

Exploring the spatial sensitivity of environmental parameters: emission source location, building layout, and emission intensity in urban microscale CFD modeling

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ABSTRACT

Computational Fluid Dynamics (CFD) is essential for simulating urban micro-meteorology and pollutant dispersion, yet high computational costs necessitate the simplification of building layout and source parameters. This study investigates the spatial sensitivity of modeling fidelity in a characteristic high-density residential neighborhood in Nanjing ($H_{max} = 20$ m) under prevailing southeasterly wind conditions. We innovatively introduced the Structural Similarity Index Measure (SSIM) to evaluate similarities in concentration magnitude (luminance) and spatial patterns (structure), transcending traditional point-wise error analysis. Nine scenarios were analyzed by varying source locations, downstream layouts, and emission strengths. Results for this specific neighborhood morphology show: (1) The emission source location significantly impacts a characteristic near-field zone ($y < 900$ m, i.e., $20H_{max}$ from the neighborhood boundary; $z < 100$ m or $5H_{max}$), but sensitivity decays rapidly, with SSIM values approaching 1 beyond these spatial thresholds. (2) Downstream sparse buildings induce only localized perturbations with negligible impact on macro-scale dispersion in this texture. (3) Variations in source strength only linearly scale concentration magnitudes, while the spatial structure remains invariant (SSIM structure ≈ 1). Finally, a sensitivity hierarchy for this type of neighborhood-scale modeling is established: source location is the most critical, followed by near-field building layout, while source strength allows for flexible simplification. Operationally, explicit geometric resolution and precise source localization are strictly required only within $20H_{max}$ horizontally and $5H_{max}$ vertically. Beyond these case-specific thresholds, far-field geometries can be safely simplified (e.g., replacing sparse downstream buildings with aerodynamic roughness) to reduce computational cost without sacrificing dispersion accuracy.

1. Introduction

Computational Fluid Dynamics (CFD) has emerged as the preferred tool for high-fidelity numerical simulations of micro-meteorology and micro-environments at the street-canyon and community scales. This preference stems from its robust ability to resolve complex three-dimensional flow structures and the intricate physical processes of pollutant transport within the urban canopy [1]. Compared to mesoscale meteorological-chemical models operating on kilometer-scale grids (e.g., WRF-Chem) or statistical approaches based on synoptic weather patterns [2], CFD offers superior resolution in characterizing building-induced wake flows, local vortex formation, and near-source pollutant dispersion [3]. This level of detail is crucial for assessing

urban ventilation potential [4], the urban heat island (UHI) effect [5–7], and associated public health risks. Furthermore, CFD provides an essential technical foundation for fine-grained environmental management, bridging the scale gap from urban agglomerations [8,9] to local communities [10].

However, high-fidelity CFD simulations invariably incur prohibitive computational costs. To accurately reproduce complex urban morphologies, researchers must construct detailed building geometries and define intricate boundary conditions. This often necessitates using unstructured meshes to conform to irregular building shapes. These requirements not only impose significant computational burdens but also frequently trigger numerical instability and convergence issues related to mesh quality, turbulence model selection, or boundary condition

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parameterization [3]. Therefore, to ensure both numerical robustness and practical feasibility for engineering applications, it is highly desirable to rationally simplify CFD configurations—such as by adopting streamlined meshing strategies or reducing boundary complexity—provided that the essential physical processes are faithfully captured.

Essentially, this simplification represents a rational abstraction of real-world conditions. Prevalent strategies in urban CFD modeling include omitting buildings or isolated obstacles that exert negligible aerodynamic influence on the target flow field [11]; neglecting minor facade details (e.g., window frames and balconies) [12]; and abstracting the indirect effects of indoor spaces on street-canyon ventilation [13]. Additionally, for subsequent pollutant dispersion simulations, researchers frequently simplify the quantity [14], geometry, location [15], and intensity [16] of emission sources. The primary objective of these "simplified modeling" strategies is to strike an optimal balance between computational efficiency and simulation accuracy.

However, a critical scientific question remains: What are the spatial sensitivity boundaries of these modeling simplifications regarding the final simulation outcomes? Specifically, how do they impact the spatiotemporal distribution of airflow and pollutant concentrations at micro-scales of several hundred meters? In other words, beyond what spatial extent (e.g., the downwind distance normalized by maximum building height) do simulation discrepancies become practically negligible? Such discrepancies are typically induced by adding or removing buildings, adjusting layouts, or modifying the location and intensity of emission sources. To date, the literature lacks universal consensus or quantitative thresholds regarding these boundaries.

Several studies indicate that at the neighborhood or district scale, statistical urban morphological parameters—such as building density, sky view factor (SVF), and frontal area index—are the primary drivers of urban heat island (UHI) intensity and ventilation potential [4,17]. This suggests that securing accurate macro-scale morphological data may be more critical than modeling the precise geometric details of individual buildings. For instance, parameters like building height and floor area ratio (FAR) dictate variations in the ventilation potential coefficient [4]. Meanwhile, vegetation coverage and building density explain most of the variance in surface UHI intensity [17]. At the micro-scale, however, the exchange of energy, momentum, and mass between the urban canopy and the atmosphere is highly spatially heterogeneous [18–20]. Driven by specific building layouts, this non-uniformity modulates mesoscale circulations [21] and shapes micro-scale ventilation corridors [22].

Furthermore, several CFD studies explicitly warn that geometric simplifications can introduce substantial errors. For instance, minor variations in building arrangements can alter local flow fields, significantly impacting the spatial distribution of pollutants—particularly reactive species—within street canyons [23]. On windward facades, the presence of balconies can restrict airflow penetration, thereby reducing internal wind speeds [24]. Moreover, roof shapes and building heights directly govern airflow patterns and pollutant dispersion in isolated street canyons [25,26]. Other research highlights that the distance and angular position of emission sources distinctly alter pollutant dispersion around high-rise buildings [27]. Additionally, street trees create aerodynamic blockage effects that vary depending on wind speed, leaf area density (LAD), drag coefficient, canopy morphology, and blockage ratio [28]. Reinforcing this perspective, the recently developed Inhomogeneous Wind Scheme for Urban Streets (IWSUS-v1) demonstrates that parameterization schemes accounting for urban canopy heterogeneity yield significantly higher simulation accuracy than traditional homogeneous models [1].

Despite these insights, significant knowledge gaps persist. First, most studies on simplification sensitivity are confined to specific cases or idealized street canyons. They lack a systematic approach to quantify the impact magnitude and spatial attenuation patterns of various simplification strategies (e.g., geometry, layout, and source location) on

simulation outcomes. Second, existing findings fail to identify the spatial thresholds beyond which micro-scale details become negligible. This threshold is a crucial metric for guiding the rational simplification of CFD setups in realistic, complex communities. Finally, few studies have integrated building detail sensitivity with emission source characteristics (e.g., emission height) to explore their coupled effects and relative importance in local pollutant dispersion.

Consequently, this study systematically investigates the following core questions regarding CFD simulations of urban near-surface environments (at a scale of several hundred meters): to what extent do minor building layout alterations (e.g., adding or removing individual buildings) and spatial shifts in emission sources impact local airflow and spatiotemporal pollutant distribution? How do these impacts attenuate with downwind distance? Moreover, how does the magnitude of influence vary when these adjustments occur at different upstream or downstream locations? Ultimately, this research seeks to quantitatively identify the critical spatial threshold beyond which discrepancies induced by these variations become practically negligible for regional assessments. Through controlled numerical experiments, this study provides a scientific foundation and practical guidelines for defining the "requisite modeling fidelity" in complex urban communities. This approach optimizes the efficiency of high-resolution environmental modeling without compromising reliability.

2. Methodology

To systematically address the spatial boundary questions regarding modeling fidelity raised in the Introduction, this study employs a parametric simulation approach. First, a "baseline scenario" (Case 1) is established. Subsequently, a series of comparative scenarios are constructed by systematically varying specific parameters: emission source locations (Cases 2–4), downstream building layouts (Case 5), and emission intensities (Cases 6–9). By comparing these experimental cases against the baseline, we aim to decouple and quantify the independent effects of each modeling dimension. Furthermore, the Structural Similarity Index Measure (SSIM) is employed to spatially quantify these discrepancies and determine their downwind attenuation patterns.

2.1. Study area and emission scenarios

This study focuses on the Ruijin-Xincun neighborhood and its vicinity in the Qinhuai District, Nanjing (Fig. 1(a)). The area features typical 6- to 7-story slab-style residential buildings constructed in the 1990s. Kitchen exhausts, primarily located on the northern building facades, operate as decentralized direct-discharge vents. The star symbol in the figure indicates the monitoring station used for observational validation in Section 3.1. Based on best practice guidelines [29], the inlet, lateral, and top boundaries must be positioned at least $5H_{max}$ from the target building region, while the downstream boundary requires a minimum distance of $15H_{max}$ to ensure full wake flow development. Here, H_{max} denotes the maximum building height. In this study, H_{max} is 20 m (Fig. 1(c)), and the target building zone occupies a volume of $500 \text{ m} \times 500 \text{ m} \times 20 \text{ m}$. Consequently, the overall CFD computational domain spans $2500 \text{ m} \times 2500 \text{ m} \times 200 \text{ m}$ (Fig. 1(d)). Furthermore, Reynolds number independence is a critical criterion for simulating isothermal flows and pollutant dispersion around buildings [14]. The characteristic Reynolds number (Re) is defined as $Re = U_{ref}H/\nu$. Given an inlet reference wind speed (U_{ref}) of 3 m/s, a characteristic building height (H) of 20 m, and the kinematic viscosity of air (ν), the calculated Re is approximately 4.0×10^6 . This value significantly exceeds the critical threshold, confirming that the flow field is fully turbulent and invariant to further increases in the Reynolds number.

