

Team Control Number: 26MS0992

Problem Chosen: A

Urban Residential Air Quality Assessment Under Point-Source Pollution Events: Outdoor Dispersion and Indoor Infiltration Modeling

Summary

Urban residential communities can face acute health risks when hazardous pollutants are released from nearby point sources. Because residents spend most of their time indoors, a realistic risk assessment must connect outdoor dispersion to indoor exposure through infiltration and ventilation.

For Problem 1 (Outdoor): We construct an outdoor dispersion module using classical Gaussian theory. Continuous emissions are represented by the **Gaussian plume model**, and short-duration accident/attack releases are modeled by the **Gaussian puff model**. To handle arbitrary wind directions while keeping residential locations fixed, we introduce a **geographic coordinate system** (X,Y,Z) and a **wind-aligned system** (x,y,z), linked by a rotation transformation. Ground reflection is incorporated via the **mirror-source method**, under assumptions of steady meteorology, flat terrain, and inert pollutants.

To quantify worst-case neighborhood impact, we analyze the **ground-level centerline concentration** ($z = 0, y = 0$) for the plume model. An extremum analysis yields the condition for peak ground concentration,

$$\sigma_z(x) \approx \frac{H}{\sqrt{2}},$$

showing that a larger effective release height H shifts the peak farther downwind and decreases peak magnitude (approximately $C_{\max} \propto 1/H^2$). For puff scenarios, the time-dependent concentration field supports emergency indicators such as **arrival time**, **peak time**, and **hazardous duration** using urban-modified Pasquill–Gifford (Briggs) dispersion parameters under typical neutral stability (Class D).

For Problem 2 (Indoor): We build an indoor air-quality module that takes the outdoor concentration near the building envelope as the driving input and predicts indoor exposure dynamics. The indoor process is formulated as a **transport–diffusion (PDE) model** with key parameters including indoor airflow speed u , diffusion coefficient D , and

deposition/removal coefficient k . To reflect realistic building operation, we evaluate three ventilation regimes: **(I) crack infiltration**, **(II) natural ventilation**, and **(III) mechanical ventilation (with filtration)**. Boundary conditions are specified using a **Robin (third-type) inlet condition** and an outlet condition to close the PDE system, and the model is solved numerically.

Simulation results show that indoor concentration depends strongly on ventilation mode: under long-term ventilation, pollutant influence is most significant within a few meters of the window (with a clear rise–fall–stabilize pattern at a monitoring point), while under crack-only infiltration the impacted zone shrinks to within about half a meter near the window and peak levels are much lower. Mechanical ventilation with filtration produces the largest reduction in indoor concentration, demonstrating the effectiveness of engineered ventilation for emergency protection.

Keywords: Gaussian plume; Gaussian puff; outdoor–indoor coupling; transport–diffusion PDE; Robin boundary; ventilation scenarios; urban residential risk.

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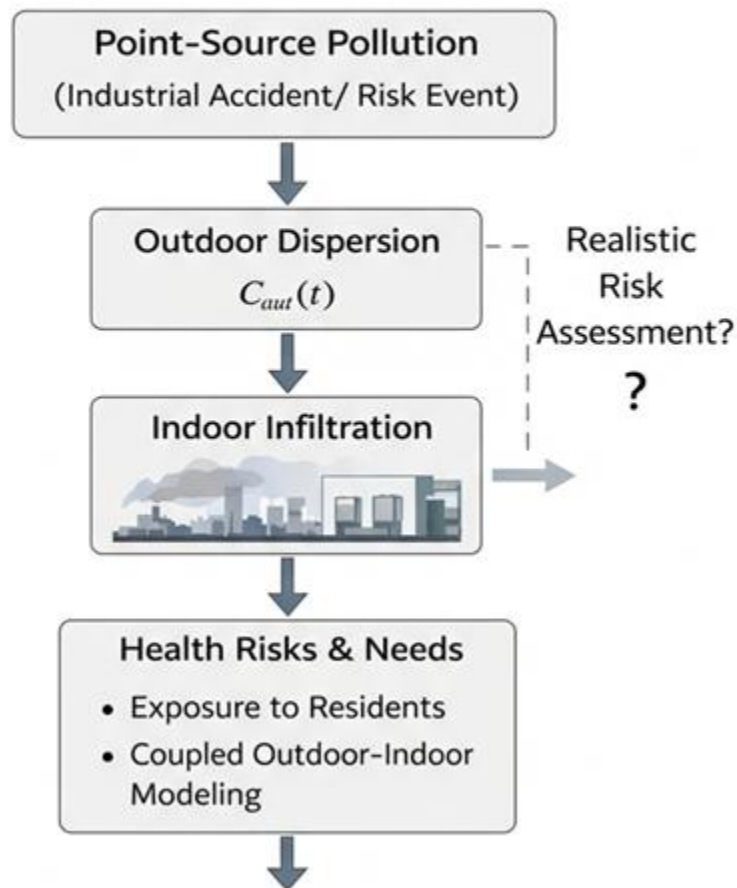
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1 Introduction

1.1 Problem Background

Figure 1: Problem Background



With increasing urban density and the concentration of high-rise buildings, modern cities face growing risks from air pollution incidents caused by industrial accidents, infrastructure failures, or malicious attacks. Once hazardous substances are released into the atmosphere, they can be transported over long distances by wind and turbulence, posing serious threats to nearby residential communities. In such scenarios, residents are exposed not only outdoors but also indoors, as pollutants infiltrate buildings through ventilation and leakage pathways.

