ANALYSIS OF PM 2.5 EXPOSURE IMPACT IN DIFFERENT ATMOSPHERIC CONTEXTS: A DETAILED FEM SIMULATION ANALYSIS IN A VIRTUAL LOAC DEVICE

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Abstract: PM 2.5 concentration is a significant factor in fine particulate matter pollution, causing adverse health impacts, particularly respiratory health. Different sources of PM 2.5 pollutants can also damage human lungs. A comparative impact analysis on lungs in high and low-AQI-ranked cities can help regenerate urban air quality improvement guidelines and future land-use planning. A study of human lung mechanism simulation using a microfluidic device's virtual 3D model called Lung on a Chip (LOAC), by analyzing fine particle transport, deposition, cell uptake, and inflammatory response, shows how changes in PM 2.5 concentration cause damage to health conditions. The deposition level is not proportional to the PM 2.5 concentration; it depends on the source, breathing style, outdoor exposure, and exposure duration. This research helps identify harmful PM 2.5 concentration thresholds and guides future research on healthy zoning in future cities, considering air quality's impact on human health in urban areas.

Keywords: *PM 2.5 impact, air quality index, virtual simulation, health impact, transportation and deposition*

1. Introduction

PM 2.5 is mainly particulate matter, smaller than 2.5 microns, and floats in the air as a pollutant (*Particulate Matter (PM) Basics | US EPA*, 2024). PM 2.5 is essentially a liquid droplet-solid particle mixture in the air and can cause various types of respiratory diseases, lung damage, and even cancer when inhaled (Air Quality: PM2.5, 2019; *PM 2.5 - What Does It Mean, and Why Does It Matter?*, 2021). This mixture mainly carries heavy metal particles, organic carbon such as soot and elemental carbon particles, nitrates, sulfates, secondary organic aerosols, and other particulate matter. These particles are most responsible for air pollution in various cities (*PM 2.5 - What Does It Mean, and Why Does It Matter?*, 2021; Wang et al., 2020; Combes & Franchineau, 2019). Most PM 2.5 concentrations are generated from construction sites, industries, automobiles, power plants, etcetera (*Particulate Matter (PM) Basics | US EPA*, 2024). In cities where pollution exposure from these sources is high and there is a lack of air filtration facilities, PM 2.5 concentrations are highest. U.S. Environmental Protection Agency (EPA) has set a level or standard for the concentration of this PM 2.5 in cities so that we understand how harmful and unhealthy we live. At the same time, we try to mitigate and counteract the detrimental effects of this pollutant (*PM 2.5 - What Does It Mean, and Why Does It Matter?*, 2021). This standard is called the PM 2.5 concentration level, based on the concentration of all particulates that generally harm the respiratory system, and is measured in micrograms per cubic meter (ug/m3). The city with higher PM 2.5 particulates in the air is called a higher PM 2.5 concentration-based polluted city. Various organizations, such as IQAir, measure these levels and prepare reports. The report is prepared by collecting, processing, and analyzing data from ground-level monitoring stations, revealing cities' pollution ranking ("2020 World Air Quality Report," 2020). According to IQAir, the most polluted city based on PM 2.5 concentration in 2022 is Lahore, located in Pakistan. Dhaka ranks 49th in this ranking, one of the most densely populated cities in the world, but Dhaka's concentration rate is almost half that of Lahore (IQAir, 2020).

On the other hand, according to Rethinking Future and Airly.org, the lowest pollution in the world in 2021 and 2022 is in Zurich, Switzerland, a significant city geographically and economically (10 World's Least Polluted Cities in 2021, 2022; The 7 Cities with the Cleanest Air in the World - Ranking - Airly WP | Air Quality Tracker Airly, n.d.). The sources and types of pollutants in these three cities have some individual characteristics (Begum et al., 2013; Ahmad et al., 2020; *Air Pollution Country Fact Sheets 2022*, n.d.). Numerical analysis of these characteristics will help to indicate individual and city-based variations in the harmful effects of inhalation, respiratory effects, and health effects of different particulates due to differences in particle type. Besides, it will also help to determine the kind of pollution and the problems arising based on it and its solutions. Since this analysis indicates adverse effects on the human respiratory system, the study's main objective is to analyze the effects of these particles on the human lungs. The Lung on a Chip device is a microfluidic device that mimics the human lung by mimicking the physiological properties of alveolar tissue. It is an organ-on-a-chip device that combines

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MEMS, biotechnological techniques, and microcellular architecture (Bhatia & Ingber, 2014). It is used in lab simulations for drug delivery and disease modeling (Arefi et al., 2020). We have developed a CAD kernel 3D model of this lab-on-a-chip device for virtual Multiphysics simulation. We followed that model, mimicking the lung-on-a-chip device designed by Hancock (Huh et al., 2010; Hancock, M.J. and Elabbasi, N., 2018). This is a proven model so we can analyze it with proper data through COMSOL simulation (Arefi et al., 2020). Because PM 2.5 is particles under 2.5 microns, ultrafine nanoparticles are particles less than 100 nanometers in diameter (*Nanoparticle*, 2024), and nanoparticles above that are coarse nanoparticles. Numerical analysis and epidemiological research require that these two types of particles be measured separately (Wilson & Suh, 1997). Simulating the transport, deposition, and adsorption inflammation response of N.P.s on LOAC requires two different approaches: the Eulerian approach for ultra-fine nanoparticles and the Lagrangian particle tracking approach for coarse nanoparticles (Arefi et al., 2020). From the transportation-deposition rate of different particle type, size, and concentration and their response to the epithelial layer of the LOAC device, the absorption and desorption rate will help us understand the critical aspects of the impact of different AQI levels along with different contexts, and at how rate the harmful impact changes compared to the changes in AQI level along with PM 2.5 pollutant type. Prasad et al. (2023) already monitored, analyzed, and reviewed the impact of PM concentration on specific health conditions, including carcinogenicity effects, type II diabetes, and cardiovascular diseases. In this paper, through comparative analysis, we will understand the health impact of different pollution sources and their levels and guide our real-time actionable and respiratory hazard prevention at different PM 2.5 concentration levels. Through this, we will also provide direction for future research on what kind of ventilation system is preferable in different contexts for indoor air quality improvement. There are specific particle types in PM 2.5 concentration that are incredibly harmful to health and create cardiovascular disease, such as combustible particles, metal particles, organic particles, sulfate, and nitrate particles (*What Is Particle Pollution? | US EPA*, 2024; *Health and Environmental Effects of Particulate Matter (PM) | US EPA*, 2024).

