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Analyzing Dispersion Characteristics of Fine Particulate Matter in High-Density Urban Areas: A Study Using CFD Simulation and Machine Learning

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Abstract: This study examines how urban morphology, road configurations, and meteorological factors shape fine particulate matter (PM_{2.5}) dispersion in high-density urban environments, addressing a gap in block-level air quality analysis. While previous research has focused on individual street canyons, this study highlights the broader influence of building arrangement and height. Integrating computational fluid dynamics (CFD) simulations with interpretable machine learning (ML) models quantifies PM_{2.5} concentrations across various urban configurations. CFD simulations were conducted on different road layouts, block height configurations, and aspect ratio (AR) levels. The resulting dataset trained five ML models with Extreme Gradient Boosting (XGBoost), achieving the highest accuracy (91–95%). Findings show that road-specific mitigation strategies must be tailored. In loop-road networks, centrally elevated buildings enhance ventilation, while in grid-road networks, taller perimeter buildings shield inner blocks from arterial emissions. Additionally, this study identifies a threshold effect of AR, where values exceeding 2.5 improve PM_{2.5} dispersion under high wind velocity. This underscores the need for wind-sensitive designs, including optimized wind corridors and building alignments, particularly in high-density areas. The integration of ML with CFD enhances predictive accuracy, supporting data-driven urban planning strategies to optimize road layouts, zoning regulations, and aerodynamic interventions for improved air quality.

Keywords: fine particulate matter; pollutant dispersion; urban morphology; road layout; block height configuration; aspect ratio



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1. Introduction

Fine particulate matter (PM_{2.5}), a major air pollutant, poses severe health risks in urban centers, contributing to respiratory and cardiovascular diseases and premature mortality [1–3]. The urban environment, characterized by dense populations and diverse anthropogenic activities, amplifies PM_{2.5} exposure, necessitating effective urban design strategies to minimize its impact. Urban design interventions that account for pollutant dispersion mechanisms offer a promising pathway toward sustainable urban development.

PM_{2.5} concentration in cities is influenced by an intricate interplay of factors. Traffic emissions, industrial activities, and human behavior contribute substantially to pollutant levels, while meteorological conditions such as wind velocity, atmospheric pressure, and temperature dictate dispersion patterns [4–7]. Among these, urban morphology—including the layout of buildings, road networks, and open spaces—plays a pivotal role in shaping microclimate conditions and pollutant dispersion [8–10]. Road patterns, building heights,

and spatial configurations can create stagnation zones or facilitate pollutant dispersion, emphasizing the critical need to study these factors in depth [11,12].

Various methods have been developed to quantify and model particle concentrations, each with its strengths and limitations. These methods broadly include Computational Fluid Dynamics (CFD) simulations, field measurements, and statistical approaches. CFD is used to model concentration fluctuations from atmospheric releases and employs methods like ENVI-met [13], OpenFOAM [14], and ANSYS Fluent [15,16]. CFD provides a detailed analysis of pollutant transport and dispersion, accounting for complex urban geometries and environmental factors [17]. It serves as a cost-effective virtual tool for policy-making and urban planning by simulating hypothetical scenarios, offering advantages over large-scale wind tunnel experiments. Globally, CFD studies have informed policies to improve urban environments, including traffic systems, and have provided a scientific foundation for urban design guidelines [18–20].

Field measurements are crucial for environmental monitoring, providing real-time, location-specific data to validate CFD simulations and predictive models [12,21,22]. They help identify pollution hotspots, track temporal variations, and assess policy impacts [23], but their spatial and temporal limitations necessitate complementary analytical approaches. To address these gaps, statistical methods analyze spatial and temporal particulate matter (PM) trends, using techniques like land-use regression and partial correlation analysis to identify key environmental and socio-economic factors [24–27]. Machine learning (ML) models, such as Random Forest (RF) and Extreme Gradient Boosting (XGBoost), further enhance predictions by integrating diverse datasets and capturing nonlinear relationships [28–30].