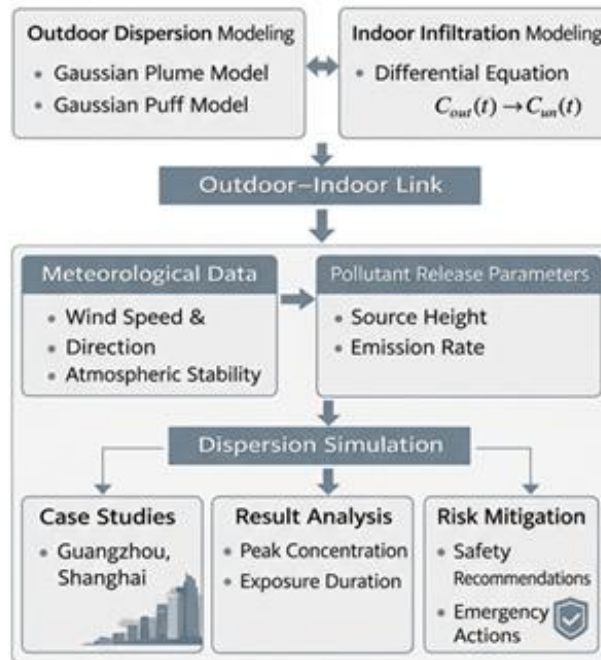
Traditional air quality assessments often focus exclusively on outdoor concentrations, neglecting the indoor environment where people typically spend more than 80% of their time. This omission may lead to a significant underestimation or mischaracterization of actual human exposure. Therefore, an integrated modeling approach that links outdoor dispersion with indoor air dynamics is essential for realistic risk evaluation.

1.2 Restatement of the Problem

The objective of this study is to:

- Establish a mathematical model to describe the outdoor dispersion of pollutants released from a point source near residential areas.
- Quantitatively analyze the effects of source height and distance on ground-level pollutant concentration.
- Develop an indoor air quality model that links outdoor concentration to indoor exposure under different ventilation conditions.
- Apply the models to realistic urban scenarios and provide actionable insights for emergency response and risk mitigation.

1.3 Our Work



To address the above objectives, we construct a coupled outdoor-indoor modeling framework. The outdoor module is based on classical atmospheric dispersion theory, while the indoor module relies on mass conservation principles. The models are analytically tractable, physically interpretable, and suitable for scenario analysis in urban environments.

2 Model Preparations

2.1 Assumptions and Justifications

Assumption 1 (Steady meteorological conditions): Wind speed, wind direction, and atmospheric stability remain constant during the short simulation period.

Justification: For emergency scenarios lasting several hours and covering distances of a few kilometers, assuming steady meteorological conditions is a common and reasonable simplification.

Assumption 2 (Point source approximation): The pollution source is treated as a point source with an effective height H .

Justification: When the source dimensions are small compared to the dispersion scale, the point source approximation is valid.

Assumption 3 (Flat terrain and full ground reflection): The terrain is flat, and the ground reflects pollutants without absorption.

Justification: This allows the use of the mirror-source method to simplify boundary conditions.

Assumption 4 (Inert pollutant): The pollutant does not undergo chemical reactions or deposition during transport.

Justification: For short-distance and short-duration events, chemical loss is often negligible.

Assumption 5 (Well-mixed indoor air): Indoor air is spatially uniform in concentration.

Justification: This assumption is widely used in indoor air quality modeling and is suitable for single-zone analysis.

Assumption 6(**Dominant one-dimensional transport**): Indoor air motion is assumed to have a prevailing direction from the window (or supply inlet) toward the opposite side of the room, defined as the x -axis. Concentration is considered well mixed on each cross-section normal to x , so gradients in y and z are neglected.

Assumption 7(**Time-invariant parameters over the event window**): The indoor advective speed u (linked to the ventilation mode) and the effective diffusion coefficient D remain constant during the short simulation period.

Assumption 8(**Removal by deposition/adsorption**): For fine particles such as $PM_{2.5}$, indoor deposition and surface adsorption are represented by a first-order decay term with coefficient k .

Assumption **9(internal sources)**: There is no additional indoor emission source; indoor concentration changes are driven solely by outdoor infiltration/ventilation and removal processes.

2.2 Notations

Symbol	Meaning
C	Pollutant mass concentration
Q	Pollution source concentration
M	Total mass of pollutants
H	Effective source height
u	Average wind speed
θ	Wind direction angle
σ	Atmospheric diffusion coefficient
k	Indoor pollutant deposition coefficient
t	Time
F	Buoyancy flux parameter
V	Volume
λ	Barrier efficiency factor
D	Diffusion coefficient

3 Problem 1: Outdoor Dispersion Modeling

3.1 Coordinate System Transformation

To accommodate arbitrary wind directions and fixed residential locations, we introduce two coordinate systems: a geographic coordinate system (X,Y,Z) and a wind-aligned coordinate system (x,y,z). The transformation between the two systems is achieved using a rotation matrix determined by the wind direction angle. This approach enables a unified formulation of the dispersion model under varying wind conditions.

Let θ be the wind direction angle (angle of the wind vector from due east), (X,Y) be the geographic coordinates, and (x,y) be the wind-aligned coordinates. The conversion relation is given by:

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix}$$

3.2 Gaussian Plume Model for Continuous Emissions

For continuous emissions under steady conditions, the outdoor concentration is described by the Gaussian plume model. In the wind-aligned coordinate system $O - xyz$, considering the full reflection effect at the ground ($z=0$), we introduce the mirror-source concept, i.e., a virtual source at $-H$ below ground. The concentration C at any point (x,y,z) is obtained by superposition of the real and virtual sources:

$$C(x, y, z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right) \right]$$

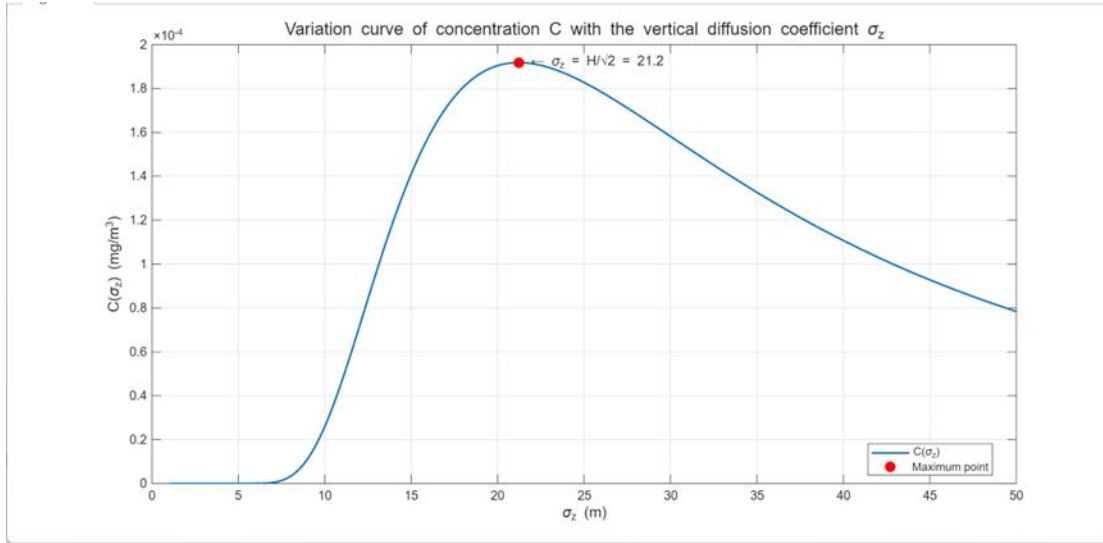
Since residents primarily live and work near ground level, we focus on ground-level concentration at $z = 0$. Substituting $z = 0$, the formula simplifies to:

$$C(x, y, 0) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{H^2}{2\sigma_z^2}\right)$$

For a fixed downwind distance x , the crosswind concentration term $\exp(-y^2/(2\sigma_y^2))$ follows a standard normal distribution centered at $y = 0$. Since the exponential function e^{-ky^2} attains its maximum at $y = 0$, the highest pollutant concentration is along the plume's centerline. To analyze the most severe impact on the community, we focus on the centerline concentration model at $y = 0$:

$$C(x, 0, 0) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{H^2}{2\sigma_z^2}\right)$$

Expressing the concentration C as a function of the vertical dispersion parameter σ_z and assuming the horizontal dispersion parameter σ_y to be proportional to σ_z , we obtain the following plot.

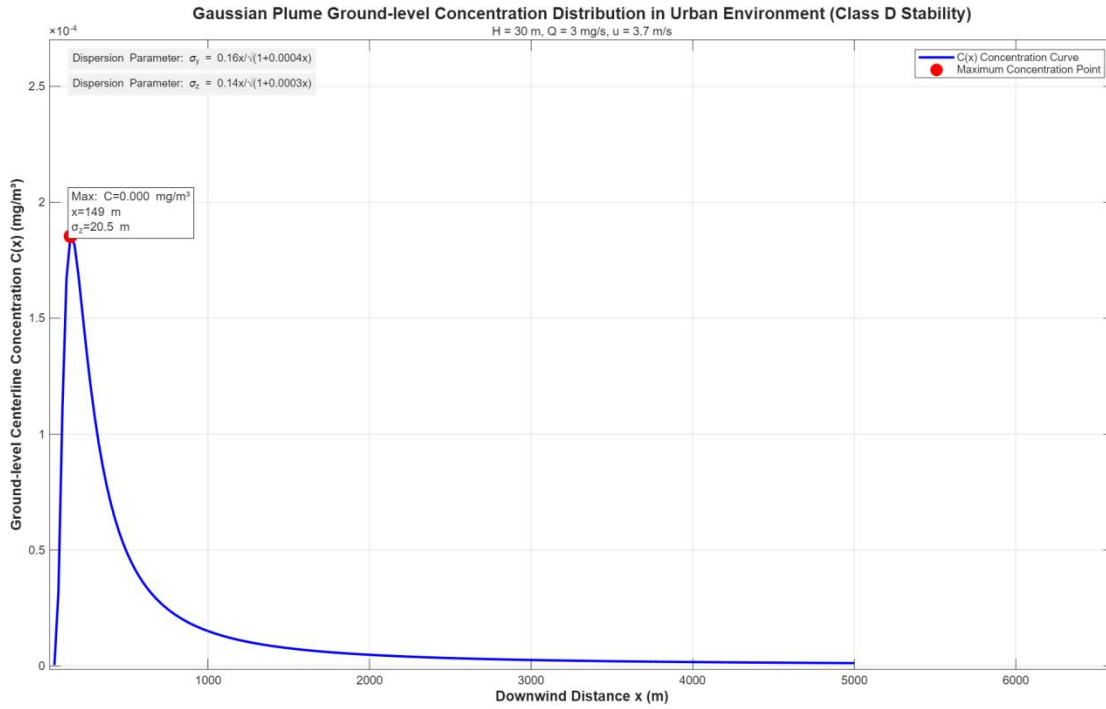


To investigate the influence of source height H and distance x on ground concentration, we perform an extremum analysis on the above equation. Assuming a roughly constant ratio of growth between horizontal and vertical dispersion parameters ($\sigma_y \propto \sigma_z$), we differentiate the concentration equation with respect to σ_z and set the derivative to zero: $dC/d\sigma_z = 0$. The derivation yields:

$$C \propto \sigma_z^{-2} \exp(-H^2/2\sigma_z^2)$$

$$\frac{d(\ln C)}{d\sigma_z} = -\frac{2}{\sigma_z} + \frac{H^2}{\sigma_z^3} = 0 \implies \sigma_z^2 = \frac{H^2}{2} \implies \sigma_z = \frac{H}{\sqrt{2}}$$

By substituting the expressions for σ_y and σ_z into the equation, we plot their corresponding graphs.



3.3 Influence of Source Height and Distance

Critical Distance: The maximum ground-level concentration occurs when $\sigma_z(x) \approx 0.707H$. Since σ_z is a monotonically increasing function of x , a higher effective source height H pushes the distance x_{\max} where the maximum concentration occurs farther downwind. This means increasing the height of an industrial stack can "push" the high pollution zone away from nearby communities toward less populated areas.

