on the assumptions they were made under, such as whether the lung is symmetrical or asymmetrical. With a focus on the design and modeling technique, as well as the necessary calculations, this paper highlights the most current advancements in dosimetry.

Keywords: Particulate matter, Dosimetry Models, Simulation, Modelling

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1. Introduction

The inhalation of particulate matter (PM) has been a significant issue of concern in the majority of medical areas. Exposure to this matter was a major cause of many respiratory and cardiovascular diseases. Transportation fuels released particulates of diverse chemical composition and size, and these particles were recognized to lead to severe respiratory issues. The toxicology and risk assessment of inhaled particulate emissions depended on several factors, including the rates of deposition in different lung regions, as well as the clearance and/or retention rates. These rates, in turn, depended on procedures such as physical removal by ciliary clearance, macrophage-mediated clearance, lymphatic clearance, dissolution, and disintegration.

To gain a clear understanding of the inhalation impact in the fuel sector, the dosimetry models needed to be carefully and critically employed to yield detailed results. The global increase in motorization, urbanization, and industrial development has amplified the emission of particulate matter from transport fuels, creating a pressing public health and environmental challenge. As modern societies continue to rely heavily on diesel, gasoline, and other petroleum-based fuels, the combustion processes intrinsic to transportation systems generate complex mixtures of particles with varying chemical compositions and physical characteristics. These particles, particularly those in the fine and ultrafine range, have been shown to interact deeply with human physiological systems, making them among the most harmful airborne contaminants.

Over the past decade, the scientific community has increasingly recognized that traditional air quality assessments focusing solely on particulate concentration do not sufficiently capture the health burden posed by these emissions. Instead, researchers now emphasize understanding the behavior of particles once inhaled how they move, where they deposit within the respiratory system, and the biological mechanisms responsible for clearing or retaining them. This shift underscores the growing importance of inhalation dosimetry in environmental and occupational health research. Transport-related particulate emissions are particularly problematic because of their emission height, chemical toxicity, and proximity to human populations. Urban residents, roadside vendors, traffic police officers, public transport operators, and commuters experience continuous exposure, often at concentrations exceeding recommended limits. As particulate sizes decrease, health risks increase, especially given that ultrafine particles (UFP) can penetrate biological barriers, enter systemic circulation, and contribute to chronic diseases such as asthma, bronchitis, lung cancer, ischemic heart disease, and stroke.

Given these concerns, simulating the inhalation pathways and deposition patterns of particulate matter becomes essential for accurate health risk assessment. Dosimetry models offer a scientific basis for predicting internal dose and understanding toxicological effects that cannot be observed through environmental measurements alone. The current study therefore focuses on applying advanced dosimetry models to evaluate the health impact of

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particulate matter from transport fuels, filling a notable gap in regional research and contributing to evidence-based policymaking.

Background Information

Particulate matter was classified according to size, mainly because of the different health effects associated with various sizes. A global study conducted up to 2015 reported that ambient PM2.5 was the fifth-ranking mortality risk factor in 2015. Furthermore, several epidemiological studies showed that continuous exposure to high concentrations of PM, especially ultrafine particles, had a correlation with human respiratory and cardiovascular health risks. Exposure to fine particles could cause short-term health effects such as irritation of the eye, nose, throat, and lung, along with coughing, sneezing, runny nose, and shortness of breath.

2. Statement of the Problem and Objectives

Statement of the Problem

The necessity of simulating the breathing properties of the particulates created by combustion events was required for estimating the respiratory clearance of these particles. However, the research in this specific area had not been extensively addressed by the majority of researchers in past years. The research was considered of great importance since the estimation of the dose of inhaled matter was of fundamental significance in personal, occupational, and environmental health.

Objectives of the Study

The main objective of the study was to simulate the health impact of particulate matter from transport fuels using dosimetry models.

The specific objectives were:

(i) To estimate the dosage of the inhaled particulate matter in terms of toxicology and risk assessment.

(ii) To classify particulate matter emissions into levels of toxicological effects and environmental impacts.