2. PM 2.5 concentration

2.1. PM 2.5 CONCENTRATION, PARTICLE PROPERTIES, AND HARMFUL IMPACT

PM 2.5 particles come in many sizes and shapes and can be made of different chemicals. Some harmful particles are emitted from direct sources, and some are produced from complex chemical reactions. Construction sites, fires, and uneven, brittle roads are responsible for direct emissions. Various industrial entities, such as power plants, chemical industries, factories where chemicals are used, and vehicles, are responsible for indirect emissions and chemical reactions (*Particulate Matter (PM) Basics | US EPA*, 2024). Combustion of automobile engine fuel, emissions from various factories, and combustion of various biomaterials are among the primary emission sources of PM 2.5.

On the other hand, secondary sources include various chemical reactions and the resulting formation of new pollutant particles. PM 2.5 fine particulate matter includes various carbon species derived from fuel combustion, such as O.C. and E.C., ionic species, such as nitrate, ammonia, and sulfate, and various secondary organic aerosols generated from various heterogeneous reactions. Sulfate and nitrate particles significantly affect PM 2.5 concentration levels (Chen et al., 2014). The health impact, attributes, and general concentrations of these harmful particles are described in Table 1 below:

Table 1: Harmful Particles of PM 2.5 Concentration

Name	Impact	Size & variation	Concentration
Fine Sulfates ($SO4^{2-}$):	Sulfate particles can aggravate lung disorders, including asthma and chronic obstructive pulmonary disease, by irritating the respiratory system (COPD) ("Sulfur Dioxide Effects on Health - Air (U.S. National Park Service)," n.d.; *Particle Pollution and Respiratory Effects	US EPA*, 2024).	Size: 0.1 - 2.5 μm Density: Varies (typically around 1.04 - 1.5 g/cm^3)	Harmful Particles: Ammonium sulfate, sodium sulfate Concentration: Varies according to context.
Fine Nitrates ($NO3^{-}$):	Nitrates can worsen respiratory conditions and cause airway irritation (*Basic Information About NO2 | US EPA*, 2024).	Size: 0.1 - 2.5 μm Density: Varies (approximately 1.18 - 1.84 g/cm^3)	Variable, influenced by urban and industrial emissions. Other Entities: Ammonium nitrate
Elemental Carbon (E.C.) and Organic Carbon (O.C.):	Polycyclic aromatic hydrocarbons (PAHs), which are carcinogenic and can cause respiratory problems and other health issues, are among the potentially dangerous substances that may be present in these particles. They are frequently linked to combustion activities (*Polycyclic Aromatic Hydrocarbons (PAHs)	Public Health Statement	ATSDR*, n.d.).	Size: 0.1 - 2.5 μm Density: EC - approximately 2.1 g/cm^3, OC - around 1.5 g/cm^3	It can be substantial in urban areas. Other Entities: Includes polycyclic aromatic hydrocarbons (PAHs)
Metals and Metal Compounds:	Lead, cadmium, and nickel are hazardous metals that can affect the respiratory system. When taken into the bloodstream, they can potentially result in systemic health problems (METALS - International Occupational Safety & Health Information Centre, n.d.).	Size: Varies (can be in the PM2.5 range) Density: Variable, depending on the specific metal	Depends on industrial and combustion processes. Other Entities: Lead, cadmium, nickel, arsenic, mercury, chromium

Ultrafine Particles:	Ultrafine particles (smaller than 0.1 um) may be particularly dangerous because they can penetrate the circulation and the deepest parts of the lungs. These particles may result in cardiovascular and respiratory issues (*Ultrafine Particle*, 2024; *Particle Pollution Exposure | US EPA*, 2024; *IQAir | First in Air Quality*, n.d.; *Particle Pollution*, n.d.).	Size: Smaller than 0.1 μm Density: Variable, typically around 1 g/cm^3	It can be significant near emission sources. Other Entities: Often not specified individually but can include combustion-generated nanoparticles.
Biological Particles:	While many biological particles are not directly harmful, they can trigger allergies and respiratory sensitivities in susceptible individuals. Mold spores, pollen, and certain types of bacteria can cause respiratory symptoms (*Allergies and the Immune System*, 2024). Due to their ability to penetrate the circulation and deep into the lungs, ultrafine particles (smaller than 0.1 m) can be particularly dangerous and may result in cardiovascular and respiratory issues (*Particle Pollution*, n.d.; *Allergies and the Immune System*, 2024).	Size: 0.1 - 2.5 μm Density: Comparable to water (around 1 g/cm^3)	It is influenced by vegetation, pollen, and microbial activity. Other Entities: Mold spores, pollen, bacteria

Recent studies show urban air pollution is responsible for 3.5 million annual deaths (Flood-Garibay et al., 2023) due to respiratory and cardiovascular diseases (*Short-term Exposure to High Levels of Air Pollution Kills 1 Million Globally Every Year*, 2024). Current studies also depict that long-term PM 2.5 exposure impacts mental health, even in low PM 2.5 levels (Lyons et al., 2024).