Based on meteorological data collected in Qinhuai District, Nanjing, from January to December 2021, a wind rose diagram was generated (Fig. 2). This diagram indicates that southeasterly winds dominate the

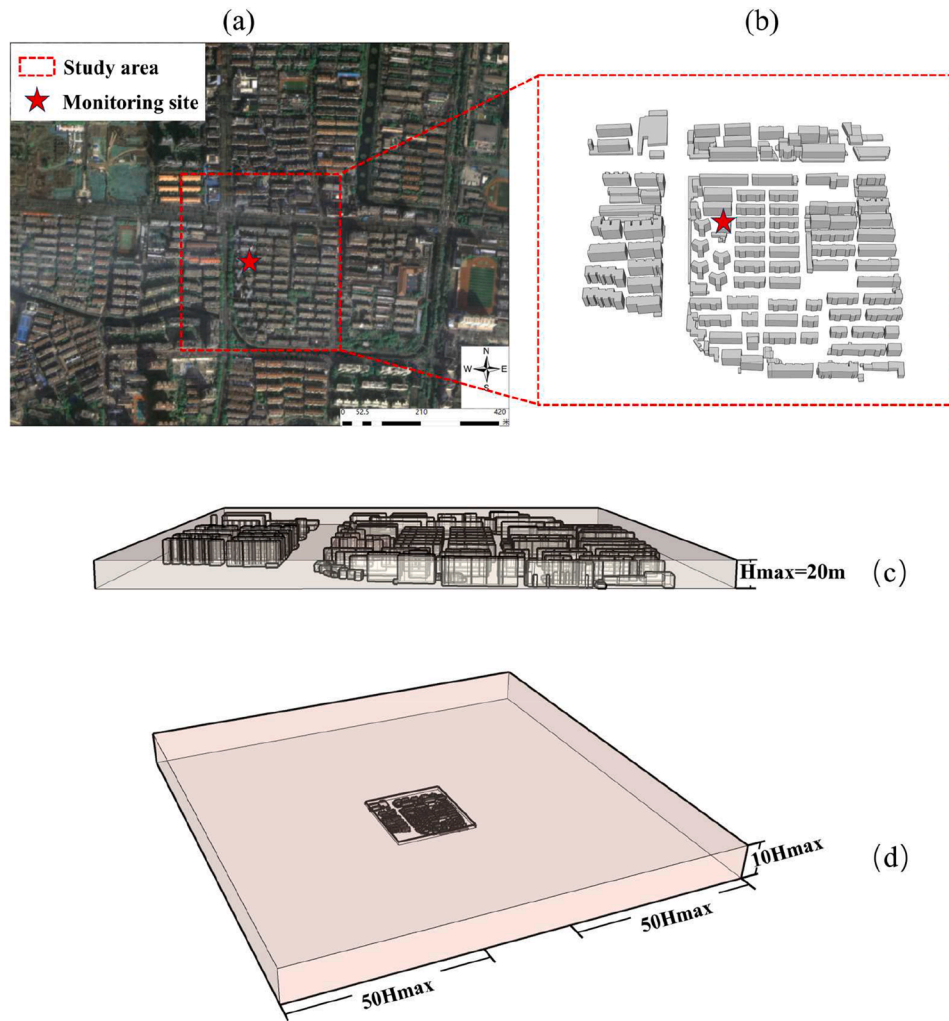


Fig. 1. the study area: (a) satellite imagery; (b) 3D building model; (c) maximum height out profiles of the building, and (d) computational domain for the CFD simulation.

study area. Consequently, the numerical simulations in this study investigate the spatial distribution of microclimatic variables and pollutant dispersion characteristics under a prevailing southeasterly wind with a reference speed of 3 m/s.

Fig. 3 illustrates the spatial distribution of emission sources and the delineation of building domains within the simulation cases. Based on their geographic locations, potential emission zones are classified into three categories: Zones A, B, and C. Fixed emission points within each zone are denoted by blue, red, and brown dots, respectively. In the computational setup, these are explicitly prescribed as mathematical point sources. To guarantee that the pollutant behaves strictly as a passive scalar without inducing artificial aerodynamic interference, the emissions are implemented purely as a scalar mass source term, completely devoid of any associated momentum flux (i.e., they are not prescribed as velocity inlets). Across the numerical experiments (Cases 1–9), active emission sources are arranged in four spatial patterns: exclusively in Zone A, Zone B, Zone C, or simultaneously across all three (A+B+C). To isolate the variables of interest, the total emission rate remains strictly constant across all scenarios, with intensity uniformly distributed among the active source points. This setup serves as a rational abstraction, deliberately simplifying the heterogeneity of real-world emissions to focus on the core research objectives. Regarding the building environment, Area 1 encompasses only the primary building clusters of the Ruijin-Xincun neighborhood (indicated by the yellow bounding box). Area 2 expands this domain by incorporating sparser

buildings to the west and north (indicated by the green bounding box).

As summarized in Table 1, the numerical experiments are systematically structured. Cases 1–4 are designed to investigate sensitivity to emission source locations by varying the active source zones while keeping emission intensity and the building domain constant. Comparing Case 1 with Case 5 isolates the aerodynamic impact of sparse downstream buildings; here, the explicitly modeled building domain is altered, but source locations and intensity remain fixed. Furthermore, evaluating Cases 6–9 against Cases 1–4 examines the effect of emission intensity. These scenarios maintain identical source locations and building layouts but amplify the emission strength by an order of magnitude. Collectively, these scenarios form a robust experimental matrix explicitly designed to decouple the independent effects of these key modeling parameters.

2.2. Structural similarity index measure (SSIM)

This study employs the Structural Similarity Index Measure (SSIM) to quantitatively evaluate the similarity of pollutant concentration distributions across different emission scenarios within the same spatial domain. Originally developed by the Laboratory for Image and Video Engineering (LIVE) [30], the SSIM algorithm compares two input arrays—represented in this context as 2D spatial concentration fields. It calculates the overall index by integrating three distinct evaluation components: luminance, contrast, and structure. The SSIM yields a

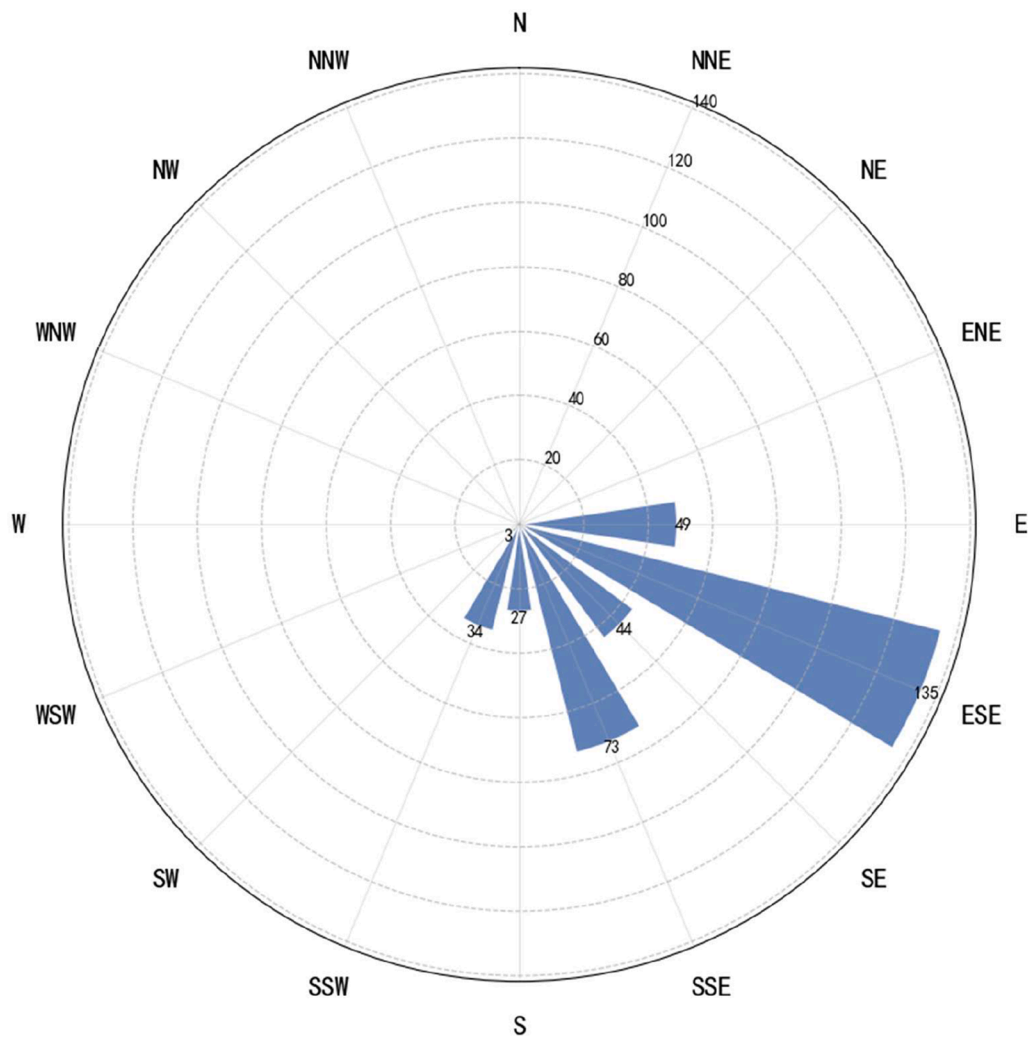


Fig. 2. Wind rose diagram of the host city of the study area from January to December 2021.

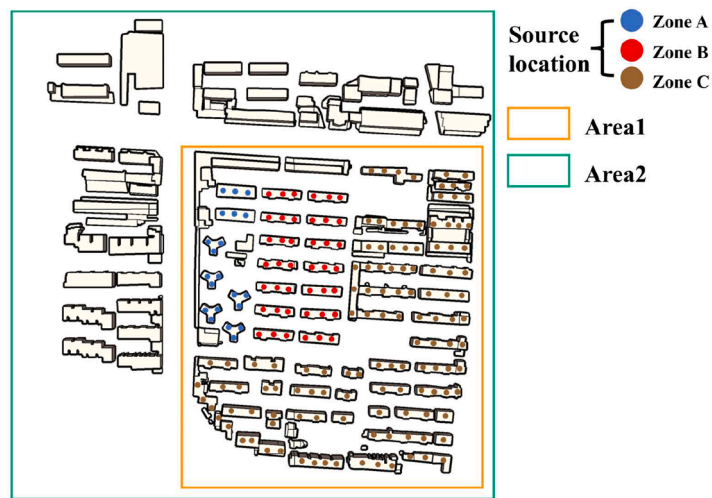


Fig. 3. Study area and potential emission source locations. The blue, red, and brown dots represent emission sources in zones A, B, and C, respectively. In the numerical experiments (Cases 1–9), emissions were allocated exclusively in zone A, B, C, or simultaneously in all zones (A+B+C), with the total emission rate kept constant across all cases. All source points within a given case share the same emission intensity.

maximum value of 1, with values approaching 1 indicating a higher degree of spatial similarity between the two compared concentration

Table 1

Configuration of simulation scenarios for the Ruijin Xincun neighborhood in Nanjing.

simulation scenario	Active Source Zones	Total Emission Intensity (g/s)	Building Domain
Case1	A+B+C	1	Area 1
Case2	Only A	1	Area 1
Case3	Only B	1	Area 1
Case4	Only C	1	Area 1
Case5	A+B+C	1	Area 2
Case6	A+B+C	10	Area 1
Case7	Only A	10	Area 1
Case8	Only B	10	Area 1
Case9	Only C	10	Area 1

fields.

First, for discrete signals, the mean intensity μ_x is utilized as an estimate of luminance. This mean intensity is then used to define the luminance comparison function, $l(x,y)$, which measures the similarity in average luminance between two images:

$$\mu_x = \frac{1}{N} \sum_{i=1}^N x_i \quad (1)$$

$$l(x,y) = \frac{2\mu_x\mu_y + C_1}{\mu_x^2 + \mu_y^2 + C_1} \quad (2)$$

where μ_x and μ_y are the mean intensities of images x and y , respectively. $C_1 = (K_1L)^2$ is a constant introduced to maintain stability (i.e., to avoid instability when the denominator is close to zero), and L represents the dynamic range of the pixel values (the number of grayscale levels). For an 8-bit image, $L = 255$. K_1 is a small constant ($K_1 \ll 1$), which is set to 0.01 in this study.