Peak Concentration: Substituting $\sigma_z^2 = H^2/2$ into the original equation gives the maximum ground concentration $C_{\max} \propto 1/H^2$. That is, the peak ground concentration is inversely proportional to the square of the effective source height. This mathematically demonstrates that "high-stack emission" is an effective measure to reduce ground-level pollution in residential areas.

By analyzing the centerline concentration, we show that the maximum ground-level concentration occurs when $\sigma_z \approx H/\sqrt{2}$.

3.4 Gaussian Puff Model for Instantaneous Releases

To address the complex process of pollutant dispersion following a sudden fire, this paper models the dispersion in two coupled stages: *thermodynamic plume rise* and *Gaussian puff diffusion*.

In the thermodynamic plume rise stage, we first estimate the total instantaneous pollutant release mass using a volume-mass scaling method. Based on the World Trade Center event as a reference, this yields approximately 2,500 kg of PM_{2.5}. Subsequently, employing the Briggs buoyant rise formula and accounting for fire-induced thermal buoyancy and wind speed profile corrections at high altitudes, we calculate the *effective source height*, H (physical height + plume rise). For instance, under typical meteorological conditions (atmospheric stability Class D), the effective source height for Shanghai's Oriental Pearl Tower is adjusted to approximately 595 m, and for the Canton Tower to about 1,198 m.

This effective height then serves as the initial center location for the second stage—Gaussian puff dispersion—thereby providing a more realistic representation of the hot smoke plume's behavior within the urban canopy.

For accidental or attack scenarios characterized by short-duration releases, we adopt the Gaussian puff model. For assumed major accidents or terrorist attacks where the pollutant release duration is extremely short (much less than the transport and diffusion time), the source can be abstracted as a geometric point, and the release approximated as an instantaneous pulse emission at time $t = 0$. The Gaussian plume model cannot describe the temporal dynamics of such sudden events. Therefore, we introduce the Gaussian puff model to analyze the transient behavior of pollutants. This model allows us to calculate key time-dependent indicators such as the arrival time of the toxic cloud, resident exposure duration, and longitudinal puff dispersion along the wind direction. These factors are crucial for emergency response planning in cities like Guangzhou and Shanghai.

Physical Process: The accident releases a large mass of pollutant in a very short time ($\Delta t \rightarrow 0$), forming a high-concentration "puff."

Motion Characteristics: This puff moves with the mean wind field while simultaneously expanding in three-dimensional space (x, y, z).

Key Difference: The model includes the time dimension t , and diffusion occurs also in the downwind direction (x -axis) characterized by σ_x .

In the wind-aligned coordinate system $O - xyz$, at time $t = 0$, a total mass M of pollutant is instantaneously released at $(0, 0, H)$. Assuming wind direction is along the positive x -axis with average speed u . At time t , the puff center moves to $(ut, 0, H)$. The concentration distribution at any point (x, y, z) and time t follows a three-dimensional Gaussian distribution. Considering full ground reflection, the concentration formula is:

$$C(x, y, z, t) = \frac{M}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \cdot E_1 \cdot E_2 \cdot E_3$$

$$E_1 = \exp \left[-\frac{(x - ut)^2}{2\sigma_x^2} \right]$$

$$E_2 = \exp \left[-\frac{y^2}{2\sigma_y^2} \right]$$

$$E_3 = \exp \left[-\frac{(z - H)^2}{2\sigma_z^2} \right] + \exp \left[-\frac{(z + H)^2}{2\sigma_z^2} \right]$$

$$C(x, y, z, t) = \frac{M}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left[-\frac{(x - ut)^2}{2\sigma_x^2} \right] \exp \left[-\frac{y^2}{2\sigma_y^2} \right] \left\{ \exp \left[-\frac{(z - H)^2}{2\sigma_z^2} \right] + \exp \left[-\frac{(z + H)^2}{2\sigma_z^2} \right] \right\}$$

Here, E_1, E_2, E_3 represent the downwind, crosswind, and vertical diffusion factors, respectively.

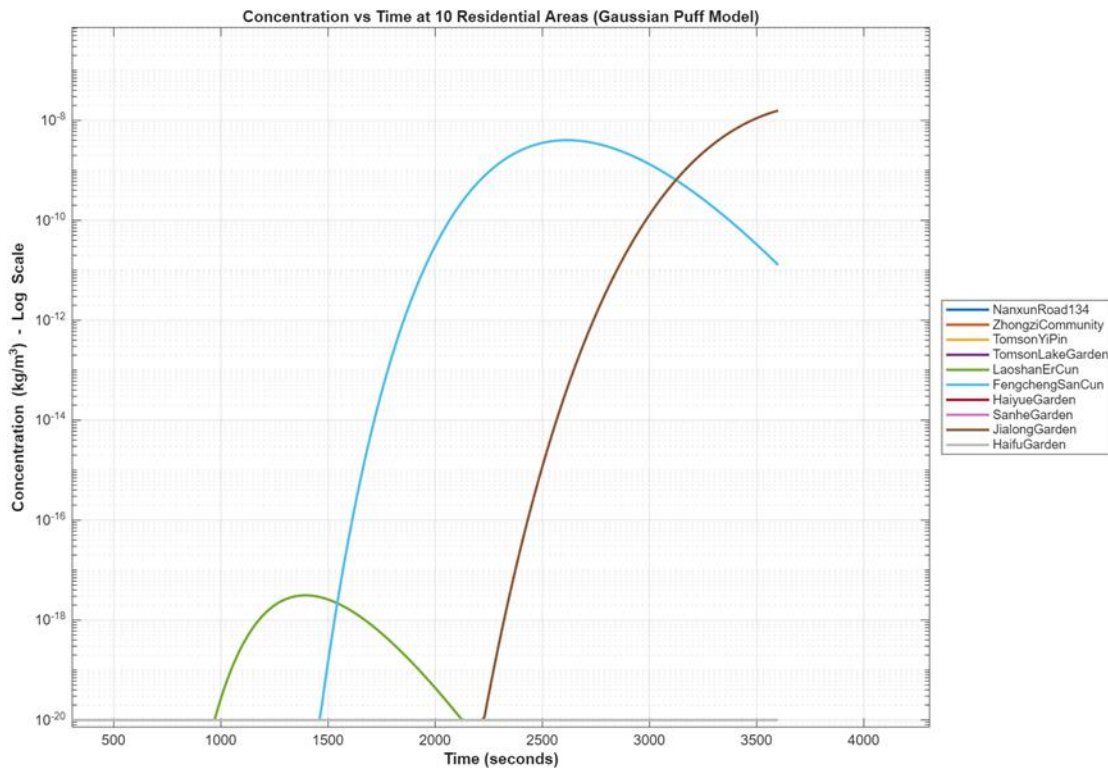
For our study object (air quality in communities near the source), we set $z = 0$, simplifying the formula to:

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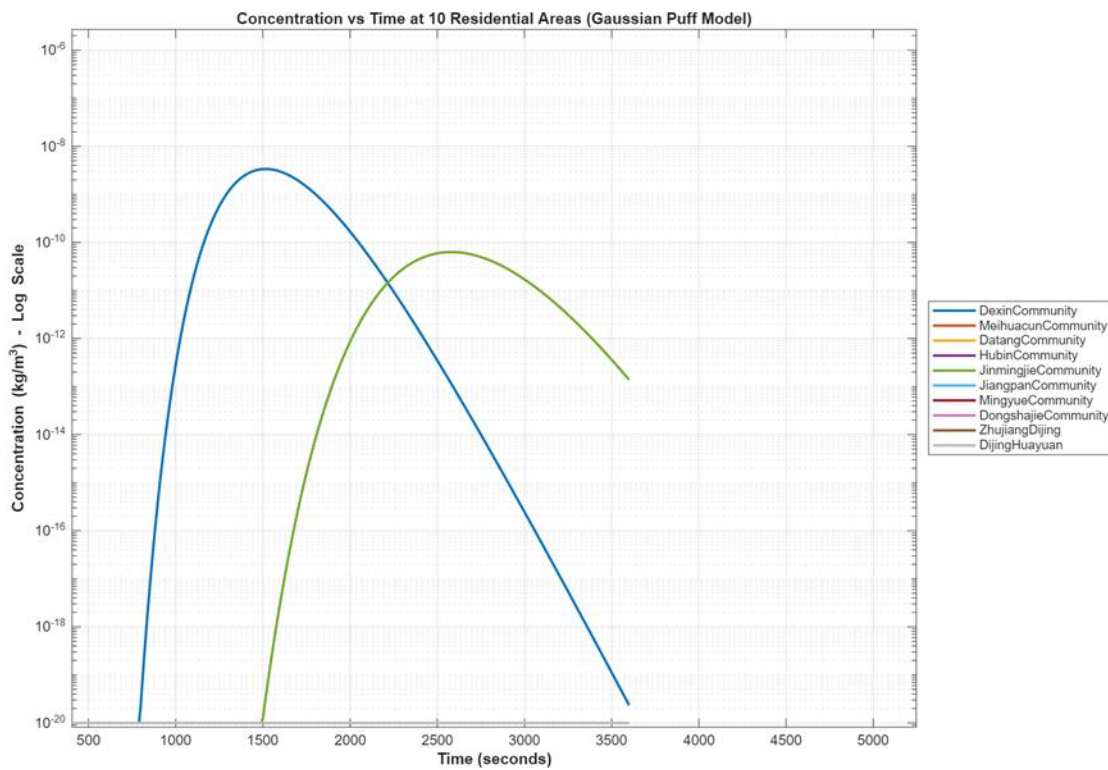
$$C(x, y, 0, t) = \frac{2M}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left[-\frac{(x - ut)^2}{2\sigma_x^2} \right] \exp \left[-\frac{y^2}{2\sigma_y^2} \right] \exp \left[-\frac{H^2}{2\sigma_z^2} \right]$$

3.5 Guangzhou & Shanghai Case Study

ten residential communities surrounding the Oriental Pearl Tower in Shanghai



ten residential communities surrounding the Canton Tower



The results show:

1. Whether a residential area is located downwind significantly affects pollutant concentration.
2. Both downwind distance and crosswind distance jointly influence concentration (as illustrated by combining data from Shanghai and Guangdong: in Guangdong, concentrations are higher in the morning and lower in the evening; in Shanghai, they are lower in the morning and higher in the evening, because the impact of crosswind distance in Shanghai outweighs that of downwind distance).

3.6 Determination of Key Parameters

Determination of Dispersion Parameters

$\sigma_x, \sigma_y, \sigma_z$ reflect the atmosphere's dilution capacity for pollutants and can be derived from Pasquill-Gifford empirical formulas. Although puff dispersion coefficients are typically smaller than those for continuous plumes, complex urban terrain introduces significant ground roughness and urban heat island effects, enhancing turbulent mixing. Therefore, to capture urban dispersion characteristics, we employ Briggs' modified Pasquill-Gifford dispersion parameters for urban environments in both scenarios (for the Gaussian puff model, assuming $\sigma_x = \sigma_y$):

Stability Class	$\sigma_y(m)$	$\sigma_z(m)$
A-B (Very Unstable)	$0.32x(1 + 0.0004x)^{-0.5}$	$0.24x(1 + 0.001x)^{0.5}$
C (Unstable)	$0.22x(1 + 0.0004x)^{-0.5}$	$0.20x$
D (Neutral)	$0.16x(1 + 0.0004x)^{-0.5}$	$0.14x(1 + 0.0003x)^{-0.5}$
E-F (Stable)	$0.11x(1 + 0.0004x)^{-0.5}$	$0.08x(1 + 0.00015x)^{-0.5}$