Recent advances in CFD simulation and ML models offer a powerful, integrated approach to assess and predict $PM_{2.5}$ distribution in urban areas [31]. CFD models provide a granular understanding of pollutant dispersion within the flow field, accounting for localized effects of urban morphology and meteorological conditions [32,33]. ML models, on the other hand, efficiently analyze large datasets to identify complex, multifactorial relationships between urban form and pollutant concentration [34,35]. Together, these methodologies address the limitations of traditional approaches, including the computational intensity of numerical simulations, high costs, and static, site-specific constraints of field measurements [36,37]. However, conventional ML models function as black boxes, limiting their interpretability for urban design and policy. Interpretable ML overcomes this challenge by ensuring accurate predictions while uncovering complex, previously unidentified relationships within datasets [38].

Building on these advancements, this study integrates CFD simulation and interpretable ML techniques to quantify the impact of urban morphology on $PM_{2.5}$ concentrations. It examines key factor interactions in high-density urban areas, analyzing $PM_{2.5}$ dispersion across road patterns and building configurations under varying meteorological conditions. Beyond academic contributions, these findings offer practical insights for policymakers and urban planners, supporting sustainable development through healthier and more resilient urban environments.

2. Materials and Methods

Figure 1 illustrates the integration of CFD simulations and ML approaches used in this study. Various urban geometry scenarios are created and simulated using ANSYS Fluent, producing particle concentration data for different urban morphology configurations, including road layout, block height, and aspect ratio (AR). These simulation outputs form a dataset that captures the relationships between input factors and particle concentrations.

This dataset is then utilized to train ML models, enabling the quantification of the influence of urban morphology and meteorological factors on PM_{2.5} dispersion.