Next, the local standard deviation σ_x is employed to reflect the dynamic range of pixel values, thereby defining the contrast comparison function, $C(x,y)$, which evaluates the similarity in contrast:

$$\sigma_x = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \mu_x)^2} \quad (3)$$

$$c(x,y) = \frac{2\sigma_x\sigma_y + C_2}{\sigma_x^2 + \sigma_y^2 + C_2} \quad (4)$$

where the stability constant is $C_2 = (K_2L)^2$ with $K_2 \ll 1$. In this study, K_2 is set to 0.03.

Subsequently, the structural comparison function, $s(x,y)$, is defined using the local standard deviations (σ_x, σ_y) and the local covariance (σ_{xy}) to measure the similarity in structural information between the two images:

$$\sigma_{xy} = \frac{1}{N-1} \sum_{i=1}^N (x_i - \mu_x)(y_i - \mu_y) \quad (5)$$

$$s(x,y) = \frac{\sigma_{xy} + C_3}{\sigma_x\sigma_y + C_3} \quad (6)$$

where the stability constant is defined as $C_3 = C_2/2$.

Finally, the three components are combined to formulate the overall SSIM index function:

$$SSIM(x,y) = [l(x,y)]^\alpha [c(x,y)]^\beta [s(x,y)]^\gamma \quad (7)$$

where the exponents $\alpha, \beta, \gamma > 0$ are parameters used to adjust the relative importance of the three components.

In this study, local statistical analysis is performed using an 11×11 Gaussian weighting window with a standard deviation of $\sigma = 1.5$. The Gaussian window is initially generated via a one-dimensional

Gaussian function, subsequently constructed into a two-dimensional Gaussian kernel through the outer product, and normalized to ensure the sum of the weights equals 1. Compared to a uniform mean filter, Gaussian weighting effectively amplifies the influence of the central pixel, thereby capturing local spatial structural features more accurately. The illustrative validation of the specific functions of each SSIM component has been detailed in Appendix A. This research primarily utilizes the luminance and structural components of the SSIM to compare the pollutant dispersion fields across different emission scenarios. Specifically, the luminance component evaluates the similarity in the absolute magnitude of pollutant concentrations, whereas the structural component quantifies the topological similarity of the spatial distribution patterns. It is crucial to clarify the data preprocessing methodology: rather than applying the SSIM algorithm directly to post-processed RGB contour plots, this study implements a direct mapping of the raw physical data. Prior to evaluating the luminance component, varying pollutant concentration values are strictly mapped to corresponding 8-bit grayscale levels (i.e., higher physical concentrations are assigned proportionally higher grayscale values). This mapping guarantees that the SSIM algorithm rigorously evaluates the actual physical concentration differences rather than artificial rendering colors. Furthermore, an idealized validation experiment is presented in Appendix B to demonstrate the irreplaceable superiority of SSIM over traditional global metrics (e.g., spatial RMSE).

2.3. Governing equations, computational grid, and boundary conditions

Given the exceedingly high Reynolds numbers inherent in atmospheric boundary layer (ABL) flows, resolving all turbulent scales via Direct Numerical Simulation (DNS) or Large Eddy Simulation (LES) incurs prohibitive computational costs [29,31–33]. Furthermore, this study primarily focuses on the statistical mean flow fields within the target domain, rather than transient turbulent structures. Consequently, the Reynolds-Averaged Navier-Stokes (RANS) approach is adopted. This framework has been extensively validated for reliably predicting pollutant dispersion in both 2D and 3D urban models. By time-averaging the instantaneous Navier-Stokes equations, RANS substantially reduces computational demands. The governing equations for mass and momentum conservation are expressed as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (8)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}(-\rho \overline{u'_i u'_j}) \quad (9)$$

where ρ denotes the fluid density; u_i and u_j represent the time-averaged velocity components in the i and j directions, respectively; p is the time-averaged thermodynamic pressure; σ_{ij} denotes the components of the molecular viscous stress tensor; u'_i and u'_j represent the velocity fluctuation components in the i and j directions; and $-\rho \overline{u'_i u'_j}$ designates the Reynolds stress tensor.

Compared to alternative RANS models—such as the $k-\omega$ shear stress transport (SST), renormalization group (RNG) $k-\epsilon$, and realizable $k-\epsilon$ (RKE) models—the standard $k-\epsilon$ (SKE) model has proven highly capable of simulating a broad spectrum of turbulent phenomena [13,33]. Furthermore, it effectively characterizes airflow and pollutant transport within urban street canyons. Consequently, this study adopts the SKE model to simulate pollutant dispersion under various emission scenarios in the Ruijin-Xincun area. The conservation equations for turbulent kinetic energy (k) and turbulent dissipation rate (ϵ) are expressed as follows:

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \epsilon \quad (10)$$

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_1 \frac{\varepsilon}{k} P_k - C_2 \frac{\varepsilon^2}{k} \quad (11)$$

$$P_k = \nu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \quad (12)$$

In the above equations, ν denotes the kinematic molecular viscosity of the fluid; ν_t is the turbulent kinematic viscosity; P_k represents the production of turbulent kinetic energy induced by mean velocity gradients; and u_i and u_j are the time-averaged velocity components in the i and j directions, respectively. The empirical constants C_1 , C_2 , σ_k , and σ_ε are generally determined through data fitting from a multitude of simple turbulent flow experiments, granting them considerable universal applicability. In this study, the values for C_1 , C_2 , σ_k , and σ_ε are set to 1.44, 1.92, 1.00, and 1.30, respectively.

The numerical simulations were executed using the open-source CFD toolbox OpenFOAM v8. The steady-state incompressible turbulence solver (simpleFoam) was employed. To ensure computational convergence, the iterative process was maintained until the scaled residuals for all governing equations stabilized and dropped below 1×10^{-6} .

Grid generation is critical for CFD simulations, as computational accuracy and efficiency depend heavily on mesh quality, topology, and spatial adaptability. To balance computational efficiency with high-resolution flow capture in critical regions, this study employs a multi-level grid refinement strategy (detailed in Appendix C). First, the blockMesh utility generates a structured background mesh. This far-field domain consists entirely of hexahedral cells that progressively coarsen outward from the target buildings via proportional grading, thereby optimizing resource allocation. Next, the snappyHexMesh utility performs local refinement and surface snapping around complex building geometries. By defining multiple refinement zones on and around the buildings, the mesh achieves smooth, progressive densification in the near-field. The finalized grid ensures a seamless transition from the coarse far-field to the highly resolved near-field, which is essential for accurately capturing flow separation and wake characteristics. Finally, a comprehensive grid sensitivity analysis (Section 2.4) confirms the grid independence of the simulation results.

The inlet of the computational domain is designated as a velocity inlet, where a constant time-averaged velocity of $U_{ref} = 3\text{m/s}$ is prescribed to simulate specific low-wind-speed meteorological conditions. To ensure the accurate specification of inflow turbulence characteristics, the turbulent kinetic energy (k) and turbulent dissipation rate (ε) at the inlet are determined using the following expressions:

$$k = \frac{3}{2} (I |U_{ref}|)^2 \quad (13)$$

$$\varepsilon = \frac{C_\mu^{3/4} k^{3/2}}{l} \quad (14)$$

where k is the turbulent kinetic energy; I is the turbulence intensity; U_{ref} is the reference velocity; l is the turbulence length scale; and C_μ is the model constant ($C_\mu = 0.09$).

Subsequently, the turbulent kinematic viscosity (ν_t) is derived from k and ε as follows:

$$\nu_t = C_\mu \frac{k^2}{\varepsilon} \quad (15)$$

2.4. Grid sensitivity analysis

To evaluate grid sensitivity, three mesh systems with varying resolutions were generated: a coarse mesh (approximately 219,000 cells), a medium mesh (641,709 cells), and a fine mesh (3683,462 cells). Fig. 4 compares the vertical profiles of wind speed (Fig. 4(a)) and normalized pollutant concentration (Fig. 4(b)) in the leeward wake region across these three grid densities. The results demonstrate that as the mesh is refined, both the velocity and concentration profiles exhibit clear convergence.

A quantitative analysis was conducted using the Grid Convergence Index (GCI) method [34], with the results summarized in Table 2. At the critical study height of $z = 15\text{ m}$, the apparent order of convergence for

Table 2

Summary of grid sensitivity analysis data for flow and concentration fields ($z = 15\text{ m}$).

Parameter	Symbol	Coarse mesh (N_3)	Medium mesh (N_2)	Fine mesh (N_1)
Total number of cells	N	219,008	641,709	3683,462
Grid refinement ratio	r	-	$r_{32} = 1.43$	$r_{21} = 1.79$
Flow field variable (U)				
Wind speed (m/s)	ϕ_u	1.0443	0.5412	0.5754
Apparent order of convergence	p_u	-	-	4.62
Extrapolated value	ϕ_{ext}	-	-	0.5778
Extrapolated relative error	e_{ext}	-	-	0.43%
Grid convergence index	GCI_{fine}	-	-	0.54%
Concentration field variable (T)				
Normalized concentration (10^{-5})	ϕ_t	2.5	2.6	2.6
Apparent order of convergence	p_t	-	-	3.45
Extrapolated value (10^{-5})	ϕ_{ext}	-	-	2.6
Extrapolated relative error	e_{ext}	-	-	0.02%
Grid convergence index	GCI_{fine}	-	-	0.03%

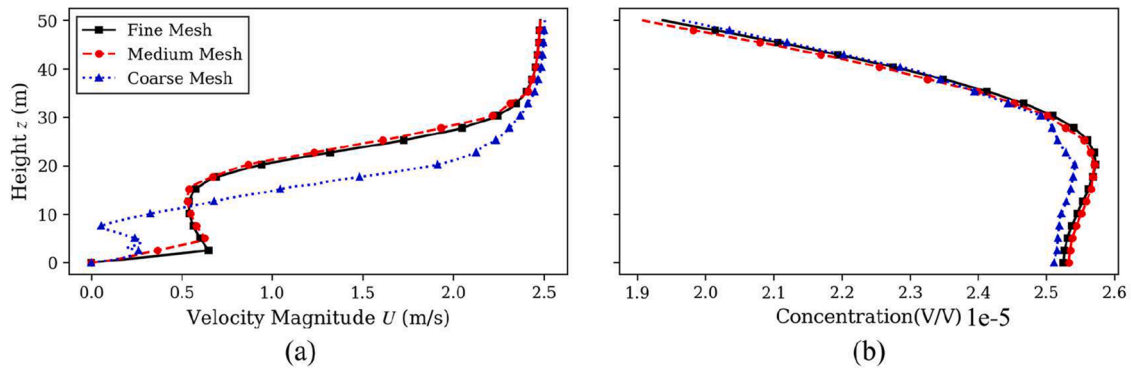


Fig. 4. Grid sensitivity analysis comparing three mesh resolutions in the building leeward wake region: (a) vertical profiles of wind speed, and (b) vertical profiles of normalized pollutant concentration.

the flow field (p_t) is 4.63, the fine-grid GCI (GCI_{fine}) is 0.54%, and the extrapolated relative error (e_{ext}) is 0.43%. For the concentration field, the apparent order of convergence (p_t) is 3.45, with a GCI_{fine} of 0.03% and an e_{ext} of 0.02%. Comparison reveals that the coarse mesh lacks sufficient resolution to capture intricate flow structures. Conversely, the medium and fine meshes demonstrate high consistency in aerodynamic characterization and pollutant transport simulation. Although minor non-monotonic oscillations occur in complex flow regions, numerical discrepancies between the fine and medium meshes remain marginal. Therefore, balancing computational cost and predictive accuracy, the medium mesh is adopted for all subsequent simulations. This choice ensures grid independence, guaranteeing that variations observed in comparative scenarios stem from physical modifications rather than discretization errors.