Considering the continuity of pollution and that accidents can occur at any time, we simulate using the most common meteorological condition—atmospheric stability Class D (neutral). The functional expressions for σ_y, σ_z with respect to x are:

Continuous Source (x is downwind distance)	Instantaneous Source (X is puff travel/diffusion distance)
$\sigma_y(x) = 0.16x(1 + 0.0004x)^{-0.5}$	$\sigma_x = \sigma_y = 0.16X(1 + 0.0004X)^{-0.5}$
$\sigma_z(x) = 0.14x(1 + 0.0003x)^{-0.5}$	$\sigma_z = 0.14X(1 + 0.0003X)^{-0.5}$

Theoretical Analysis of Key Parameter Influence

Selection of Key Pollutant Indicator: Fine Particulate Matter (PM_{2.5})

This study selects fine particulate matter with an aerodynamic diameter less than $2.5\mu m$ (PM_{2.5}) as the core simulation indicator, for the following reasons:

1. **Physical Properties:** In high-temperature flue gases from combustion and

- explosions, most of the mass is concentrated in sub-micron particles (e.g., soot and condensed aerosols). $PM_{2.5}$ has an extremely low gravitational settling velocity (almost negligible), allowing it to be transported over longer distances with atmospheric turbulence, posing a greater threat to downwind areas far from the incident site.
2. **Health Hazard:** $PM_{2.5}$ can penetrate alveoli directly into the bloodstream, causing acute respiratory and cardiovascular damage. Under high-concentration exposure from terrorist attacks, its IDLH (Immediately Dangerous to Life and Health) risk is significantly higher than that of coarse particles.
 3. **Monitoring Relevance:** Referring to post-event environmental monitoring reports (e.g., EPA, 2002), $PM_{2.5}$ typically constitutes over 90% of the mass in combustion-generated smoke and dust.

4 Problem 2: Indoor Air Quality Modeling

4.1 Model Objective and Coupling with Problem 1

After obtaining the outdoor concentration field around residential communities in Problem 1, the final concern is how outdoor pollution penetrates buildings and affects indoor air quality. This is exactly the focus of Problem 2: to model the transport of pollutants from the building envelope into the indoor space under different ventilation conditions. In our framework, the outdoor module provides the time-varying boundary input $C_{out}(t)$ at the window/air-inlet location, and the indoor module predicts the spatiotemporal indoor concentration $C_{in}(x, t)$ (abbreviated as $C(x, t)$ below).

4.2 Model Analysis and Physical Mechanisms

In Problem 1, we obtain the time-varying outdoor concentration near the residential building, denoted $C_{out}(t)$. The core goal of Problem 2 is to describe how outdoor pollutants enter the indoor space through the building envelope (windows, cracks, ventilation inlets) and then spread within the room.

Because the dominant transport direction is from the inlet toward the interior, we idealize the indoor domain as one-dimensional and model the process as a **convection–diffusion transport problem** with removal. Indoor pollution dynamics are governed by three competing mechanisms:

- **Convection:** bulk airflow carries pollutants into and through the room.
- **Diffusion:** concentration gradients and turbulent mixing spread pollutants in space.
- **Blocking and removal:** penetration through cracks/filters reduces entering mass, and indoor deposition further attenuates concentration.

We represent the three ventilation conditions by modifying the inlet boundary condition and the airflow parameter u

4.3 General Governing Equation

Let the room have length L along the x -direction and (constant) cross-sectional area A . Denote the indoor concentration by $C(x, t)$. The one-dimensional convection–diffusion–reaction equation is:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} - kC$$

Here u is the airflow speed along x , D is the effective diffusion coefficient in air, and k is the indoor removal (deposition/adsorption) coefficient.

The initial condition is taken as a clean indoor state at the start of the event:

$$C(x, 0) = 0.$$

4.4 Parameterized Modeling for Three Ventilation Conditions

This step is the core of Problem 2: we specify u and the inlet boundary condition for each physical scenario.

4.4.1 Unified Inlet Boundary (Robin Boundary)

At the inlet $x = 0$, we impose a **Robin (third-type) boundary condition** that describes the combined effect of advective inflow and diffusive exchange:

$$-D \frac{\partial C}{\partial x} \Big|_{x=0} + u C(0, t) = u \lambda C_{\text{out}}$$

where $\lambda \in [0, 1]$ is an effective entering factor. It compactly represents either crack penetration ($\lambda = P$) or mechanical filtration ($\lambda = 1 - \eta$).

At the outlet $x = L$, an outlet boundary condition is applied to close the PDE system (consistent with airflow leaving the domain).

4.4.2 Condition I: Crack Infiltration (Windows Closed)

When windows are closed, pollutants can only enter through small cracks in the envelope.

- **Physical features:** very low air exchange; small inflow speed; partial blocking/adsorption through tortuous leakage paths.
 - **Parameter setting:** choose a small infiltration-driven speed $u = u_{\text{inf}}$, and set $\lambda = P$ where $P < 1$ is the penetration factor through cracks.
 - **Boundary form:** the unified Robin boundary applies with $\lambda = P$.
-

4.4.3 Condition II: Natural Ventilation (Windows Open)

When windows are open, indoor–outdoor air exchange is strong and primarily driven by outdoor wind.

- **Physical features:** high air exchange; inflow speed dominated by wind; negligible blocking.
 - **Parameter setting:** choose u consistent with the ventilation-driven indoor flow; set $\lambda = 1$.
 - **Boundary form:** the unified Robin boundary applies with $\lambda = 1$.
-

4.4.4 Condition III: Mechanical Ventilation with Filtration

A mechanical system supplies air at a controlled flow rate and removes pollutants at the inlet using a filter.

- **Physical features:** stable and controllable flow; filtration reduces the entering pollutant mass.
- **Parameter setting:** set u based on device flow rate (conceptually $u = Q/A$); set $\lambda = 1 - \eta$, where η is filter efficiency.
- **Boundary form:** the unified Robin boundary applies with $\lambda = 1 - \eta$.