2.2. PM 2.5 CONCENTRATION PROPERTIES OF DIFFERENT ATMOSPHERIC CONTEXT:

Lahore, the world's most polluted city, occupies the top spot in the world in PM 2.5 concentration-based population ranking (IQAir, 2020). Dhaka, on the other hand, is one of the most densely polluted megacities in the world, with PM concentration levels almost half that of Lahore ("2020 World Air Quality Report," 2020; IQAir, 2020). A correlation exists between Dhaka and Lahore in terms of pollution sources. The main difference is in the pollutant concentration level (Begum et al., 2013; Ahmad et al., 2020). On the other hand, Zurich is one of the least polluted cities globally and a significant economic zone for Europe. This city's pollution type is different from that of previous cities because the city of Zurich is wholly exposed to indirect pollution. This means Zurich suffers from pollution and PM 2.5 concentrations produced by other countries or cities (*Air Pollution Country Fact Sheets 2022*, n.d.).

The details of PM 2.5 concentration level, specific concentration of different harmful particles, pollution source and its effect, and their percentage in these three cities are given below:

1) Dhaka: Dhaka, the capital of Bangladesh, where 30-50% of PM 10 particles fall within the EPM 2.5 concentration level. Most of this particulate pollution is emitted from different types of combustible automobile engines, construction sites, road dust, and construction industries. Although Dhaka's PM 2.5 particle pollution is half that of Lahore, some specific particles, such as B.C. and sulfur from combustible engines and elemental carbon from other pollutants, are in excess. Table 2 shows data on PM 2.5 pollution in Dhaka (Begum et al., 2013):

Table 2

Harmful Nano Particles and Impact in Dhaka (Begum et al., 2013):	
Seven types of sources, particle types, and share-	
Type-1	Source: Lead Battery Industries Major Particle: Pb, Bc, Na Trace Particle: Si, K, Mn, Fe Share: 6.59%
Type -2	Source: Galvanizing factories Major Particle: E.C., Cl, Zn, Pb Trace Particle: K, Ca, Fe Zn comes from reflective properties (BEGUM, 2004) Pb comes from manufacturing (Krepski, 1985)
Type -3	Source: Sea salt contributed in monsoon season, atmospheric acid displacement reactions, Salt (NaCl, replaced by Sulphur) Major Particle: B.C., Na, S Trace Particle: Mg, Al, Si, Cl, K, Fe, Zn Share: 6.3% of fine particle mass

Type -4	Source: Brick klin, coal burning in klin (contain 4-6% Sulphur) Major Particle: B.C., S, K, Pb, Trace Particle: crustal element During the burning of waste material - Cl, Zn, and Pb emitted from plastic burn		
Type -5	Source: Soil Dust Major Particle: B.C., Mg, Al, Si, S, Cl, K, Ca, Ti, Fe, Cu Share: 9.5% of the fine particle mass		
Type -6	Source: Road Dust Major Particle: B.C. other Particle: Mg, Al, Si, P, S, Cl, K, Ca, Fe Share: 15% of the fine particle mass		
Type -7	Source: Automobile Major Particle: B.C. & S Share: 36% of fine particle mass		
Harmful PM 2.5 Particulates Exposure In Dhaka			
Particle	*Concentration ($\mu g/m^3$)*	*Found in*	*Other Properties*
BC & EC	Max: 22.417 Mean: 8.208	In every pollution	Carbon particles
Si Particulates	Max: 8.889 Mean: 1.194	Industries, Road, soil Dust	Silica (SiO_2)
Salfer Particulates (Fine Sulfates)	Max: 15.531 Mean: 2.476	Almost every pollution	Sulfur Dioxide (SO_2)
Zn Particulates	Max: 8.078 Mean: .827	Sea salt and industrial pollution	
Main Sources:			
Source	*Share*	*Particles*	
Vehicular Pollution	36% of total mass	BC & S	
Road Dust	15%	BC, Mg, Al, Si, P, S , Cl, K, Ca, Fe	
Brick Klin & Construction	22%	B.C., S, K, Pb	

2) Lahore: Lahore is the most polluted city in the world in terms of PM 2.5 concentration ranking. Vehicle combustible engines, various burners, and road and soil dust are significant sources of fine particle pollution. Table 3 below shows the various pollutants and their percentage, source, and concentration data (Ahmad et al., 2020):

Table 3

Harmful Nano Particles and Impact in Lahore (Ahmad et al., 2020):			
Top Harmful Particulates:	*Percentages*	*Source*	*Concentrationn ($\mu g/m^3$) 24-h average*
Sulfate	20.1%	Vehicle	14.8
SOA (Secondary Organic Aerosol)	16.2%	Smoke	
EC	11.0%		8.6
Nitrate	11.6%	Industries	21
POA (Particulate Organic Aerosol)	18.2%	Biomass Burning	
O.C. (Organic Compounds)		Waste Material	63

3) Zurich: Zurich is the world's least polluted city, which does not pollute itself, but recently, Zurich has been an indirect victim of pollution from neighboring countries. This resulted in a net increase in pollution and PM 2.5 concentration levels in Zurich. Although this pollution is lower than other cities, Zurich is still one of the most livable cities in the world. However, it is crucial to determine the extent to which this new pollution may affect the health of the people of Zurich (*Air Pollution Country Fact Sheets 2022*, n.d.). The increase in the incidence of COVID-19 in European cities helps us understand that even cities with clean air are not far from health risks. The particle transportation and deposition rules cannot be verified from particle concentration alone. Instead, measuring the relationship between increasing or decreasing health risks with the increase in particle concentration and the amount of damage caused by any source is essential. Zurich is our example, which will help us fully understand the effect of concentration on respiratory health risks. The pollutant concentrations found in Zurich are listed in Table 4 below (*Health and Environmental Effects of Particulate Matter (PM) | US EPA*, 2024; *Particle Pollution and Respiratory Effects | US EPA*, 2024):