2.5. Parameterization of roughness for non-target areas

In practical urban CFD simulations, due to computational constraints, while the target residential neighborhood is explicitly modeled with fine geometric detail, the surrounding areas (upwind, downwind, and lateral) often cannot be fully resolved and must be simplified. Using the aerodynamic roughness length to characterize complex terrain and features in non-target areas is a common and well-validated approach to address this challenge. Previous studies have clearly indicated that, in CFD simulations, detailed building geometries should be explicitly resolved only within a radius of at least three times the maximum dimension of the target building; beyond this range, the roughness approach can be applied. The results show that the mean wind velocity obtained using this simplified method deviates by approximately 5.5% from that of a fully geometry-resolved simulation, which is acceptable for most applications [11].

Based on the above literature support, the present study treats the non-target areas outside the explicitly resolved building cluster within the OpenFOAM framework as follows: the wall function is set to `nutk-RoughWallFunction` (with a `noSlip` velocity boundary condition), mathematically representing the underlying ground surface in non-target areas as an aerodynamically rough surface with horizontally homogeneous characteristics, consistent with the geometric parameters of the street canyon (e.g., mean building height and street width). To quantify the aerodynamic roughness length of the surrounding areas, this study adopts the morphometric method proposed by Grimmond and Oke [35]. That study indicates that for an area with mean building height H , the roughness length can be approximated as $z_0 = f_0 H$, where the empirical coefficient f_0 is typically taken as 0.1. According to the actual conditions of the study area and its surroundings, the mean building height in the surrounding areas is comparable to that of the target neighborhood (Ruijin-Xincun, $H = 20$ m). Therefore, the roughness length for the surrounding areas is estimated as $z_0 \approx 0.1 \times 20 = 2.0$ m. This value is in good agreement with the typical aerodynamic roughness length range for urban central areas (1.0–3.0 m), further validating the consistency of our simplification.

It should be noted that the objective of this study is to determine far-field spatial convergence thresholds through comparative analysis (using the SSIM metric), rather than to predict absolute values with high precision. Therefore, the simplified treatment of the surrounding areas has limited impact on the core conclusions of this paper.

3. Results and discussion

To systematically decouple the effects of key factors on pollutant dispersion, this section investigates three primary dimensions based on the scenarios outlined in Table 1: (1) the sensitivity of spatial plume distribution to emission source locations (Section 3.2); (2) the aerodynamic impact of sparse downstream buildings on far-field pollutant transport (Section 3.3); and (3) the response of plume dispersion

patterns to varying emission intensities (Section 3.4). To ensure analytical rigor, this study employs a dual-perspective evaluation approach. First, macroscopic dispersion trends are qualitatively analyzed by comparing pollutant concentration contours across various horizontal and downstream vertical cross-sections. Second, the Structural Similarity Index Measure (SSIM) is utilized to quantitatively evaluate spatial structural conformity and concentration agreement between the experimental and baseline scenarios.

3.1. Validation of CFD simulation reliability and baseline concentration field analysis

This section presents a comparative validation between field-measured tracer data and CFD simulation results. Furthermore, it comprehensively analyzes the spatial distribution characteristics of the wind and concentration fields within the study area under Case 1 (the baseline scenario). A continuous release experiment utilizing sulfur hexafluoride (SF_6) as a tracer gas was conducted on the southeastern perimeter of the Ruijin-Xincun neighborhood, with a constant emission rate of 1 g/s. To ensure a quasi-steady-state concentration field, gas release commenced one hour prior to sampling. A fixed monitoring station (indicated in Fig. 1(a) and (b)) was deployed within the neighborhood to continuously record tracer concentrations at a 10-minute temporal resolution. Specifically, air samples were collected using an EM-1500 portable atmospheric sampler (Shenzhen Guoji Instrument Co., Ltd.) equipped with 1 L polytetrafluoroethylene (PTFE) gas bags (Dongguan Lanbo Experimental Equipment Co., Ltd.). The quantitative analysis of SF_6 concentrations was performed using Gas Chromatography with an Electron Capture Detector (GC-ECD) utilizing a GS-AL/KCl capillary column (50 m length, 0.530 mm inner diameter). The limit of detection (LOD) for this method is 0.004 ppb (v/v), which is two to three orders of magnitude lower than the experimentally observed concentrations, thereby guaranteeing an exceptionally high signal-to-noise ratio. The monitoring site was strategically positioned on the roof of a single-story building at a height of 7 m above ground level. To minimize and document localized aerodynamic interference, the horizontal distances from the sampling inlet to adjacent buildings were strictly verified: approximately 30 m to the north, 27 m to the west, 23 m to the east, and 56 m to the south. This setup coincides with a National Environmental Monitoring Station that has reliably served multiple previous research projects, further empirically verifying its spatial representativeness of the neighborhood's typical dispersion characteristics. While this single-point validation confirms the general order of magnitude and baseline transport behavior, its limitations in fully resolving the complete three-dimensional concentration topology are acknowledged. The field measurements were conducted from 08:00 to 16:00 on January 4, 2023. During this observational window, the regional background meteorology featured a stable southeasterly wind with an average velocity of 3 m/s. Moreover, deviations of instantaneous wind speeds from this mean were maintained within a 20% margin. Consequently, this period provides an exceptionally stable meteorological background for model validation.

Fig. 5(a) compares the time series of CFD-simulated tracer concentrations with field observations. Overall, the simulated and observed concentrations fall within the same order of magnitude. Following the calibration of relevant CFD model parameters, systematic biases—such as consistent overestimation or underestimation—have been effectively eliminated. Notably, the model slightly underestimates peak concentrations compared to the observations. This underestimation is a typical limitation of the Reynolds-Averaged Navier-Stokes (RANS) approach in resolving transient turbulent fluctuations [32,36,37]. Additionally, a slight time lag is observed during the concentration decay phase.

Fig. 5(b) displays the scatter regression plot of the observed versus simulated concentrations, where the black dashed line represents the ideal 1:1 reference line. Regression analysis indicates a slight overall

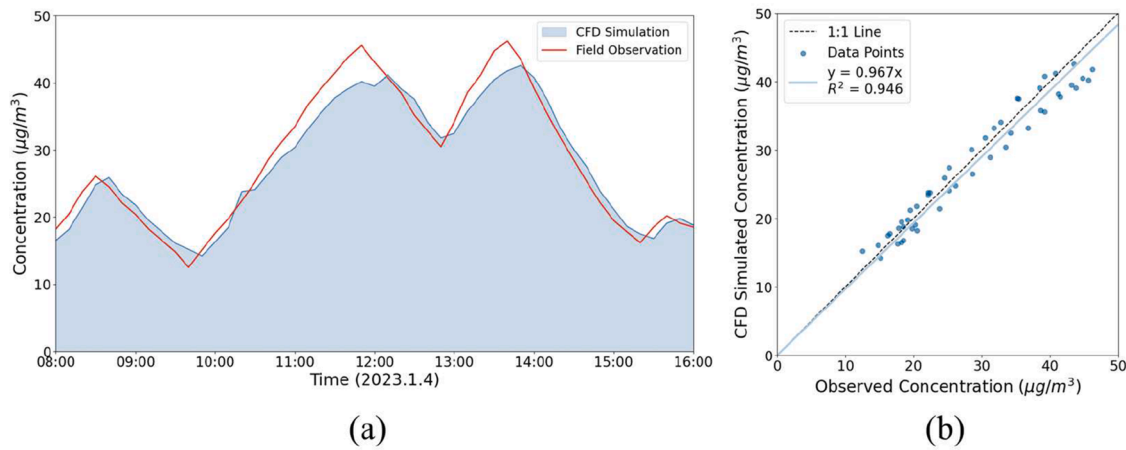


Fig. 5. Comparison of the CFD-predicted and field-observed tracer concentrations: (a) time series, and (b) scatter regression plot.

underestimation of approximately 3.3% by the CFD model; this deviation primarily stems from the aforementioned under-prediction of peaks in the high-concentration regions. Despite this minor discrepancy, most data points cluster tightly along the 1:1 reference line, indicating the absence of significant systematic bias across the entire sampling range. The high coefficient of determination ($R^2 = 0.946$) and a slope close to 1 demonstrate that the current CFD configuration is sufficiently accurate for subsequent pollutant dispersion analyses within the built environment.

Previous air quality studies have employed various statistical metrics to evaluate dispersion models [10,38–41]. Table 3 summarizes the metrics used to compare predicted and observed tracer concentrations. The validation results demonstrate the robust performance of the CFD model. This high consistency is likely attributable to the high temporal data resolution and the chemical inertness of SF_6 , which allows the simulation to isolate aerodynamic effects from complex chemical reactions.

Furthermore, this section analyzes the baseline concentration field to elucidate pollutant distribution characteristics within the Ruijin-Xincun area. As depicted in Fig. 6(a), under the prevailing southeasterly wind, the shielding effect of building clusters causes a substantial accumulation of pollutants within the neighborhood at $z = 15$ m. Although some pollutants are transported downstream into the near-field, far-field concentrations remain relatively low. As shown in Fig. 6(e), at an elevation slightly above $H_{\max}$ ($z = 25$ m), the spatial distribution strongly resembles that at $z = 15$ m; however, absolute concentrations within the neighborhood are markedly lower compared to the lower layer. Conversely, as illustrated in Fig. 6(i), at higher altitudes ($z = 100$ m), pollutant concentrations are negligible, indicating that localized emissions within the neighborhood minimally impact the atmospheric environment at this altitude.

3.2. Spatial sensitivity to the fine-tuning of emission source locations

This section investigates how minor adjustments to emission source

Table 3
Statistical validation metrics for comparing the predicted and observed tracer concentrations.

	SF_6	Ideal	Accept Range
HIT RATE	1	1	≥ 0.66
FAC2	1	1	$0.3 \leq \text{FAC2} \leq 1$
FB	0.022	0	$-0.67 < \text{FB} < 0.67$
MG	1.013	1	$0.7 < \text{MG} < 1.3$
NMSE	0.007	0	≤ 1.5
VG	1.006	1	< 1.6

locations impact pollutant dispersion and plume spatial distribution under prevailing southeasterly winds. Using pollutant concentration as the primary metric, this analysis delineates the horizontal and vertical extents where these source displacements significantly alter the plume. Furthermore, the Structural Similarity Index Measure (SSIM; detailed in Section 2.2) quantitatively evaluates spatial structural conformity and concentration agreement. This comparison is conducted between the realistic baseline (Case 1) and the experimental scenarios with shifted sources (Cases 2–4; Section 2.1). Consequently, this approach precisely identifies the sensitivity of simulated concentration fields to minor spatial modifications.