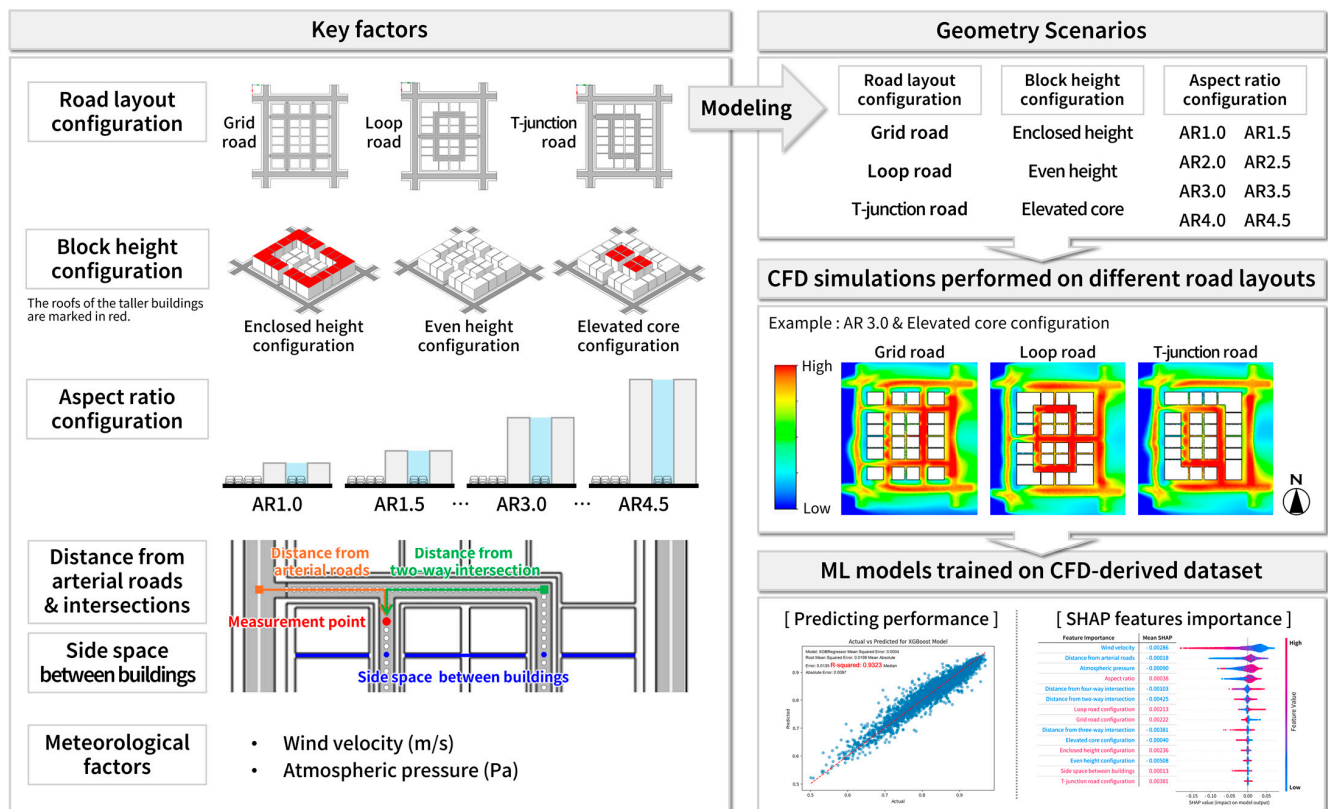


Figure 1. Research framework for integrating computational fluid domain (CFD) simulation and machine learning (ML).

2.1. CFD Simulation

2.1.1. Mathematical Models

This study used ANSYS Fluent 2023 R2 as the primary computational tool for modeling fluid dynamics and pollutant dispersion in urban environments. ANSYS Fluent, a widely used CFD software provided by ANSYS, Inc. (Canonsburg, PA, USA), is employed in this study to simulate the concentration and dispersion of air pollutants in urban environments. Its robust capabilities allow for intricate modeling of fluid dynamics, thermal transfer, and species dispersion, rendering it appropriate for the analysis of complicated urban microclimates [39]. Moreover, ANSYS Fluent supports customizable boundary conditions and mesh generation, allowing for an accurate depiction of various urban morphology [40]. Our model simulates air turbulence within a fully three-dimensional system, accounting for variations in altitude and the dynamics of vertical vortex formations [41]. The simulation framework is constructed using the Reynolds-averaged Navier–Stokes equations, with the Shear-Stress Transport $k-\omega$ (SST $k-\omega$) turbulence model [42]. This model, which combines the advantages of $k-\omega$ modeling for near-wall flows and $k-\epsilon$ modeling for free-stream zones, has been validated in previous studies and is particularly suited for complex flow conditions in urban areas [43–45]. The turbulent viscosity values were analyzed to assess the impact of ANSYS Fluent’s default viscosity ratio limit of 10^5 . The maximum recorded value of approximately 1, well below the limit, aligns with the SST $k-\omega$ model’s near-wall sensitivity.

The passive scalar transport equation simulates the dispersion and concentration of particulates in the air. Equation (1) models the transport of a scalar field representing particulate concentration as follows:

$$\frac{\partial}{\partial x_i} \left(\rho u_i \phi - \Gamma \frac{\partial \phi}{\partial x_i} \right) = S_\phi \quad (1)$$

where Γ is the diffusion coefficient for the scalar, and S_ϕ is the source term representing emissions of the scalar when only one scalar was set [46]. This equation effectively models the interplay of advection, diffusion, and source dynamics, providing comprehensive insights into pollutants' behavior under different environmental conditions. This analysis assumes a steady-state flow, neglecting particle interactions, heat effects, and unsteady dynamics, with the particles' negligible impact on the air attributed to their sufficiently small volume fraction [47]. The simulation achieved convergence after 500 iterations, with residuals below 10^{-6} for major flow variables, demonstrating numerical stability and ensuring the accuracy of the solution. Furthermore, the turbulent Schmidt number was set to 0.7 to represent the relationship between turbulent viscosity and scalar diffusivity in pollutant dispersion modeling [48,49].