Table 4

Zurich Harmful PM 2.5 Exposure Particulate (PM 2.5 Pollution from other countries)			
Particle	*Percentage*	*Source*	*Concentration (μg/m^3)* *24-h average*
Nitrate	22%	Passive	2.4
Sulphate	36%	Passive	4.3

3. Theories & kinetics

In nanoengineering and computational molecular research, various approaches and methods exist to assess the effects of fine and coarse particles on the respiratory system. Theory and kinetics are used together depending on the data we use in the research. Further discussion of this research is possible with fluid-particle interactions on various biomaterials or microfluidic lab chips. The main objective of our study is to analyze the comparative effects of PM 2.5 concentrations based on context, source, and magnitude, which will then provide a path for in-depth research and in-detail causal collection. Another objective of ours is to develop the role and thinking of multidisciplinary engineers such as Urban Designers and Planners, Architects, and HVAC Engineers in making a sustainable living plan to make a city pollution-free and minimize the health effects of pollution (Combes & Franchineau, 2019; The 7 Cities with the Cleanest Air in the World - Ranking - Airly WP | Air Quality Tracker Airly, n.d; Huh et al., 2010; Arefi et al., 2020; Wilson & Suh, 1997; Tian et al., 2016).

3.1. AQI LEVEL AND PM 2.5 CONCENTRATION
There is a proportional relationship between AQI and PM 2.5 concentration. Generally, AQI or Air Quality Index expresses how polluted the air is or how high the concentration of pollutants is. This level is expressed in an index of good, moderate, unhealthy for the sensitive group, unhealthy, very unhealthy, and hazardous. Each of these groups has its own specific PM 2.5 concentration level. This level is usually expressed as micrograms per meter cubed, which means how many micrograms of PM 2.5 particles are in one cubic meter of air, which is hazardous. Now calculated on a weighted basis, a summation of the mass of all hazardous particles yields a PM 2.5 level. However, it is impossible to know the amount of individual damage of this particle or its transportation or deposition in human lungs from this PM 2.5 level. Because the spread of different particles is not the same everywhere, it depends on the particle's mass, the source of everything. In that case, it is necessary to know the molar mass of the individual particle according to its source, and by searching the attributes of that particle, it is possible to determine the degree of deposition. As can be seen, the particle concentration mass and molar concentration differ significantly, significantly impacting the deposition prediction. Considering the particles we inhale is also essential (Combes & Franchineau, 2019; "2020 World Air Quality Report," 2020; IQAir, 2020; *AQI Basics | AirNow.gov*, n.d.).

3.2. KEY ASPECT OF LOAC DEVICE
Lung on A Chip Device (LOAC) is a microfluidic lab-on-a-chip device representing the critical physical aspect of human lungs consisting of MEMs as an epithelial layer. A microfluidic computation can establish the inhalation and exhalation environment with particle transportation deposition. We use a reference of the Virtual LOAC device developed by Hancock, M.J. and Elabbasi, N. (2018) from the Huh et al. (2010) LOAC device. The device design has two separate chambers for air and blood vessels, separated by a thin epithelial layer (PDMS). We took the air channel for our simulation and omitted the blood vessels. Since blood vessels do not play an influential role in the transportation and deposition of air particulates. We treat the substrate and the rest of the walls as rigid, except for the inlet and outlet. Although there is stretching in Huh's model, this is not vital for our research. The dimension of the device is 2mm in length (L), 400 μm in width (W), and 70 μm in height (H). The inlet is 400*70 μm^2 and the outlet is too. The substrate dimension is 400 x 2000 μm^2, with PDMS as material, a type of MEMS that can represent epithelial tissue well (Arefi et al., 2020).

3.3. TRANSPORTATION AND DEPOSITION
Transportation refers to how Nanoparticles transport or move and stick to the epithelial layer or lung tissue. The process of sticking or attachment of particles onto the surface of lung tissue is called adsorption. If the particles are harmful, it affects lung health. The thin layer of lung cells is defined as the epithelial layer, which is the crucial element of our simulation. The deposition of N.P.s varies and depends on particle size, diameter, shape and density, and the airflow pattern of breathing within the respiratory channel. Coarse particles can deposit in the upper ways of the respiratory tract, while fine particles can deposit in the deeper parts of the lungs (Arefi et al., 2020).

3.4. ADSORPTION & DESORPTION KINETICS
When the particles come into contact with the lung tissue, they can adsorb on the surface through various mechanisms and physical aspects. Different kinds of force and biological interaction take place to consume. We will define the adsorption kinetics using two models, one rapid uptake by cells model and another using Langmuir kinetics to explain adsorption and desorption in an unidirectional microfluid flow. With these, we will develop two equations of Surface reaction rate; one uses a rapid uptake mechanism, and another uses Langmuir kinetics. Langmuir and Frumkin's kinetics can describe finite adsorption and desorption on a substrate surface. Bulk concentration, maximum surface coverage, and surface saturation

rate equation are needed to develop Langmuir Frumkin kinetics for simulation (Huh et al., 2010; Bhatia & Ingber, 2014; Arefi et al., 2020).

3.5. EULERIAN APPROACH

Eulerian is a scientific method that defines the transportation and formation of particles in fluid. Eulerian approach defines a steady state and fixed point, from which we can analyze particle movement and behavior. We will use the advection-diffusion model of the Eulerian approach. As our experimental particle has negligible inertia, adapting the Eulerian Approach is suitable for the simulation (Arefi et al., 2020).

3.6. ADVECTION-DIFFUSION MODEL

Advection defines the bulk movement of particles with the fluid, like carrying the particle along with the air (as a fluid). Diffusion is particles' random movement from high to low concentrated fluidic area. Through mathematical equations, these two models summarize how the N.P.s will be transported (advection) and how they will spread and deposit on the substrate. Studying the behavior of particles is essential for air quality improvement and aerosol health environment research (Huh et al., 2010).