3.2.1. Impact on near-field concentration distribution

As illustrated in Fig. 6, to comprehensively analyze horizontal plume distribution, three typical heights were selected: within the urban canopy ($z = 15$ m), slightly above the maximum building height ($z = 25$ m), and in the higher airspace ($z = 100$ m). The results indicate that varying emission source locations significantly alters concentration distributions within the building clusters and near-field downwind regions across the four scenarios. In Case 2, where sources are exclusively in Zone A (Fig. 6(b, f)), the pollutant transport distance significantly exceeds that of the control group (Case 1; Fig. 6(a, e)). Because Zone A is situated further downwind within the cluster, the emitted plume experiences weaker physical blockage and aerodynamic perturbations from downstream buildings. Case 3 (Fig. 6(c, g)) confines emissions solely to Zone B. Although Zone B lies further upwind, the lower building heights in Zone A fail to significantly obstruct the advancing plume. Consequently, apart from localized discrepancies within Zone B (at $z = 15$ m and 25 m), Case 3 exhibits a concentration distribution largely similar to Case 2 across Zone A and its northwestern downwind regions. In contrast, Case 4 (sources restricted to Zone C; Fig. 6(d, h)) exhibits the weakest far-field transport capacity. Dense downstream buildings trap most pollutants, leading to considerably higher concentrations within the neighborhood and its immediate vicinity compared to the reference group, while far-downwind concentrations remain exceptionally low. These findings demonstrate that greater downstream building density and height exert stronger aerodynamic perturbations on pollutant dispersion, significantly altering the plume structure near the maximum building height. However, at higher altitudes ($z = 100$ m), the impact of minor source displacements on the overall plume distribution diminishes substantially (Fig. 6(i–l)). Therefore, when simulating complex urban street canyons, spatial source locations must be meticulously configured if the research focuses on or below the urban canopy. Conversely, the system's sensitivity to source location remains relatively low if the focus lies well above the canopy within the atmospheric boundary layer. Furthermore, dense buildings immediately downwind necessitate precise source

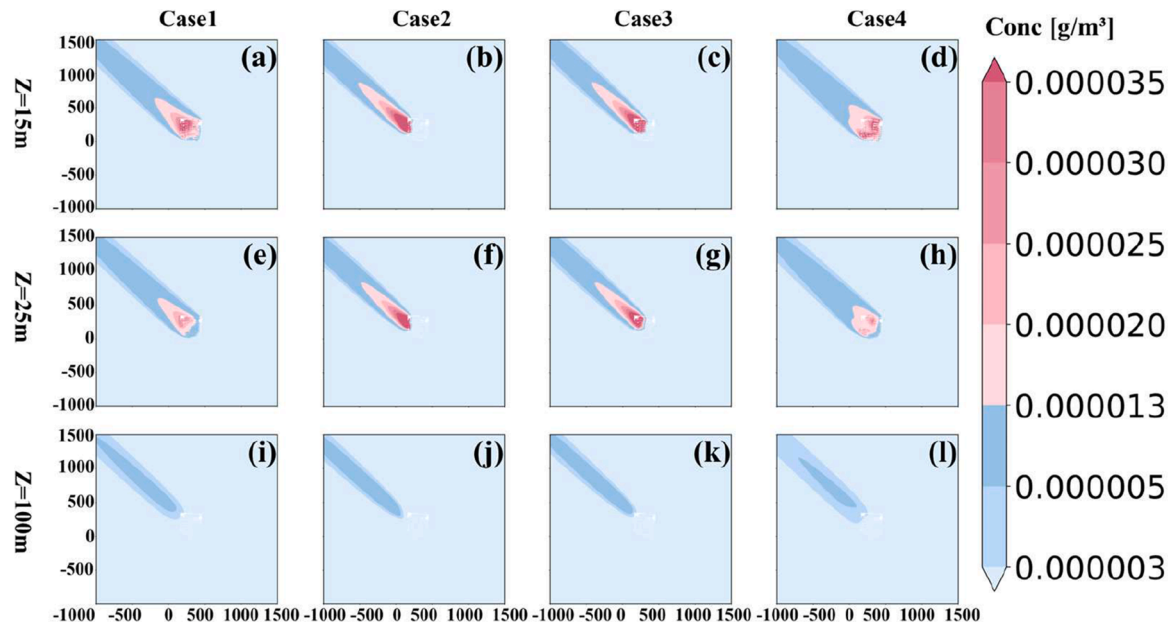


Fig. 6. Horizontal contour plots illustrating the spatial distributions of pollutant concentrations at various heights for Cases 1–4 under the prevailing southeasterly wind condition.

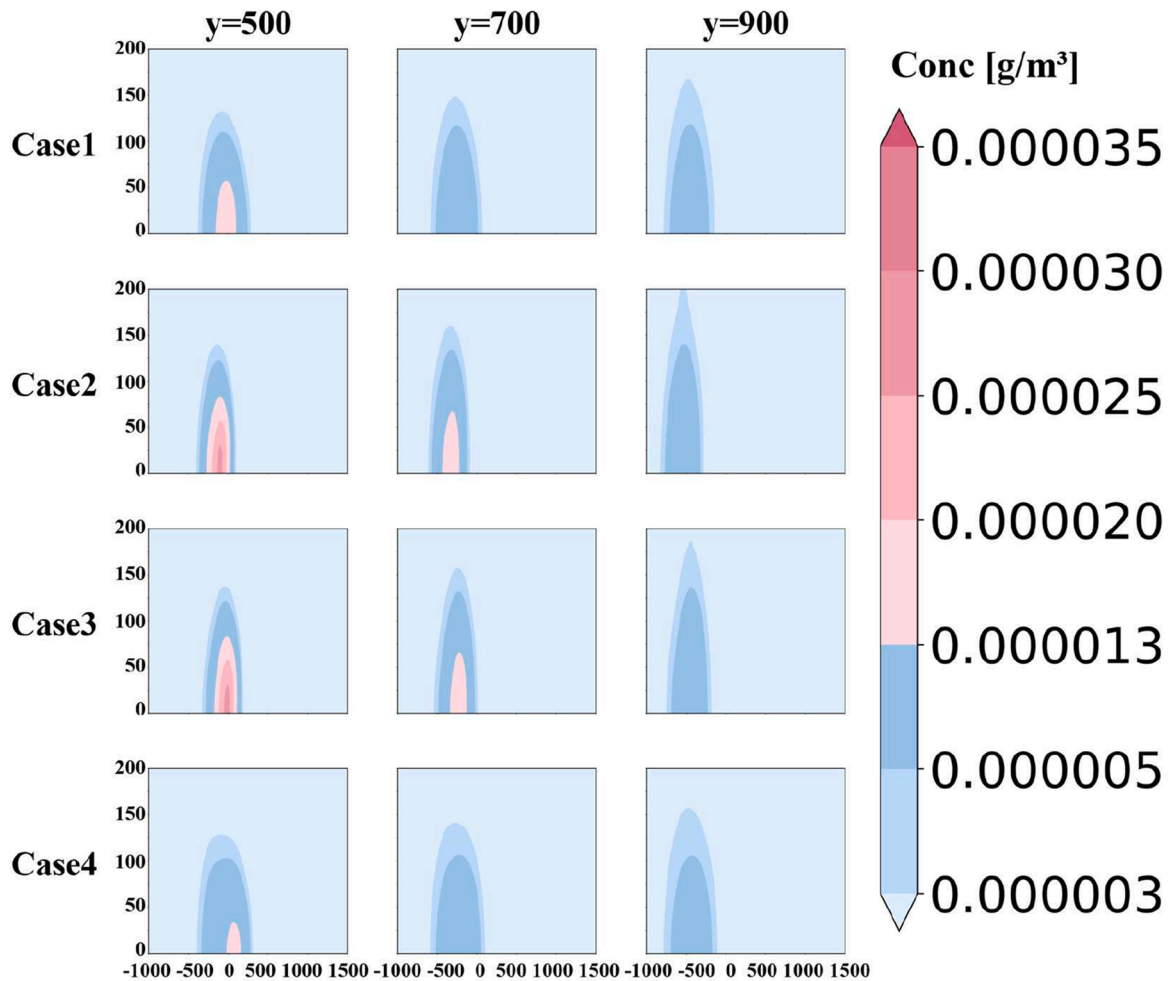


Fig. 7. Spatial distribution and downstream evolution of pollutant concentrations across vertical cross-sections (x - z planes) under various emission scenarios (Cases 1–4).

positioning; otherwise, these precision requirements can be appropriately relaxed.

Fig. 7 illustrates the plume concentration distributions for Cases 1–4 across vertical cross-sections at various downwind distances ($y = 500, 700, \text{ and } 900 \text{ m}$). Specifically, the $y = 500 \text{ m}$ plane aligns with the neighborhood's northern boundary, whereas the $y = 700 \text{ m}$ and 900 m planes lie further north. In the near-field regions ($y = 500 \text{ m}$ and 700 m), the four scenarios exhibit significant disparities. Below $z = 100 \text{ m}$, Cases 2 and 3 demonstrate markedly higher concentrations than the control group (Case 1). This indicates that positioning emission sources in the further downwind Zones A or B elevates concentrations in near-field, low-altitude regions. Conversely, Case 4, with sources situated in the upwind Zone C, exhibits substantially lower near-field concentrations than the control group. However, in the far-field region ($y = 900 \text{ m}$), the impact of minor source displacements becomes negligible, and the concentration distributions across the four scenarios tend to converge. This demonstrates that for spatial regions sufficiently far downwind ($y \geq 900 \text{ m}$, i.e., beyond $20H_{max}$ from the neighborhood edge) and at sufficient altitudes ($z \geq 100 \text{ m}$, i.e., above $5H_{max}$), the aerodynamic effects of source adjustments can be safely ignored. Within these spatial thresholds, however, aerodynamic perturbations caused by building morphology prevent pollutants from fully mixing and diluting. Consequently, variations in source locations induce non-negligible concentration discrepancies in localized areas.

3.2.2. Attenuation characteristics of the spatial influence: a quantitative evaluation based on SSIM

To further quantify these qualitative observations, Figs. 8 and 9 present the Structural Similarity Index Measure (SSIM) components, evaluating spatial similarities between the modified-source scenarios (Cases 2–4) and the baseline (Case 1) across horizontal cross-sections at the three specified heights. A lower SSIM value at any grid point indicates a more pronounced deviation from the baseline distribution. The results demonstrate that as altitude increases, both the SSIM luminance and structural components between Cases 2–4 and Case 1 exhibit a gradual ascent. At the height of $z = 100 \text{ m}$ (equivalent to $5H_{max}$), the SSIM values across the entire computational domain universally approach 1. From a mechanistic perspective, this elevation lies well above the urban canopy layer, transitioning into the upper roughness sublayer or inertial sublayer. In this regime, vertical dispersion is predominantly driven by larger-scale atmospheric boundary layer eddies rather than the localized mechanical shear generated by individual buildings. Consequently, intense vertical turbulent mixing effectively

homogenizes the localized concentration perturbations induced by specific ground-level source configurations. This confirms that as elevation increases, horizontal pollutant distributions converge, and spatial rearrangements of low-level emission sources exert virtually no influence on high-altitude concentration fields.