2.1.2. Computational Domains and Meshing

As shown in Figure 2, the geometric model dimensions are estimated to be approximately 284 m in length and 264 m in width. The computational domain was constructed in accordance with the AIJ guidelines [50]. The inlet boundary was positioned 5H away from the geometry, where H is the average height of the entire geometry, whereas the outlet boundary was set 15H away. In accordance with the influence of the prevailing westerlies in South Korea, the velocity-inlet is set to the west wind and the average wind velocity of 2 m/s, considering background airflow at the investigated site. The boundary condition for the outlet was pressure-out, and the boundary conditions of the ground and building surfaces were no-slip walls and isothermal heating conditions. All other boundaries were also placed at a distance of 5H from the geometry. A symmetry boundary condition was applied to the computational domain. This model comprises only fluid regions without any voids, which is crucial for accurately simulating PM_{2.5} dispersion within the complex geometry of high-density urban environments.

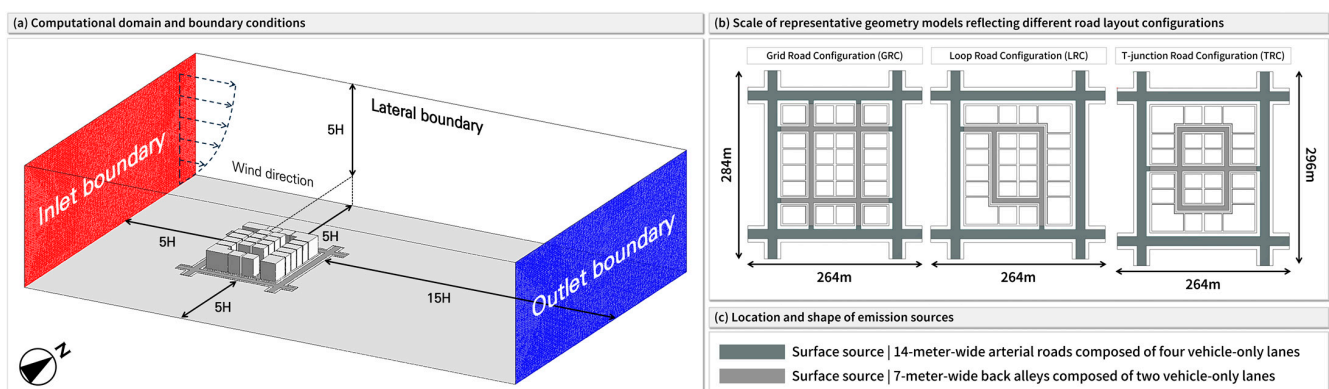


Figure 2. (a) Computational domain and boundary conditions, (b) scale of representative geometry models reflecting different road layout configurations, and (c) location and shape of emission sources.

This study assumes that PM was treated as a non-reactive air pollutant to analyze the direct effects of road emissions on dispersion. The emission source is set with a width of 14 m for arterial roads and 7 m for back alleys at the ground to cover the entire roads for vehicles without pedestrian roads. The background concentrations are set to zero to focus

on the influence of selected features on traffic-emitted PM concentrations as well [51]. The amount of PM_{2.5} emitted from the roads was calculated, as referenced in Guo's study [8], based on traffic flow and the PM emission factor. The total amount of PM_{2.5} emitted by road vehicles, M , is calculated as follows:

$$M = \frac{\sum N_x \cdot E_x}{3600} \cdot \frac{S}{1000} = 2.8e^{-04} \text{ (kg/s)} \quad (2)$$

here, N_x (h^{-1}) represents the number of vehicles traveling on the road per hour; E_x ($\text{g}/(\text{km} \cdot \text{h})$) is the PM_{2.5} emission per hour, per unit length and per vehicle, and S (km) is the total length of the road. The emitted pollutants are assumed to be fully mixed near the road surface across the entire road length due to vehicle movement, based on the homogeneous emission method [52]. Hourly traffic volumes, heavy-duty vehicle rates, and idling times are based on traffic observation during field measurements in our previous study [53].