3.7. RAPID UPTAKE MODEL

In this model, the tissue instantly absorbs or takes up particles (endocytosis and phagocytosis), called internalization. In the rapid uptake model, no desorption or surface saturation happens. It defines c=0 as a boundary condition (Arefi et al., 2020).

4. Methodology

4.1.MODELING TECHNIQUE

As we study nanoparticles' transport, adsorption, and related physics, a virtual CAD kernel model simulation of the LOAC device will be performed using COMSOL Multiphysics software to define model building, physics, and boundary conditions. Table X lists the parameters used in our simulation model. Our simulation 3D model is shown in Figure 1.

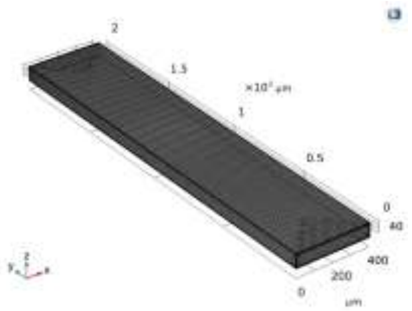


Figure 1, 3D Model of LOAC Device.
(Source: Author; Hancock, M.J. and Elabbasi, N. (2018))

4.2. SOLVING LAMINAR FLOW

In the simulation's first step, we have to solve the microfluidic air flow; fundamentally, we solved the laminar flow using the standard Navier Stokes equation. To represent what a lab-on-a-chip would be, we used a Reynolds number of several hundred (Arefi et al., 2020). Here, such turbulent flow would not work and would be highly linear. The standard Navier-Stokes equation used in our model is stated below-

$$\rho \frac{\partial u}{\partial t} + \rho(u \, . \nabla)u = \nabla . [-pI + K] + F \qquad (1)$$

$$\rho \nabla . u = 0 \qquad (2)$$

Here u and p is the velocity and pressure of the fluid flow, and the ρ and μ are the density and dynamic viscosity of airflow. We have calculated time-dependent unidirectional flow to observe the deposition scenarios on continuous inhalation. Every parameter rate is calculated from the literature. The K in equation (1) is the reference temperature, and the F is a help variable. Temperature is a factor in our research as we simulate different contexts.

4.3 SOLVING TRANSPORTATION OF DILUTED SPECIES

The core part of the research is analyzing and simulating the transport and deposition of Nanoparticles with the support of adsorption-desorption kinetics and modifying the Langmuir-Frumkin equation for surface reaction rate. We use the transport of Diluted Species (tds) module to simulate the mechanism. Modifying the surface reaction rate equation can define whether the simulation is in a rapid uptake or finite adsorption-desorption model.

i) Adsorption-desorption models and equations

We use the Langmuir-Frumkin model, which describes the surface reaction rate (adsorption) through the bulk concentration of particles and maximum surface coverage. The standard equation is,

$$\frac{dc_s}{dt} = k_{ads}c(\gamma_s - c_s) - k_{des}c_s \qquad (3)$$

In equation (3), k_{ads} is the adsorption rate constant, which unit is mol/(m^2.s) for zero-order reaction, where s^{-1} is for first-order reaction. Our adsorption is a zero-order reaction so that we will adapt the rate to the first unit. On the other hand, k_{des} is a first-order reaction, as the reaction is proportional to the concentration of adsorption; the unit should be s^{-1} for the desorption rate constant, c is the initial concentration of the species or the bulk volume concentration, where c_s are the concentration of species onto the surface. Both unit of c and cs is mol/m^3. γ_s is the maximum surface coverage; we can adapt it to a unitless normal, or we can calculate the actual molar rate. For our case, we have calculated the γ_s.

The $k_{ads}c(\gamma_s - c_s)$ define the rate of adsorption, which is proportional to the rate of adsorption constant and the bulk volume concentration of the particle at the inlet and the unoccupied surfaces $(\gamma_s - c_s)$. The increase in concentration of the particles could increase the particle number for adsorption; the rate of surface occupancy describes how much species will be absorbed. Additionally $-k_{des}c_s$ describes the desorption rate as proportional to the constant desorption rate and surface concentration. The increase of cs is proportional to the rise of desorption. By subtracting these two terms, the overall equation for the net rate change of the surface concentration of a particle (for adsorption and desorption) evolves. R represents this rate, so the equation is-

$$R = k_{ads}c(\gamma_s - c_s) - k_{des}c_s \qquad (4)$$

ii) Modified adsorption-desorption models and equations

We have modified the standard equation with the Langmuir-Furmkin kinetics to solve more accurately with the dimensionless maximum surface coverage term, θ.

$$R_{ads} = k_{ads} \,.\, c_0 \,.\, \frac{(1-\theta).(K_{ads}.\theta)}{1+K_{ads}.\theta} \qquad (5)$$

$$R_{des} = k_{des} \,.\, c_s \qquad (6)$$

Equation (5) represents the Absorption rate, whereas equation (6) represents the Desorption rate; by subtracting these two equations, we can achieve the net reaction changes on the substrate, *R.*

We will solve the convection-diffusion equation with the previous laminar flow's Navier stokes equation, thus showing how particle diffusivity could be in action. The solved equation,

$$\frac{\partial c}{\partial t} + v.\nabla_c = D\nabla^2 c \qquad (7)$$

Where D represents the diffusivity or diffusion coefficient of the particle.

4.4 BOUNDARY CONDITIONS

We have imposed different boundary conditions to complete the numerical approach perfectly with fewer errors in the simulation. For the laminar flow, as we use a time-dependent study for unidirectional flow, we impose a fully developed flow to maintain stress-free conditions at the outlet. As the substrate has a thin lubricating condition to replicate the epithelial layer of the lungs, we will apply slip velocity on this. For the other wall, a no-slip boundary condition will be suitable, as the stretching is omitted. Finally, initial velocity will be applied with a negligible pressure condition.