Conversely, in the low-altitude regions (exemplified by $z = 15 \text{ m}$ in Fig. 8 (a–c) and Fig. 9(a–c)), dictated by the discrepancies in source locations, the SSIM component values within the neighborhood and its immediate vicinity remain notably low. This indicates substantial deviations in both the absolute concentration magnitudes and the spatial contour topologies, as near-field dispersion within the canopy is heavily governed by localized flow separation and building-induced recirculating wakes. Nevertheless, as the downwind distance extends into the unobstructed far-field, the SSIM values gradually recover. This recovery is fundamentally tied to the turbulent homogenization process and the wake recovery length scale of the entire neighborhood. As the plume exits the complex building cluster and transports over the open downstream fetch, it is no longer subjected to the continuous mechanical shear and complex recirculation zones induced by individual buildings. Instead, the momentum deficit in the neighborhood wake gradually recovers, and dispersion becomes completely dominated by the background atmospheric boundary layer turbulence. This macro-scale mixing effectively smooths out the initial spatial heterogeneity caused by different source locations. This reveals that the aerodynamic interference caused by the spatial heterogeneity of localized emissions on the downstream concentration similarity continuously attenuates with increasing distance.

In summary, altering pollution source locations within the neighborhood significantly affects pollutant concentration distributions only within a limited spatial domain. Once the altitude reaches $z = 100 \text{ m}$ (equivalent to $5H_{max}$) and the horizontal downwind distance exceeds $y = 900 \text{ m}$ (i.e., 400 m , or $20H_{max}$, from the neighborhood boundary), the concentration distributions across different emission scenarios become remarkably consistent. Crucially, these empirically derived spatial thresholds exhibit remarkable physical consistency with established urban CFD guidelines. These guidelines stipulate that the computational domain's top boundary must be at least $5H_{max}$ above the buildings, and the outflow boundary must extend at least $15H_{max}$ downstream to allow for "full wake flow development" [29]. Our identified convergence boundaries ($5H_{max}$ vertically and $20H_{max}$ horizontally) physically denote the critical limits where the neighborhood-scale aerodynamic wakes fully dissipate and background atmospheric turbulence completely regains dominance. This finding yields key

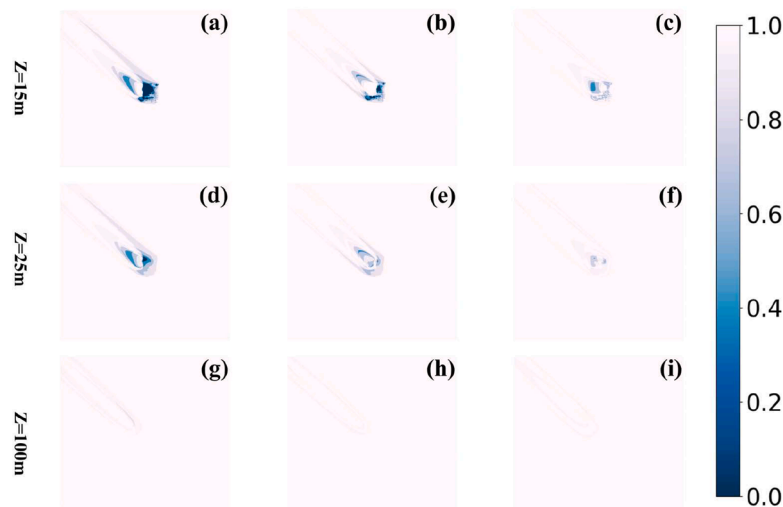


Fig. 8. Spatial distribution contour plots of the SSIM luminance component at various heights for (a, d, g) Case 2, (b, e, h) Case 3, and (c, f, i) Case 4, with the baseline scenario serving as the reference.

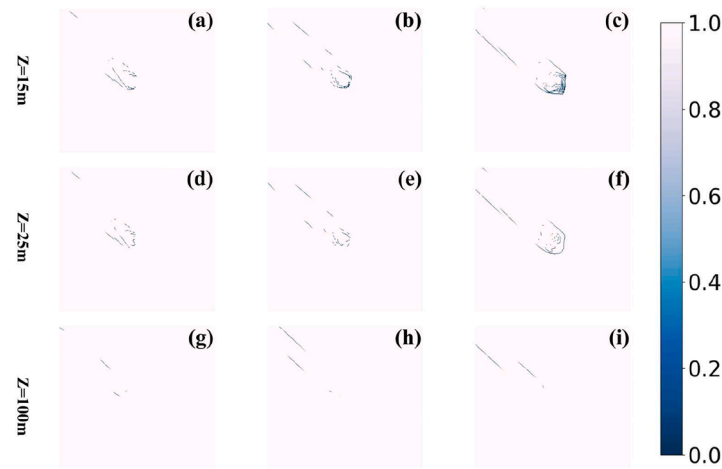


Fig. 9. Spatial distribution contour plots of the SSIM structural component at various heights for (a, d, g) Case 2, (b, e, h) Case 3, and (c, f, i) Case 4, with the baseline scenario serving as the reference.

methodological insights for future CFD modeling: when evaluating the macro-scale environmental impacts of localized emissions on the far-field atmosphere, target-area building layouts and source locations can be reasonably simplified. Conversely, if the objective is to investigate the micro-environmental details of pollutant dispersion within the urban canopy, high-fidelity modeling and meticulous configuration of both the building morphology and the emission source locations are absolutely mandatory.

3.3. Feasibility of simplifying downstream building layouts

This section investigates the impact of sparse buildings downwind of emission sources on pollutant dispersion. As discussed in Section 3.2, the concentration distributions of Case 3 closely resemble those of Case 2. This resemblance is hypothesized to stem from the scarcity of downstream obstacles in Case 3, which fail to induce substantial aerodynamic blocking. To rigorously validate this hypothesis, Case 5 was developed from the baseline scenario (Case 1) by introducing sparse buildings along the western and northern downwind peripheries of the neighborhood. This configuration specifically examines whether sparse downstream obstacles are indeed insufficient to impede far-field pollutant transport.

3.3.1. Influence of downwind sparse buildings on the shape of the dispersion plume

Comparing Fig. 10(a-c) with Fig. 6(a, e, i) reveals that, whether near the maximum building height ($z = 15$ and 25 m) or well above the urban canopy ($z = 100$ m), the pollutant concentration distributions of Cases 5 and 1 closely resemble each other both within the neighborhood and at various downwind distances. The newly incorporated sparse buildings on the northwestern periphery exert no significant aerodynamic perturbations on pollutant transport and dispersion; consequently, visual discrepancies between the two scenarios are virtually indistinguishable. Similarly, Fig. 10(d-f) illustrates the concentration distributions of Case 5 across the x-z planes at three downstream cross-sections ($y = 500$, 700 , and 900 m). Comparing these with the corresponding Case 1 results (Fig. 7) demonstrates that vertical pollutant distributions remain highly consistent across both near-field and far-field regions. These findings indicate that introducing sparse downwind buildings fails to significantly alter macroscopic pollutant transport pathways within the neighborhood and its subsequent downstream regions.

3.3.2. Local perturbation assessment based on SSIM

Given the inherent limitations of qualitative visual comparisons, this study further employs SSIM analysis to capture subtle dispersion field discrepancies between the two scenarios. The spatial distribution of the

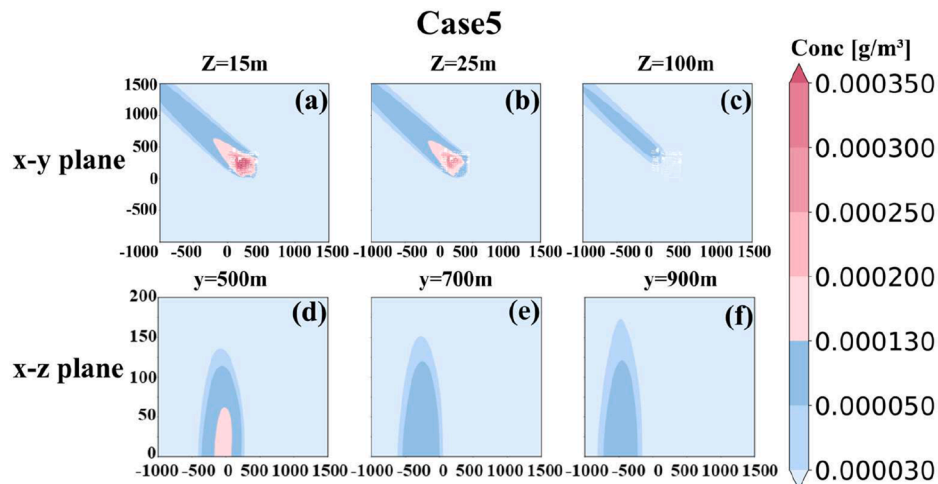


Fig. 10. Spatial distribution of pollutant concentrations for Case 5 under the prevailing southeasterly wind condition: (a-c) horizontal contour plots at various heights, and (d-f) downstream evolution across vertical cross-sections (x-z planes).

SSIM luminance component (Fig. 11(a-c)) reveals that its values approach 1 across all evaluated heights, demonstrating that Cases 5 and 1 maintain remarkably high consistency in concentration magnitude. While the downstream structures act as localized momentum sinks that exert aerodynamic drag, they do not impede the global advective mass flux nor alter the conservation of the emitted pollutant mass. This implies that the presence of sparse downwind buildings negligibly impacts overall pollutant field intensity.

Nevertheless, the SSIM structural components at various heights (Fig. 11(d-f)) indicate that at the urban canopy levels ($z = 15$ and 25 m), distinct low-value bands emerge within the neighborhood and its immediate vicinity. These near-ground structural distortions are physically driven by the local pressure field alterations and flow blockages induced by the sparse buildings, which generate distinct wake cavities and cause localized lateral channeling of the plume. Conversely, in the higher airspace ($z = 100$ m), only faint discrepancies in structural contours are observed in the far-field region. This vertical attenuation of structural deviation aligns with boundary layer theory, as the aerodynamic disturbances caused by the sparse obstacles are largely confined within the urban roughness sublayer and rapidly dissipate along the vertical gradient. These structural deviations suggest that although the sparse buildings indeed induce localized aerodynamic perturbations near the neighborhood—resulting in minor deflections of the plume trajectory—they do not fundamentally alter the macroscopic dispersion trends.

In summary, aerodynamic blocking induced by sparse downstream buildings does not significantly alter the spatial threshold of the pollutant's influence zone. The far-field distribution characteristics remain highly consistent with those observed in unobstructed scenarios. From an urban planning perspective, this finding indicates that merely deploying sparse downwind barrier zones yields marginal efficacy in mitigating far-field pollutant concentrations. Furthermore, to optimize computational efficiency in future CFD studies, such sparse peripheral buildings—which negligibly impact pollutant transport and dispersion—can be safely omitted from the computational domain.

3.4. Sensitivity analysis of emission intensity on dispersion patterns

This section investigates the influence of varying emission intensities on downstream plume spatial characteristics under fixed source locations. Specifically, Cases 6–9 share identical emission source locations with Cases 1–4, respectively, yet their prescribed emission intensities are amplified by a factor of ten. To facilitate an intuitive visual comparison, the color scale ranges for the concentration contour plots at various heights (Fig. 12) and the vertical cross-sections (x - z planes) at

different downstream distances (Fig. 13) for Cases 6–9 are scaled up by exactly ten times compared to their counterparts in Cases 1–4 (Figs. 6 and 7).