4.5 Model Solution

Since C_{out} is constant, the system will eventually reach a steady state ($\partial C / \partial t = 0$). The steady-state equation simplifies to:

$$D \frac{d^2 C}{dx^2} - u \frac{dC}{dx} - kC = 0$$

This is a second-order linear homogeneous differential equation with constant coefficients. Its general solution takes the form:

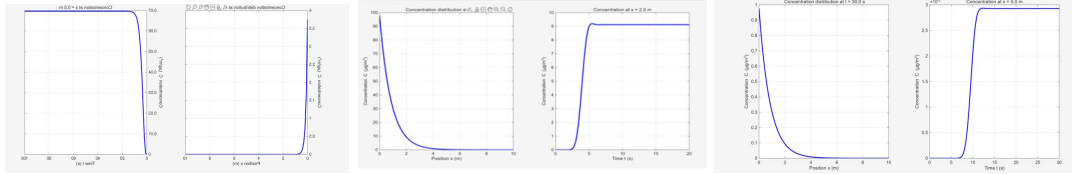
$$C(x) = Ae^{r_1 x} + Be^{r_2 x}$$

Where r_1 and r_2 are the roots of the characteristic equation $Dr^2 - ur - k = 0$:

$$r_{1,2} = \frac{u \pm \sqrt{u^2 + 4Dk}}{2D}$$

Solving simultaneously yields the coefficients A and B, thereby obtaining the complete steady-state spatial concentration distribution $C_{ss}(x)$.

Steady-State Solution: By substituting the above parameters into the steady-state solution formula, the steady-state spatial distribution of indoor pollutants $C_{ss}(x)$ under the three ventilation modes can be directly calculated.



Calculation of Key Indicators:

Average Indoor Steady-State Concentration: $\bar{C}_{ss} = \frac{1}{L} \int_0^L C_{ss}(x) dx$

Penetration Rate: Can be defined as \bar{C}_{ss}/C_{out} , used to compare the blocking effectiveness of different ventilation modes.

4.6 Results and Discussion (Based on Simulation Outputs)

The simulations show that indoor exposure is highly sensitive to ventilation mode:

- **Natural ventilation produces the largest indoor impact.** Under long-term ventilation, elevated concentrations are most evident within roughly **3.5 m** from the window. At a monitoring location around **2 m**, the concentration typically

increases rapidly, then decreases as outdoor forcing weakens, and finally approaches a stable level, forming a clear “rise–fall–stabilize” trend.

- **Crack infiltration strongly suppresses and localizes indoor pollution.** Closing windows significantly reduces penetration: noticeable impact is confined to about **0.5 m** near the window, and the overall indoor concentration is much lower than the natural ventilation case.
- **Mechanical ventilation with filtration yields the best protection.** Because filtration reduces the effective inlet pollutant fraction, indoor concentrations are substantially lowered compared with natural ventilation, demonstrating the effectiveness of engineered ventilation during outdoor pollution emergencies.

Overall, Problem 2 completes the outdoor–indoor linkage required by the prompt by converting the outdoor concentration time series into indoor spatiotemporal exposure under three realistic ventilation regimes.

5 Sensitivity Analysis

To test the robustness of our models and identify the key parameters that most influence the results, we conducted a sensitivity analysis on the core variables. We employed a one-factor-at-a-time approach, varying a single parameter by $\pm 10\%$ or $\pm 20\%$ from its baseline value in the standard scenario (Shanghai Oriental Pearl Tower case), while observing the percentage change in the target metric (peak ground concentration C_{\max}).

5.1 Selection of Key Parameters

We focused on the following two physical parameters which inherently carry uncertainty:

- **Effective Source Height H :** Although the tower height is fixed, the plume rise Δh , influenced by emission temperature and initial velocity, is subject to fluctuation.
- **Average Wind Speed u :** Meteorological conditions vary over time, introducing error in predicted wind speeds.

5.2 Definition of Sensitivity Index

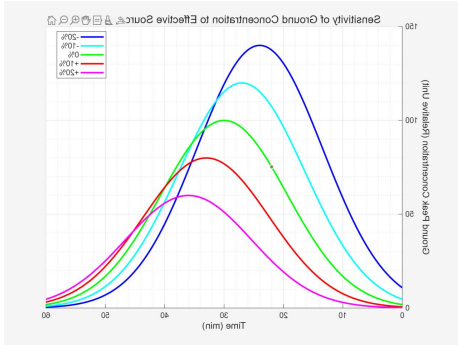
The sensitivity coefficient S is defined as the ratio of the relative change in the result to the relative change in the parameter:

$$S = \frac{\Delta C / C_0}{\Delta P / P_0}$$

where C_0 is the baseline concentration and P_0 is the baseline parameter value. A larger $|S|$ indicates greater model sensitivity to that parameter.

5.3 Analysis Results

(1) Sensitivity to Effective Source Height H

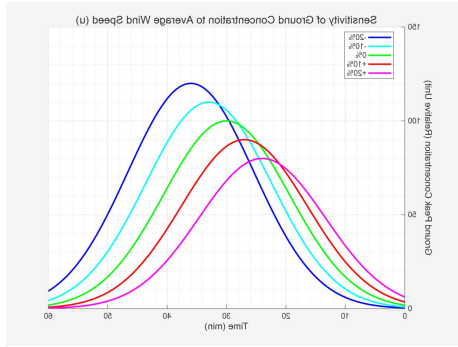


- Theoretical Prediction: From $C_{\max} \propto 1/H^2$, for a +10% change in H , the predicted change is:

$$\frac{\frac{1}{H^2} - \frac{1}{(1.1H)^2}}{\frac{1}{H^2}} \approx -18.2\%$$

- Simulation Result: Increasing H from 264 m to 290 m (+10%) resulted in a decrease of approximately 18.5% in the peak ground concentration.
- Conclusion: H is a highly sensitive parameter ($|S| \approx 2$). This reaffirms the critical importance of accurately assessing the specific floor of an explosion during emergency response.