We should work on our modified Langmuir-Frumkin kinetic-based Surface reaction rate equation for the transport of Diluted species to solve the adsorption-desorption kinetics along with the General Form Boundary PDE (gb) condition. We need a convection transport mechanism as an additional entity as we solve the convection-diffusion equation and the Navier-stokes equation in laminar flow. We took the equation of species activity as ideal. For stabilization of diffusion, we permit both streamline and crosswind diffusion. From context data, the initial concentration was our different species concentration in bulk air volume. Additionally, a concentration boundary condition has been added to calculate for imposing concentration at the inlet as cj = c0,j. The outflow represents the outlet, and the flux represents the general inward flux of the surface reaction, $-n.(J_j+uc_j)= J_{0,j}$ on the substrate to assume the convection as well. We apply symmetry conditions for non-activated walls. An additional PDE boundary condition has been imposed to settle the conservative flux according to the axis and address the dependent variable U2 and the source term quantity of net change in surface reaction rate.

4.5 PARAMETERS AND NUMERIC FOR DIFFERENT CONTEXTS:

Table 5 lists the constant parameters used in our simulation model.

Table 5: Parameters

Parameter Name	Symbol	Value
Air Channel Height	H	7E-5 m
Air Channel Width	W	4E-4 m
Air Channel Length	L	0.002 m
Diffusivity	D_s	Varies*
Volume Concentration at Inlet	C_0	Varies**
Particle Diameter	d	Varies**
Maximum Areal Concentration	T_s	5.24E-8 m
Uniform Air Velocity at Inlet	$V0$	0.000337 m/s
slip velocity on membrane	vs	1.37E-6 m
Gas constant	R_c	8.3145 J/mol
Gas Diffusivity	D	2.14E-5 m²/s
Mass Transfer Coefficient	k_c	2.9833E-7 m/s
Flow rate constant	K_{ads}	1E-6 m³/(s·mol)
Flow rate backward constant	K_{des}	1E-9 1/s

We have calculated the required parameter for each concentration level of each context, such as the volume concentration at the inlet C_0, maximum surface coverage g_s, maximum particles on surface $N_{max,}$ and number of the particle in concentration, N_c for each particle concentration of each context. We took the average and highest PM 2.5 particle concentration for each particle and the collected data for each particle concentration of each context.

Table 6 shows that each parameter is calculated for each concentration at the highest and average PM 2.5 pollution level. Table 7 shows the estimated values for the parameters relative to the actual concentration of each particle in normal air.

Table 6

Calculated Values For Individual Particle Concentration from Literature			
	PM 2.5 concentration, from literature	Maximum Surface Coverage, g_s (Mol/ m³)	Volume Concentration, C_o (μg/m³)
Dhaka			
BC	22.417 μg/m³	0.015	1.86e-6
Sillica	8.8 μg/m³	4.42e-3	1.447e-7
SO2	15.5 μg/m³	4.56e-6	2.41e-7
Lahore			
SO2	14.8 μg/m³	4.56e-6	2.31e7
EC	8.6 μg/m³	0.015	7.16e-7
Zurich			
NH4NO3	2.4 μg/m³	2.15e-3	3e-8
SO2	4.3 μg/m³	4.56e-6	6.7e-8

Table 7

Particle Name	**Concentration, from literature**	**Maximum Surface Coverage, g_s (Mol/ m³)**	**Volume Concentration, C_o**	**Molar volume (m³)**	**Max Number Of Particle On Surface**	**Number of Particle in concentration**	**Molar mass per particle(mol)**
Dhaka							
BC	65.8 μg/m³	0.015	5.47 e-6	6.67e-6	8e6	2917	1.875e-9
BC	146.4 μg/m³	0.015	1.22e-5	6.67e-6	8e6	6507	1.875e-9
Sillica- SiO2	65.8 μg/m³	4.42e-3	1.08e-6	2.26e-5	3.2e6	146	1.38125e-9
Sillica SiO2	146.4 μg/m³	4.42e-3	2.41e-6	2.26e-5	3.2e6	326	1.38125e-9
Sulfur Dioxide (SO2)	65.8 μg/m³	4.56e-6	1.03e-6	2.19e-2	8e6	1.77e6	5.81e-13
Sulfur Dioxide (SO2)	146.4 μg/m³	4.56e-6	2.29e-6	2.19e-2	8e6	3.94e6	5.81e-13
Ammonium Sulphate	65.8 μg/m³	1.343e-3	4.98e-7	7.466e-5	7.08e6	2621	1.9e-10

Ammonium Sulphate	146.4 µg/m^3	1.343e-3	1.108e-6	7.466e-5	7.08e6	5831	1.9e-10
Lahore							
Ammonium Sulphate	97 µg/m^3	1.343e-3	7.34e-7	7.466e-5	7.08e6	3863	1.9e-10
Ammonium Sulphate	192.9 µg/m^3	1.343e-3	1.46 e-6	7.466e-5	7.08e6	7684	1.9e-10
Sulfur Dioxide (SO2)	97 µg/m^3	4.56e-6	1.51e-6	2.19e-2	8e6	2.59e6	5.81e-13
Sulfur Dioxide (SO2)	192.9 µg/m^3	4.56e-6	3.01e-6	2.19e-2	8e6	5.18e6	5.81e-13
Ammonium Nitrate	97 µg/m^3	2.15e-3	1.212e-6	4.65e-5	3.2e6	1804	6.72e10
Ammonium Nitrate	192.9 µg/m^3	2.15e-3	2.41e-6	4.65e-5	3.2e6	3586	6.72e10
E.C. (Elemental Carbon	97 µg/m^3	0.015	8.08e-6	6.67e-6	8e6	4309	1.875e-9
E.C. (Elemental Carbon	192.9 µg/m^3	0.015	1.6075e-5	6.67e-6	8e6	8573	1.875e-9
Zurich							
Ammonium Nitrate	10.4 µg/m^3	2.15e-3	1.3e-7	4.65e-5	3.2e6	193	6.72e10
Ammonium Nitrate	24.1 µg/m^3	2.15e-3	3.01e-7	4.65e-5	3.2e6	461	6.72e10
Sulfur Dioxide (SO2)	10.4 µg/m^3	4.56e-6	1.623-7	2.19e-2	8e6	2.79e5	5.81e-13
Sulfur Dioxide (SO2)	24.1 µg/m^3	4.56e-6	3.76e-7	2.19e-2	8e6	6.47e5	5.81e-13