3.4.1. Linear relationship between concentration and emission intensity

Comparing Fig. 12 with Fig. 6 and Fig. 13 with Fig. 7 reveals a strict linear scaling relationship: although the numerical concentrations in Cases 6–9 are an order of magnitude higher than those in Cases 1–4, their spatial distribution contours remain remarkably consistent. Quantitative analysis based on the SSIM luminance component further corroborates this observation. With Cases 1–4 as references, the SSIM luminance spatial distributions for Cases 6–9 (Fig. 14) exhibit significant heterogeneity. Specifically, luminance values are notably low in near-source regions within the building clusters. Mechanistically, this occurs because the SSIM luminance component is highly sensitive to absolute differences in concentration. Because the emission intensities of Cases 6–9 are tenfold those of the baseline scenarios, absolute concentration discrepancies between the two sets peak in high-concentration near-source regions, thereby decreasing luminance similarity scores. Conversely, in the far-field regions, as the plume dilutes, pollutant concentrations progressively decrease. Absolute concentration discrepancies narrow accordingly, causing SSIM luminance values to gradually recover. This trend statistically confirms the strict linear scaling relationship between the pollutant concentration field and emission source intensity.

3.4.2. Stability of the spatial distribution structure

In sharp contrast to the luminance component, the SSIM structural component exhibits exceptional stability across all investigated heights. With Cases 1–4 as references, the SSIM structural distributions for Cases 6–9 (Fig. 15) demonstrate that at all three altitudes ($z = 15$, 25 , and 100 m), values remain consistently close to 1 throughout the computational domain. This high structural similarity carries significant physical implications. It demonstrates that topological features of the plume—such as transport trajectories and dispersion widths—remain invariant to changes in emission intensity. This confirms that pollutants behave strictly as passive scalars within the urban canopy, exerting no buoyancy-driven or momentum-altering feedback on the background airflow. Because trace gas concentrations are insufficient to induce density stratification or modify fluid kinematics, momentum equations governing the flow remain fundamentally decoupled from pollutant concentration. The turbulent flow field governing the dispersion process is dictated solely by meteorological boundary conditions and building geometry. Consequently, since the species transport equation is mathematically linear with respect to the scalar concentration, variations in

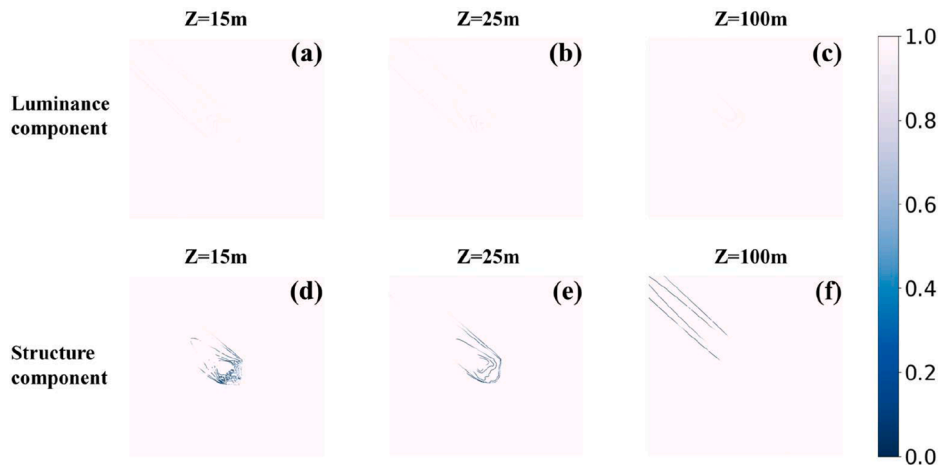


Fig. 11. Spatial distribution contour plots of the SSIM (a-c) luminance and (d-f) structural components at various heights for Case 5, with the baseline scenario serving as the reference.

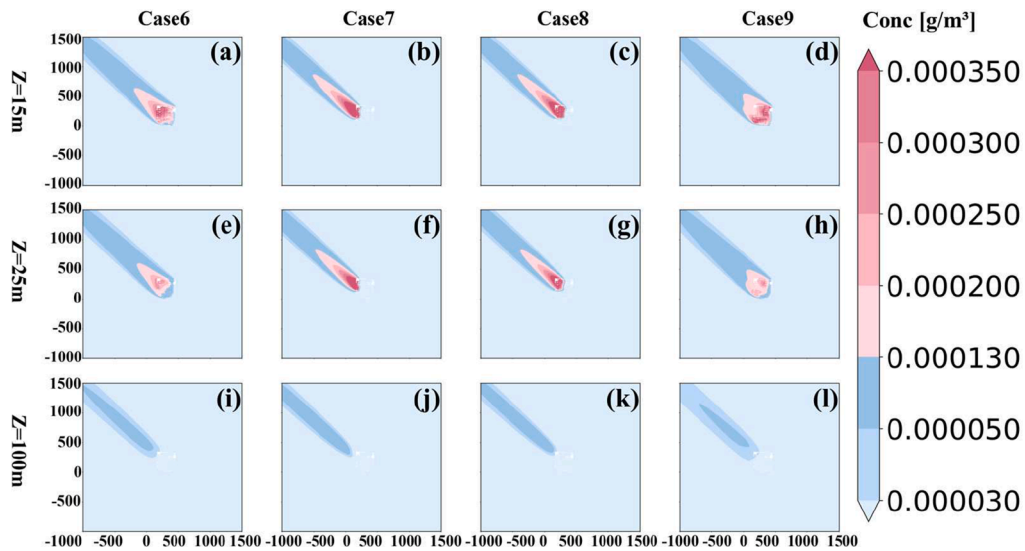


Fig. 12. Horizontal contour plots illustrating the spatial distributions of pollutant concentrations at various heights for Cases 6–9 under the prevailing southeasterly wind condition.

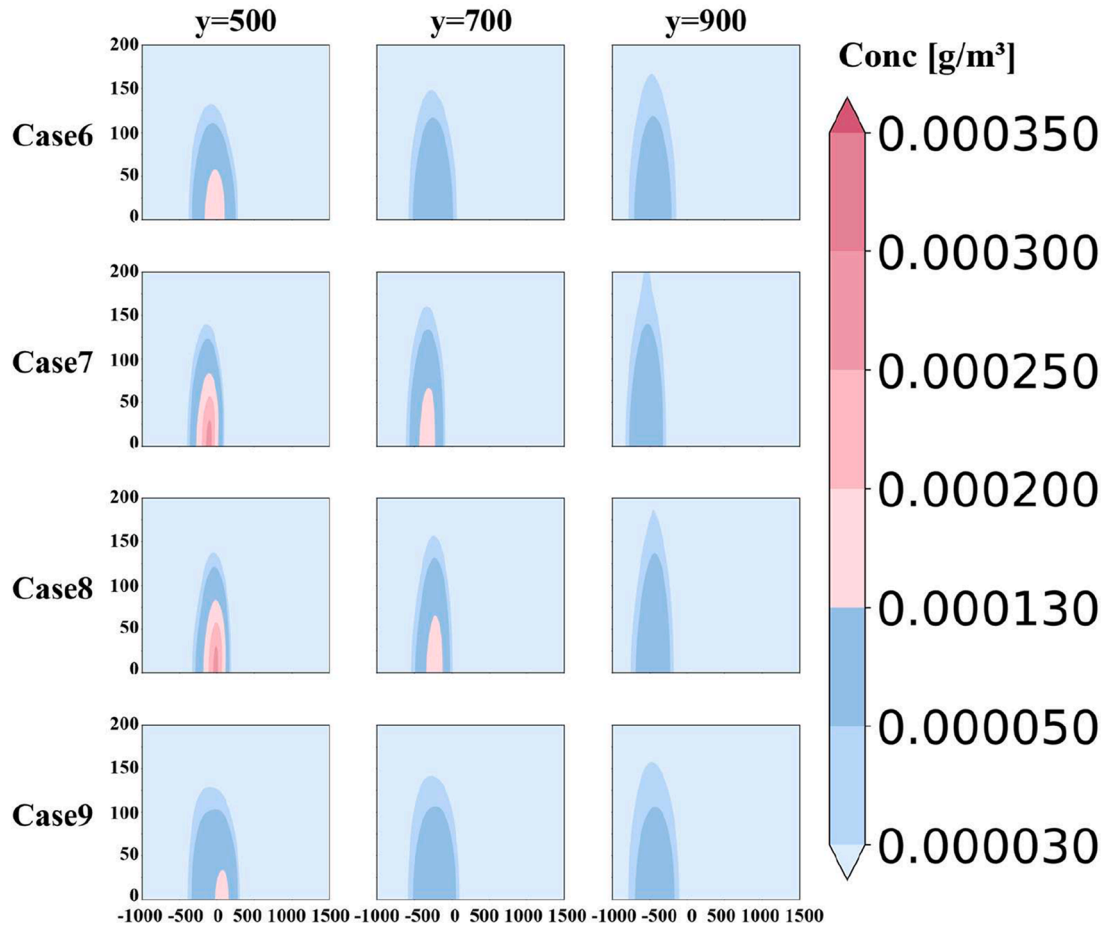


Fig. 13. Spatial distribution and downstream evolution of pollutant concentrations across vertical cross-sections (x - z planes) under various emission scenarios (Cases 6–9).

emission intensity only act as a uniform scaling multiplier. This numerically amplifies the absolute concentration field without altering the underlying advection and diffusion mechanisms.

In summary, this study demonstrates that under fixed source

locations, emission intensity variations primarily modulate the absolute magnitude of pollutant concentrations rather than their spatial distribution patterns. This indicates that source location predominantly determines dispersion field morphology, while source strength acts

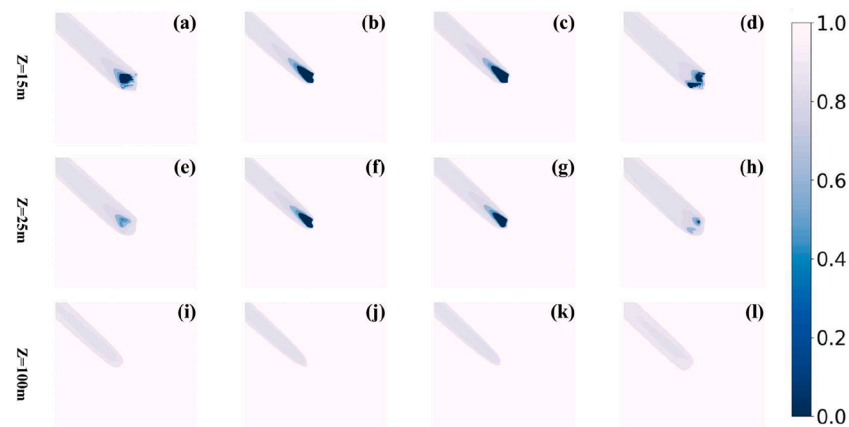


Fig. 14. Spatial distribution of the SSIM luminance component at various heights, comparing high-intensity scenarios (Cases 6–9) with their corresponding baseline references (Cases 1–4): (a, e, i) Case 6 vs. Case 1; (b, f, j) Case 7 vs. Case 2; (c, g, k) Case 8 vs. Case 3; and (d, h, l) Case 9 vs. Case 4.