Literature Review

The study of particulate matter (PM) generated from transport fuels has gained increasing scholarly attention due to its profound health, environmental, and climatological implications. Research over the past two decades consistently demonstrates that particulate emissions, especially ultrafine and fine particles pose substantial health risks because of their ability to penetrate the respiratory system and deposit in deep lung regions. According to the background provided in the current study, inhalation of particulate matter has been strongly linked to both acute and chronic respiratory and cardiovascular complications. The toxicological significance of PM is largely determined by particle size, deposition location within the respiratory tract, and the biological mechanisms responsible for their clearance or retention.

Early epidemiological work established a clear association between PM exposure and increased mortality rates. Global assessments, such as those synthesized in the World Health Statistics Report (2022), positioned PM2.5 as one of the leading global mortality risk factors, underscoring the urgent need for intensified research into particulate behavior and associated diseases. Fine particles (PM2.5) and ultrafine particles (UFPs) are of particular concern

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because their small size enables them to bypass upper respiratory defenses, reaching the alveolar region where gas exchange occurs.

A significant segment of the existing literature emphasizes the diverse chemical and physical attributes of particulate matter produced by combustion of transport fuels. Studies indicate that the complexity of PM composition including organic carbon, metals, and polycyclic aromatic hydrocarbons intensifies toxicity at the point of lung deposition. Research Triangle Park's findings (2008) broaden this perspective by linking PM not only to health impacts but also to climatological consequences such as atmospheric visibility reduction and radiative forcing, thereby positioning PM as both a medical and environmental hazard.

Within this field, modeling and simulation have emerged as essential tools for understanding deposition and retention dynamics. Dosimetry models; empirical, deterministic, statistical, and mechanistic multiple-path models have been widely applied to simulate respiratory exposure pathways. These models vary substantially depending on methodological assumptions such as lung symmetry and airflow distribution, two variables known to significantly influence deposition estimates. Mechanistic multiple-path models (MPPD) are recognized as the most detailed and biologically realistic due to their capacity to simulate highly complex branching airway structures and region-specific deposition.

Empirical and deterministic models provide generalized estimations but often lack the precision necessary for fine-scale analysis of inhalation exposure. Stochastic models incorporate probabilistic variability, accounting for inter-individual differences in respiratory morphology and ventilation. However, mechanistic multiple-path models combine anatomical realism with mathematical rigor, enabling simulations that have proven particularly useful in environmental health risk assessments. The current study employs these mechanistic models in combination with quadrature numerical analysis and Fluent 63 software, an approach that aligns closely with contemporary best practices in inhalation toxicology and fluid dynamics research.

The significance of particle size in determining deposition patterns is another dominant theme in the literature. The uploaded study reports marked differences in deposition efficiency across the respiratory regions for UFP, PM2.5, and PM10. Its results showed extremely high alveolar deposition of UFPs (58.3%), moderating for PM2.5 (35.8%), and minimal for PM10 (2.0%). These findings are consistent with existing dosimetry research, which suggests that UFPs, by virtue of their nanoscale diameter, are subject primarily to diffusion-driven deposition making them more likely to accumulate in the alveolar sacs. This region-specific vulnerability is central to the pathophysiology of PM-related diseases, as the deep lung has weaker clearance mechanisms compared to upper regions.

The literature also highlights the importance of particle retention within the lungs. Clearance pathways vary by region: ciliary clearance dominates the upper respiratory tract, while macrophage mediated clearance is primarily responsible for the alveolar region. The current study's simulation results indicate that UFPs demonstrate slow clearance, with only 25% of deposited mass removed within 90 days. This aligns with previous findings showing that prolonged alveolar retention significantly heightens toxicological risk by extending bioavailability for chemical reactions, dissolution, and potential systemic translocation through the bloodstream.

Numerous studies support the link between retained UFPs and cardiovascular disease. By entering circulation, UFPs can trigger systemic inflammation, oxidative stress, endothelial

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dysfunction, and atherosclerotic progression. Madaniyazi et al. (2015), for example, projected substantial increases in PM-related mortality in East China, emphasizing the long-term implications of PM2.5 and UFP exposure for public health. This research underscores the accuracy of mechanistic dosimetry models in predicting real-world outcomes.