5. Result Analysis

5.1 ANALYSIS OF EULERIAN SIMULATION FOR SURFACE REACTION RATE

We show the surface reaction rate for a total of 12 s over a breathing cycle of 4 s for different particle and city concentrations considering the graph base. This is essentially an Eulerian simulation, which shows the surface reaction rate and concentration on the epithelial layer in unidirectional flow; we only collected 12 seconds of graph data for proper comparison. As shown in Figure 2, our data collected from the literature is a comparative analysis of the health impact of the B.C. and E.C. particle elements, usually produced from combustible engines.

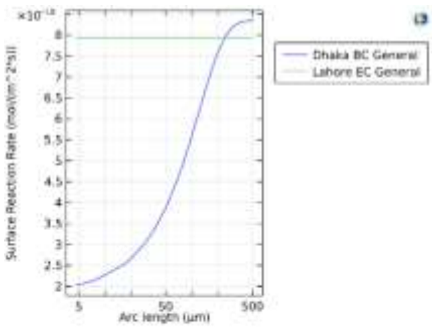
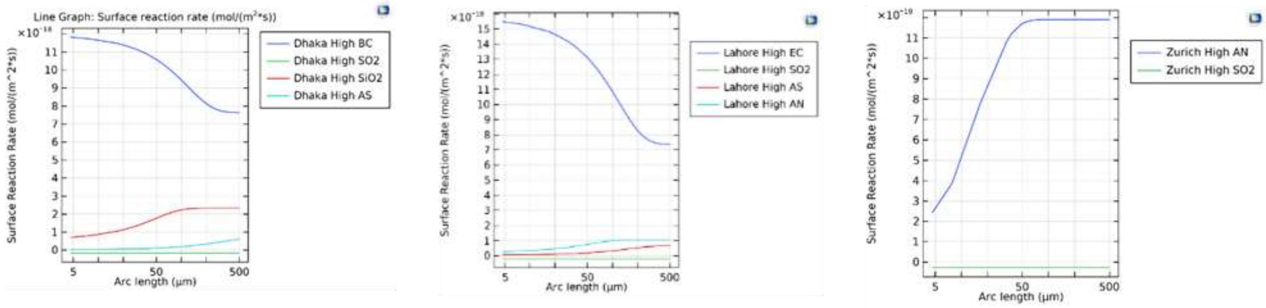


Figure 2, Comparative Graph of Dhaka and Lahore For Carbon Exposure

The graph confirms that particulate matter emitted from combustible engines threatens human health in Dhaka because of its reaction rate, which is more harmful than Lahore's in-depth adsorption, as shown in lung depth. In Figure 3, we show a comparative comparison of each city's exposures. We counted the PM 2.5 concentration of each town obtained from IQAir as the concentration for each particle, which will help us diagnose problems occurring in case of source exposure. We first show a comparative graphical representation of individual city pollutant particle sources at the same concentration (average and peak) (Figure 3).

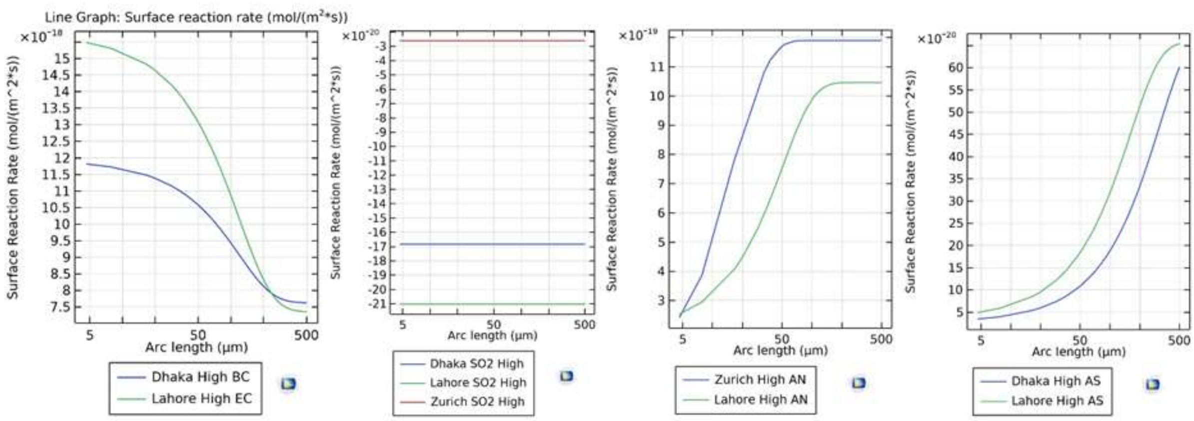
From the graph, we can see a healthy pattern of carbon particle exposure in Lahore (b) and Dhaka (a); in comparison to other particles, the carbon exposure levels in the two cities are alarming because carbon particles are generated from burning things and, from their deposition, inflammation, cause serious problems of lung cancer. Inhalation of such a high concentration will cause severe symptoms. Although Dhaka's exposure is half that of Lahore, Harmful Impact makes Dhaka's environment extremely hazardous. On the other hand, the concentration of ammonium nitrate in the air of Zurich is exposed to indirect pollution (c) (although lower than in other cities). Still, the inhalation adsorption rate is a cause for concern.