The mesh within this computational domain is categorized into two regions: surface and volume. The surface mesh size ranges from a minimum of 0.5 m to a maximum of 5 m. The volume mesh was filled with polyhedral cells, and the maximum cell length was automatically determined by the software, ranging from 6.09 m to 6.54 m. To enhance computational accuracy within the wall boundary layers, 10 layers are applied in succession, and the height of the first layer is set to 0.05 m. This mesh configuration optimizes the balance between simulation accuracy and computational efficiency, thereby improving the temporal efficiency of the simulations.

To further validate the effectiveness of this mesh, a grid independence test was conducted under steady-state conditions using the Grid road-AR1.0-even height configuration geometry scenario. PM_{2.5} concentration values were compared at the same location across four different mesh resolutions: coarse, medium, fine, and finest (Figure in Appendix A). The total number of cells in the coarse, medium, and fine meshes corresponded to approximately 45%, 60%, and 95% of the total number of cells in the finest mesh, respectively. The finest mesh was selected for the final simulations to ensure reliable results, as it provided the highest resolution for capturing airflow dynamics and pollutant dispersion patterns with greater accuracy.

2.1.3. Geometry Scenarios

Our model represents a simplified version of a commercial urban block in Pangyo, one of the new towns located south of Seoul. Commercial blocks in these new towns are typically high-density urban areas located near major transportation hubs characterized by high pedestrian activity and heavy vehicular traffic. Designed to maximize land use and economic activity, these districts serve as key business and commercial centers. In new Korean towns, floor area ratios of commercial blocks typically range from 600% to 700%, with an average building height of approximately 50 m. In this study, each geometric scenario consists of 24 buildings, 25-m-wide arterial roads surrounding the block with four lanes, and 12-m-wide back alleys between buildings with two lanes. Based on the wind speed measured during field observations in October, an average wind speed of 2 m/s was used in this study to simulate pollutant dispersion [53].

In this study, 72 geometric scenarios are generated by combining three road patterns, three block height configurations, and eight AR levels (Figure 3a). First, grid, loop, and T-junction roads are identified as the three representative road patterns for CFD simulation, selected due to their common presence in commercial blocks of new towns in Korea. In this study, three simulation models were developed based on distinct road configurations: Grid Road Configuration (GRC), representing an interconnected network linking arterial roads and back alleys; Loop Road Configuration (LRC), featuring a closed-loop with limited

connections to arterial roads; and T-Junction Road Configuration (TRC), defined by three-way intersections connecting to arterial roads. The connectivity between arterial roads and back alleys varies depending on the road configuration, leading to differences in traffic volume. In the Grid Road Layout, where connectivity is high, through traffic tends to be more prevalent. Conversely, in the Loop Road Layout, where connectivity is lower and back alleys are primarily used for parking, traffic volume is relatively lower. This study incorporates these differences by considering the varying amounts of $PM_{2.5}$ emissions generated by each road configuration.