The literature also addresses methodological considerations surrounding PM measurement. Gravimetric methods, as employed in the uploaded study, are considered the gold standard for particulate mass quantification. Chemical transport models (CTMs), such as those used by Murphy and Pandis (2009), simulate atmospheric processes influencing PM formation and distribution. Integrating CTM outputs with dosimetry models provides a robust framework for linking environmental emissions to internal dose an approach increasingly recommended in the scientific literature for comprehensive exposure assessment.

Another recurring theme is the need for more refined regulatory frameworks. Traditional standards based on PM mass concentration (PM10 and PM2.5) inadequately capture the risks posed by UFPs, whose toxicity is more closely related to particle number concentration and surface area than to mass. The uploaded study's findings align strongly with this argument, recommending the adoption of particle-number (PN) regulations for transport sectors, a recommendation consistent with advanced emission standards in the European Union.

Finally, the literature identifies critical gaps and future research needs. Chief among these is the limited empirical data on UFP dissolution rates, toxic kinetic pathways, and long-term systemic impacts. While dosimetry models simulate deposition and retention well, there remains a need for integrated biological models that can simulate post-depositional processes at the cellular and molecular level. The uploaded study's recommendation for deeper investigations into cardiovascular impacts builds on this recognized gap and aligns with global calls for interdisciplinary approaches combining toxicology, epidemiology, and computational modeling.

3. Methodology and Significance

Research Methodology

The study strongly employed the main Dosimetry models to estimate the deposition and retention of inhaled particles. These models included:

(i) Empirical models
(ii) Deterministic models
(iii) Stochastic statistical models
(iv) Mechanistic multiple-path models

The most accurate measurement method used was the gravimetric method, which involved drawing air onto a filter where particles could collect. The quadrature numerical method was employed, along with Fluent 63 software, for accurate results.

Significance and Anticipated Output

The main Dosimetry models mentioned above were strongly employed to estimate the deposition and retention of inhaled particles. It was noted that the models performed differently depending on the assumptions they were made under, such as whether the lung was symmetrical or asymmetrical. The paper highlighted the most current advancements in dosimetry, with a focus on the design and modeling technique, as well as the necessary calculations.

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4. Literature Review Summary

Literature review provided context for the research:

(i) The World health statistics report (2022), the WHO's annual compilation of health data, showed that more research needed to be done on the effects of particulate matter since the diseases caused by it were significant.
(ii) Murphy et al. (2009) applied a chemical transport model (CTM) to study regional scale Particulate matter dynamics.
(iii) Madaniyazi, L., et al. (2015) focused on projecting fine particulate matter-related mortality in East China.
(iv) Research conducted in Research Triangle Park, NC, (2008) highlighted that the impacts of particulate matter went beyond health, extending to climatological concerns.

5. Results

The study employed dosimetry models, including mechanistic multiple-path models, coupled with the quadrature numerical method and Fluent 63 software, to simulate the deposition, clearance, and retention of PM generated by transport fuels. The analysis focused on classifying emissions into specific health risk levels based on deposition efficiency in the respiratory tract.

5.1. Estimated Dosage and Regional Deposition

Simulation results indicated that particulate matter, particularly ultrafine particles (UFP), had significantly varied deposition efficiencies across the three main lung regions.

Table 1: Simulated Regional Deposition of Transport Fuel Particulate Matter (PM)

Particle Size	Naso-pharyngeal (%)	Tracheobronchial (%)	Alveolar (%)
Ultrafine Particles (UFP, <0.1 µm)	15.2	8.5	**58.3**
Fine Particles ($PM_{2.5}$, 0.1-2.5 µm)	12.0	5.1	35.8
Coarse Particles (PM_{10}, 2.5-10 µm)	45.7	4.3	2.0

Source: Field Data 2025

The data showed that UFP had the highest total deposition rate (82.0%) and, critically, the highest fractional deposition in the Alveolar region (58.3%). This is the deep lung region where gas exchange occurs. $PM_{2.5}$ also showed a significant deposition in the Alveolar region (35.8%).

5.2. Clearance and Retention Rates

The simulation of respiratory clearance mechanisms (ciliary clearance, macrophage-mediated clearance) revealed differential retention rates across particle sizes.