(a) (b) (c)

Figure 3, (a) Exposure of Dhaka, (b) Exposure of Lahore, (c) Exposure of Zurich
[All Graphs Shown The Surface Reaction Rate During Inhalation]

Figure 4 shows a comparison diagram between cities for individual particles. Figure 4 gives us some direction regarding which city sources are more dangerous.



(a) (b) (c) (d)

Figure 4, (a) Comparison Graph Between Lahore and Dhaka for PM 2.5 Level Carbon Expousure, (b) Comparison Graph Between Cities for PM 2.5 Level SO2 Expousure, (c) Comparison Graph Between Zurich and Lahore for PM 2.5 Ammonium Nitrate Expousure, (d) Comparison Graph Between Lahore and Dhaka for Ammonium Sulphate Expousure.
[All Graph Shown The Surface Reaction Rate During Inhalation]

Graph (b) clearly shows that Lahore has significant SO2 pollution, and despite the Level of SO2 concentration being similar to Dhaka, due to the climate and diffusion, people inhale a considerable amount of SO2 compared to other cities. On the other hand, from graphs (a) and (d), we consider a similar impact on carbon and sulfate inhalation between Dhaka and Lahore. Lahore and Dhaka are far different in the concentration level of PM 2.5 Sulphate and Carbon Particles, but the adsorption level is similar and significant. The most alarming situation is shown in (c), where Zurich has a substantial level of nitrate adsorption, compared to Lahore, where the nitrate pollution is high and is from a direct source. The yield scenarios of pollution in Zurich's healthy environment can be harmful and deadly.

6. Discussion & remarks

From the Eulerian simulation analysis, we conclude some decisions, which are stated below:

1. Schulze, F., et al. (2017) have already explored the physical microfluidic chips to investigate the health impact of PM 2.5 pollutants. That also emphasizes the relationship between air quality data and human biological response. Our paper also addresses a simulation process using organs on a chip's computer model, which virtually computes the health impact, supporting Schulze's method. Our virtual model of LOAC examines the lung impact of PM 2.5 in different climatic locations, creating an example of a cheaper respiratory health impact evaluation technique in multiple atmospheric contexts and expanding research toward a comparative assessment.
2. PM concentrations and pollution levels are not the only determinants of health impact. Instead, context, climate, and pollution sources are directly responsible for adverse effects on the respiratory system.
3. Although cities can resist internal pollution resources, significant exposure to indirect pollution can wreak havoc on urban health.
4. Everyone should consider the PM 2.5 concentration thresholds and deposition patterns to prevent airborne diseases in Indoor and outdoor area planning, from architects to urban planners to health engineers to HVAC engineers.
5. Sustainable and livable city and residence design decisions should consider individual particulate pollutants and their sources rather than the overall PM2.5 concentration.

6. Respiration-related considerations in both livable cities and prevention procedures should focus on how it is inhaled.
7. Industrial and Automobile exposure should be minimized through the PM concentration-based urban zonal design and implementing different exposure control urban concepts, such as the 5-minute walk city concept.
8. A detailed simulated health impact analysis based on air quality could be integrated into BIM-based design decision-making in architectural spaces. Xu et al. (2022) have already explored the integration of air quality monitoring systems into BIM in construction sites by using edge computing. In the near future, we can integrate agent-based multiphysical computation into urban-scale BIM and create prediction modeling of respiratory impact. Also, it will direct us in designing new air ventilation systems, air filters, and urban-level opening strategies, which will enable us to implement the prevention of airborne viruses like COVID-19 in the near future, which have a high deposition rate in the human lungs.
9. Recent findings suggest that highly dense leaf vegetation and ventilation corridors for natural wind flow in urban areas could impact improving air quality (Lin et al., 2024). Also, green dynamic traffic management strategies, which integrate real-time local air quality into traffic management systems, might improve the micro-climatic air condition in urban areas (Van Baalen et al., 2011). Considering the other factors that are responsible for health impact along with PM 2.5 concentration level, these strategies could be beneficial for mitigating the impact, as these approaches are practical on micro-climate, specific land use, and pollution sources.

7. Conclusion

Environmental air quality improvement is crucial for good health. PM 2.5 concentration level is a standard criterion for determining air quality. In the question of healthy urban environment design considering air quality, we need to focus on more attributes. The simulation study manifests the relationship between health impact (signifies by surface reaction rate) on different contexts and different PM 2.5 pollutants, which is not consistent according to the AQI Index; rather, it depends on the pollutant source type. Not only that, passive air pollution and clean and cold air (which is a specific climatic context) could create a comparatively more severe impact by lung deposition than in the active pollution area. Also, the source location is a significant factor; for example, sulfur dioxide creates a fatal effect in Zurich (which is a less polluted country compared to others) due to its source location. Considering COVID-19 as 100nm (Bar-On et al., 2020) particle matter, the susceptibility, incompressibility, and exposure of European countries (Kenyon, C., 2020) also support the phenomena of Zurich. To ensure a healthy urban environment and healthy respiratory system for every urban dweller, we need to adopt multidisciplinary approaches by reconciling bio microfluidic engineering, environmental science, and urban planning. The appeasement among these disciplines will also address the critical problems of the future cities. Not only that, urban planners could ensure a healthy environment by relocating the potentially harmful pollutants and their source plots, confining them into a particular category of land use, and isolating them from residential, commercial, and mixed-use areas. In this procedure, environmentalists and bioengineers would calculate the susceptibility of each pollutant and its source. From the continuation of this collaboration, multidisciplinary strategies could also be used in designing special air ventilation and filtration systems in those particular areas to reduce respiratory predicament. This research tries to explain and vindicate the overall PM 2.5 concentration impact along with other indicators through the computer simulation, which also reflects critical insights into healthy urban and residential design decisions and planning based on air quality index consideration.

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