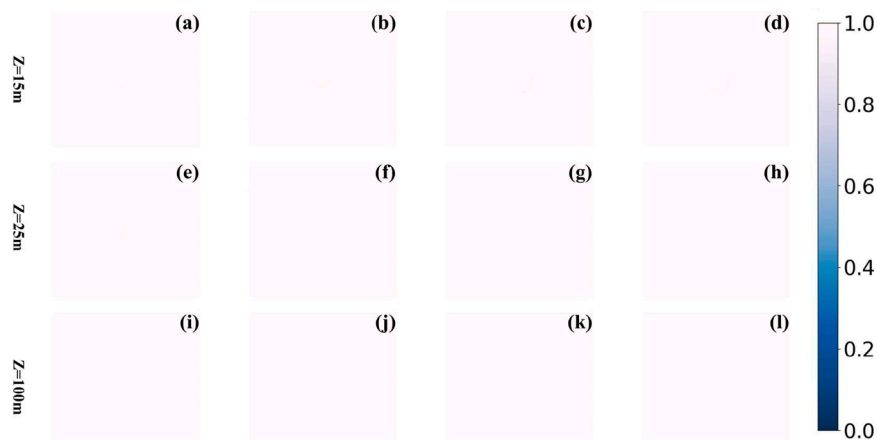


Fig. 15. Spatial distribution of the SSIM structural component at various heights, comparing high-intensity scenarios (Cases 6–9) with their corresponding baseline references (Cases 1–4): (a, e, i) Case 6 vs. Case 1; (b, f, j) Case 7 vs. Case 2; (c, g, k) Case 8 vs. Case 3; and (d, h, l) Case 9 vs. Case 4.

essentially as a proportional scaling factor. Consequently, future studies can reasonably simplify emission intensity configurations when analyzing relative dispersion trends rather than absolute concentrations.

Synthesizing the analyses in Sections 3.2–3.4, this study establishes a sensitivity hierarchy for key boundary conditions in street-canyon-scale CFD simulations. These findings offer strategic guidance for future urban environmental modeling to balance computational efficiency with predictive fidelity. Emission source location emerges as the primary sensitivity driver (Tier 1), decisively influencing micro-environmental dispersion characteristics—particularly in the source near-field; thus, high-precision configuration is mandatory. Peripheral building layout constitutes a secondary factor (Tier 2), warranting a distance-based simplification strategy: prioritizing high-fidelity modeling of near-field obstacles for localized dispersion, while reasonably simplifying downstream structures for far-field analyses. Emission intensity ranks lowest in sensitivity (Tier 3), acting merely as a linear scaling factor, and can be flexibly normalized based on specific analytical goals. In conclusion, future CFD simulations of urban pollutant dispersion should prioritize the accuracy of source positioning, followed by the detailed representation of near-field building geometry, while treating emission intensity as a scalable variable.

4. Conclusion

This study employed computational fluid dynamics (CFD) to investigate the sensitivity of pollutant dispersion simulations to emission

source locations, downstream sparse buildings, and emission intensities within a characteristic high-density residential neighborhood under neutral atmospheric conditions. By introducing the Structural Similarity Index Measure (SSIM) as a quantitative metric, spatial deviations in plume morphology and concentration magnitudes were rigorously evaluated. The primary findings for this specific urban texture are summarized as follows:

- (1) Fine-tuning of the emission source location significantly influences pollutant distribution within the building canopy and near-field regions. However, this sensitivity attenuates rapidly with increasing distance and altitude. For the simulated conditions, when the vertical height reaches $z = 100$ m ($5H_{max}$) or the downwind distance exceeds $y = 900$ m ($20H_{max}$ from the neighborhood boundary), the spatial structures of the plumes originating from different source locations tend to converge. These values serve as indicative spatial thresholds for modeling convergence in similar high-density urban morphologies.
- (2) The influence of sparse building structures located downwind of the source on macroscopic dispersion characteristics is negligible within the investigated scenario. Although these structures induce localized aerodynamic perturbations and minor trajectory deflections, they do not fundamentally alter the characteristic influence distance or the far-field distribution trends compared to unobstructed scenarios under prevailing wind conditions.

- (3) Variations in emission intensity exert a purely linear scaling effect, altering only the absolute numerical values of concentrations without affecting their spatial distribution patterns. In contrast, the spatial location of the emission source remains the predominant factor determining the plume's structural topology. This finding clarifies that precise calibration of the source location is more critical than mere corrections of emission intensity in dispersion modeling.

Based on the sensitivity hierarchy established above, we propose the following operational guideline for future CFD simulations in similar urban textures. Within the near-field region ($20H_{max}$ horizontally and $5H_{max}$ vertically), explicit geometric resolution and precise source localization are indispensable for accurate near-canopy simulations. Beyond these spatial thresholds, far-field geometries can be reasonably simplified—for instance, replacing downstream sparse buildings with an equivalent aerodynamic roughness length or omitting distant structures entirely. Such simplifications dramatically reduce mesh counts and computational costs without compromising the physical accuracy of macroscopic far-field dispersion trends.

Limitations and future outlook

While this study reveals key response patterns of pollutant distribution at the urban micro-scale, several limitations persist that warrant further investigation in future research:

- (1) This study is based on a characteristic case of a residential neighborhood in Nanjing to establish the preliminary quantitative boundaries of emission source location impacts. However, the identified influence distances (e.g., $5H_{max}$ vertically and $20H_{max}$ horizontally) are inherently coupled with the specific building heights, floor area ratios (FAR), and street aspect ratios (H/W) of the investigated site. Furthermore, it must be emphasized that the reported thresholds serve as reference values specifically derived within the RANS Standard $k-\varepsilon$ (SKE) modeling framework. Since these thresholds represent "case-specific reference scales," future studies should incorporate a broader diversity of urban textures and meteorological conditions—including varying wind directions and atmospheric stabilities—to verify the universality of these patterns and develop generalized pollutant dilution models based on urban morphological parameters. Specifically, exploring how alternative turbulence models (e.g., LES or other RANS variants), diverse building morphologies, and varying aspect ratios might induce shifts in these spatial boundaries will be a primary focus of our subsequent research.
- (2) To maintain a strategic focus on aerodynamic sensitivity, this study assumes steady-state residential emissions with uniform source strength and treats the pollutant strictly as a passive scalar. It is under these specific non-buoyant, steady-state, and identical wind-field assumptions that we concluded variations in emission intensity solely linearly scale the concentration magnitude without altering the spatial structure of the plume. However, it must be explicitly stated that this linear-scaling conclusion should not be directly generalized to complex real-world emission sources. In reality, urban emissions (such as traffic and commercial sources) exhibit pronounced temporal variability, spatial heterogeneity, and often carry strong initial momentum or thermal buoyancy. We deliberately decoupled these factors in this baseline study because different emission forms involve distinct dispersion mechanisms; conflating source dynamics with geometric factors could obscure the fundamental sensitivity hierarchy identified here. Future research will explore how non-steady-state emission patterns, initial momentum fluxes, and source-strength heterogeneity modulate the established spatial thresholds, providing deeper insights into emergency response and complex environmental management.
- (3) To balance computational efficiency, building geometries were idealized, neglecting micro-scale structural features such as roof configurations, window openings, and balconies, which can influence localized recirculation zones and near-wall turbulence production. Furthermore, the potential synergistic effects of urban vegetation—acting both as a momentum sink through aerodynamic resistance and as a pollutant sink through dry deposition—were not considered. Future research will utilize higher-fidelity models to explore the complex modulation of detailed architectural features and green infrastructure on pollutant dispersion pathways within the urban roughness sublayer.
- (4) This baseline study focuses exclusively on aerodynamic factors under neutral atmospheric conditions, thereby neglecting thermal effects and buoyancy-driven flows. In real urban microclimates, solar radiation and anthropogenic heat emissions induce strong local thermal gradients. These thermal disparities generate buoyancy forces that can significantly alter vertical turbulent mixing, modify the topological structure of localized recirculation zones, and trigger thermal stratification. Consequently, the thermally-induced flow dynamics could potentially shift the spatial convergence thresholds ($20H_{max}$ and $5H_{max}$) identified under strictly isothermal conditions. Future research should integrate non-isothermal solvers to systematically investigate the coupled effects of urban thermodynamics and aerodynamics on the spatial sensitivity of pollutant dispersion.
- (5) The "spatial attenuation of source location sensitivity" identified in this study provides a theoretical foundation for a zonal strategy in neighborhood-scale inverse modeling. Specifically, dense monitoring networks can be deployed in the near-field for precise source location inversion, while far-field measurements should focus on constraining emission strengths. Future research should explore integrating high-density near-field sensor data with sparse far-field observations. Developing such a multi-scale data assimilation framework will effectively mitigate the inherent ill-posedness of micro-scale inverse modeling.
- (6) It is also worth noting that the SKE model, despite its well-documented limitations in predicting flow separation over idealized smooth surfaces, has been validated against our field SF₆ tracer experiment (Section 3.1) and has demonstrated acceptable predictive accuracy for scalar concentrations at the neighborhood scale. Furthermore, several recent studies have shown that the SKE model can perform favorably—or even outperform—other RANS models (e.g., RNG $k-\varepsilon$ and SST $k-\omega$) in predicting scalar concentration fields within compact urban geometries, particularly when source location sensitivity is of interest [42]. One key reason is that the overprediction of turbulent kinetic energy by the SKE model in building clusters partly compensates for the systematic underestimation inherent to RANS methods [42]. Additionally, real urban building surfaces are characterized by multi-scale roughness elements (roof tiles, exposed aggregate walls, balconies, air conditioning units, etc.), which induce early turbulent transition and elevate leeward turbulent intensity. Under such high-roughness conditions, the discrepancies between different RANS models that are well documented for smooth surfaces become less pronounced, and the influence of surface roughness on wind flow is comparable to that of turbulence model choice [12,43]. Therefore, the inherent biases of the SKE model in recirculation zone prediction have limited impact on our far-field concentration similarity conclusions. Nonetheless, we acknowledge that LES or other RANS variants (e.g., SST $k-\omega$) might yield slightly different numerical thresholds, and exploring these alternatives remains a high priority for our future work.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used Google Gemini only to improve the readability and language of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

CRediT authorship contribution statement

Chao Zhang: Data curation, Formal analysis, Investigation, Methodology, Visualization, Writing – original draft. **Junrui Mi:** Data curation, Formal analysis, Validation, Writing – review & editing. **Zhenxin Liu:** Conceptualization, Formal analysis, Funding acquisition, Supervision, Writing – review & editing. **Pinliang Jiang:** Data curation, Validation, Visualization, Writing – review & editing. **Hong Liao:** Funding acquisition, Supervision. **Ning Zhang:** Funding acquisition, Resources.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in the following paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.buildenv.2026.114936](https://doi.org/10.1016/j.buildenv.2026.114936).

Data availability

Data will be made available on request.

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