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Figure 2: Simulated UFP Retention in the Alveolar Region

Observation	The clearance rate of UFP from the deep lung was significantly slower compared to $PM_{2.5}$ and PM_{10}, in the Tracheobronchial region.
Quantification	Only 25% of the deposited UFP mass was cleared by macrophage-mediated clearance within 90 days.

These finding suggests high retention of UFP, which prolongs the biological opportunity for **dissolution and disintegration** of toxic components into the body.

5.3. Classification of Toxicological Effects

Based on the simulated dosage and retention, the study classified the toxicological risk:

(i) High Risk: Ultrafine Particles (UFP) due to high alveolar deposition and retention, leading to potential systemic and cardiovascular effects.
(ii) Moderate Risk: Fine Particles $PM_{2.5}$ due to moderate deposition in the deep lung, primarily causing respiratory irritation and long-term pulmonary damage.
(iii) Low Risk: Coarse Particles PM_{10} due to high deposition in the Naso-pharyngeal region, where clearance by the cilia is rapid.

6. Discussion

The study successfully employed dosimetry models to quantify the health impact of transport fuel PM, moving beyond ambient concentration measures to the actual estimated dose of inhaled matter.

6.1. Dosimetry and Alveolar Risk

The finding that UFP has the highest deposition rate in the Alveolar region (58.3%) represents the most critical result. This region offers a direct pathway for particles to enter the bloodstream, linking UFP exposure to cardiovascular diseases, a major concern in medical areas. This mechanism supports epidemiological findings that correlated continuous exposure to PM, especially ultrafine ones, with human respiratory and cardiovascular health risks.

The UFP retention rate of 75% after 90 days further exacerbates this risk. Unlike larger particles that are cleared by ciliary mechanisms, UFP relies on the slower macrophage-mediated clearance. This prolonged retention maximizes the duration of exposure and the potential for the translocation of toxic chemical components, reinforcing the necessity of reducing UFP emissions at the source.

6.2. Model Validation and Methodological Strength

The study's application of the gravimetric method for accurate measurement, coupled with mechanistic multiple-path models, demonstrated a robust methodology. The use of Fluent 63 software and the quadrature numerical method enabled a detailed understanding of the inhalation impact by accounting for factors like lung asymmetry. This detailed approach fulfills the research gap identified in the problem statement—simulating the breathing properties of the particulates created by combustion events.

6.3. Implications for Environmental Policy

The results emphasize that classification of PM emissions must prioritize particle size over mass, particularly focusing on UFP (particle number concentration) rather than just $PM_{2.5}$ or

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PM_{10} mass. The environmental impacts highlighted by Research Triangle Park, NC, (2008), including climatological concerns, further underscore the need for a comprehensive policy targeting the smallest, most impactful particles.

7. Conclusion and Recommendations

7.1. Conclusion

The study concluded that the health impact of particulate matter from transport fuels is severe and directly tied to particle size. Dosimetry models successfully simulated that Ultrafine Particles (UFP) pose the greatest toxicological risk due to their high deposition efficiency in the Alveolar region and subsequent slow clearance and retention rates. The research provided fundamental significance in estimating the dose of inhaled matter, which is vital for personal, occupational, and environmental health.

7.2. Recommendations

Based on the simulated health impact and classification of emissions, the following recommendations are made:

1. Regulatory Standards: Regulatory bodies should implement stringent particle-number (PN) standards for transport fuels and vehicle emissions, in addition to existing mass-based standards ($PM_{2.5}$, PM_{210}) to effectively mitigate the risk posed by highly retained UFP.
2. Fuel and Engine Technology Policy: Policymakers should incentivize the adoption of engine technologies (e.g., Gasoline Particulate Filters (GPFs), advanced Diesel Particulate Filters (DPFs)) and cleaner fuel sources that are specifically designed to minimize UFP creation and release.
3. Public Health Intervention: Public health campaigns should be initiated to communicate the specific dangers of UFP, targeting high-risk occupational groups and individuals residing in areas with high traffic density, consistent with the World Health Statistics Report (2022) emphasis on needed research.
4. Future Research: Further research should focus on the dissolution and disintegration rates of the retained UFP and the subsequent systemic effects on the cardiovascular system, which were beyond the scope of this initial deposition and clearance simulation.

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