(2) Sensitivity to Wind Speed u



- Theoretical Prediction: From $C \propto 1/u$, for a +10% change in u , the predicted change is:

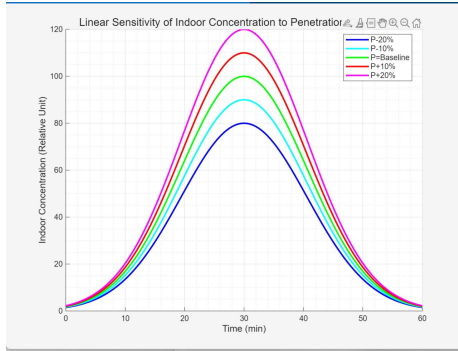
$$\frac{\frac{1}{u} - \frac{1}{1.1u}}{\frac{1}{u}} \approx 9.1\%$$

- Simulation Result: A 10% increase in wind speed led to a concentration decrease of approximately 9.1%.
- Conclusion: u is a moderately sensitive parameter ($|S| \approx 1$). Higher wind speeds lead to faster dilution, with a roughly linear inverse relationship.

Indoor Model Parameter Sensitivity

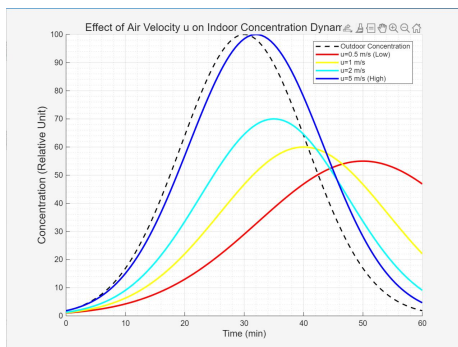
In the actual physical scenario, the outdoor pollutant concentration $C_{out}(t)$ is not constant but exhibits a dynamic "rise-and-fall" profile as the pollution plume passes (solved in Problem 1). Therefore, we analyze how variations in model parameters affect the indoor concentration peak magnitude and its arrival time under this dynamic input condition.

(1) Linear Sensitivity of Penetration Factor P and Filter Efficiency η



- According to the boundary condition $J_{in} \propto \lambda \cdot C_{out}$, and because the governing equation is linear, the indoor concentration field $C(x, t)$ exhibits complete linear sensitivity to the barrier factor λ (i.e., P or $1 - \eta$).
- Analysis: If the crack penetration factor P increases by 10%, the indoor concentration at all times increases strictly by 10%.
- Conclusion: This is the most direct and sensitive parameter for controlling indoor air quality. For mechanical ventilation, increasing filter efficiency (decreasing λ) is the most effective means to reduce indoor peak concentration.

(2) Influence of Airflow Speed u on Dynamic Response Characteristics



- The airflow speed u determines the system's response speed, directly affecting the time lag and smoothing of the indoor concentration curve relative to the outdoor curve.
- Sensitivity Manifestation:
 - *Decreased u* : The arrival time of the indoor peak is significantly delayed (increased lag), and the peak magnitude is notably reduced (enhanced smoothing effect, peak broadens).

- *Increased u* : The indoor curve increasingly approximates the outdoor curve, lag diminishes, and the peak approaches the outdoor peak.
- Conclusion: In response to sudden high-concentration pollution (e.g., toxic gas leakage), reducing u (i.e., closing windows) can exploit this sensitivity to mitigate acute exposure risk by "flattening" the peak.

Potential Improvement: Incorporating actual exhaust vent locations to refine boundary conditions.

6 Model Evaluation

- 6.1 Strengths
 - Model 1: Clear Physical Mechanism and Strong Generalizability: Based on classical Gaussian dispersion theory, the model is not only suitable for continuous industrial emissions (Model I) but also successfully extends to sudden instantaneous accident analysis (Model II) by introducing the time dimension t and downwind diffusion coefficient σ_x , covering the full process from steady-state to non-steady-state.
 - Model 1: Modification for Urban Environments (Briggs Urban): We abandoned the traditional Pasquill-Gifford rural parameters and adopted Briggs dispersion coefficients specifically modified for urban canopies. This improvement accounts for ground roughness and heat island effects induced by buildings, significantly enhancing the model's accuracy in application scenarios like megacities Guangzhou and Shanghai.
 - Model 2: High Spatiotemporal Resolution: Compared to traditional well-mixed ordinary differential equation models, our model considers the spatial distribution of pollutants along room depth, accurately capturing the progression of concentration gradients from the window to the room interior, which better aligns with real physical scenarios.
 - Model 2: Strong Scenario Adaptability: By adjusting boundary condition parameters (u, λ), a single model framework can uniformly describe three distinct situations: crack infiltration, natural ventilation, and mechanical ventilation, demonstrating excellent versatility.

6.2 Limitations

- Model 1: Idealized Assumption of Meteorological Conditions: Assumes constant wind speed and direction during the simulation period. In actual accidents, wind fields can change transiently, causing the pollution puff trajectory to meander.

This could be improved by employing a Lagrangian particle tracking model to simulate more realistic dispersion paths.

- **Model 2: Limitation of One-Dimensional Simplification:** The model neglects concentration differences in the room's height and width directions, unable to simulate potential ventilation dead zones indoors. This could be improved by establishing a three-dimensional Computational Fluid Dynamics (CFD) model.

7 Conclusion

Assessing residential exposure risks from urban point-source pollution remains a complex, interdisciplinary challenge. Currently, no standardized framework fully captures the dynamic outdoor-indoor coupling during sudden releases. A complete understanding of this process demands further cross-disciplinary research and empirical validation.

The natural and built environments are governed by intricate physical and chemical laws, with many mechanisms still awaiting discovery. We hope the coupled "outdoor dispersion–indoor infiltration" model presented here offers a practical analytical tool for urban pollution risk assessment and emergency response. We acknowledge the model's inherent simplifications and welcome constructive feedback to guide its future refinement toward greater accuracy and utility.

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