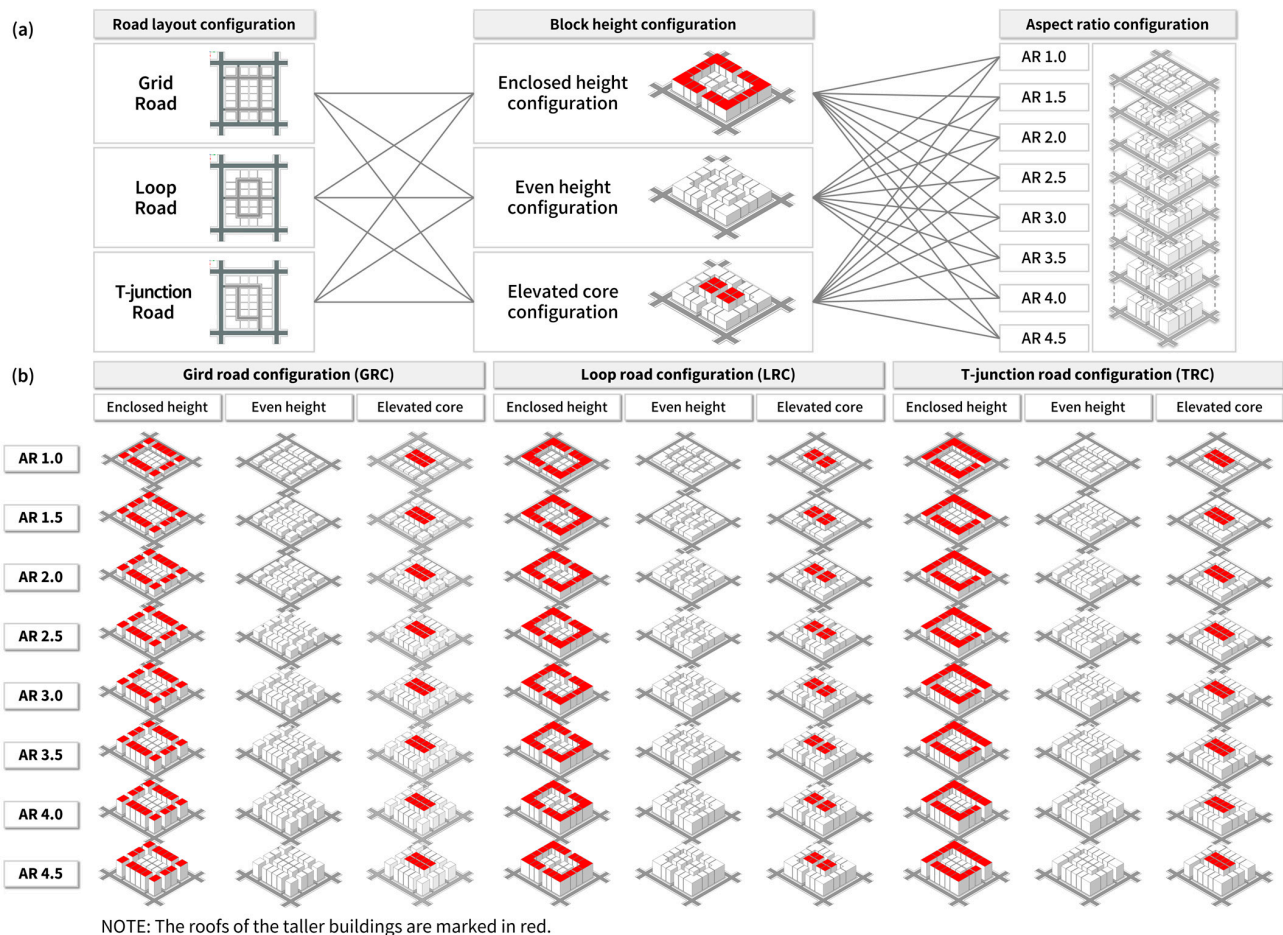


Figure 3. (a) Combination of three road patterns, three block height configurations, and eight AR levels and (b) a total of 72 idealized geometry scenarios.

Second, block height configuration consists of three morphological types: enclosed height configuration, where outer buildings are taller than inner ones; elevated core configuration, where inner buildings are taller than outer ones; and even height configuration, where inner and outer buildings have uniform heights within the block (Figure 3b). The height difference between the inner and outer buildings is 8 m, approximately equivalent to two stories. Third, AR is defined as the ratio of average building height to back alley width. In this study, a 12 m back alley width is used as the standard, while building heights are varied to establish AR values ranging from 1.0 to 4.5 in 0.5 increments, resulting in a total of eight different AR levels applied to the geometry models.

2.2. Integration of CFD and Machine Learning

2.2.1. Evaluation of CFD Simulation

This study simulated the flow field and $PM_{2.5}$ dispersion of the urban block using CFD techniques. The simulation outputs produced a dataset mapping the relationships

between input factors and particle concentrations. To account for urban morphology, road layout and block height configurations were incorporated into the geometry scenarios. The CFD results indicate that among the three configurations, loop roads exhibited the highest average $PM_{2.5}$ concentrations, followed by T-junction roads, while grid roads recorded the lowest levels, demonstrating superior pollutant dispersion capacity (Figure 4a).

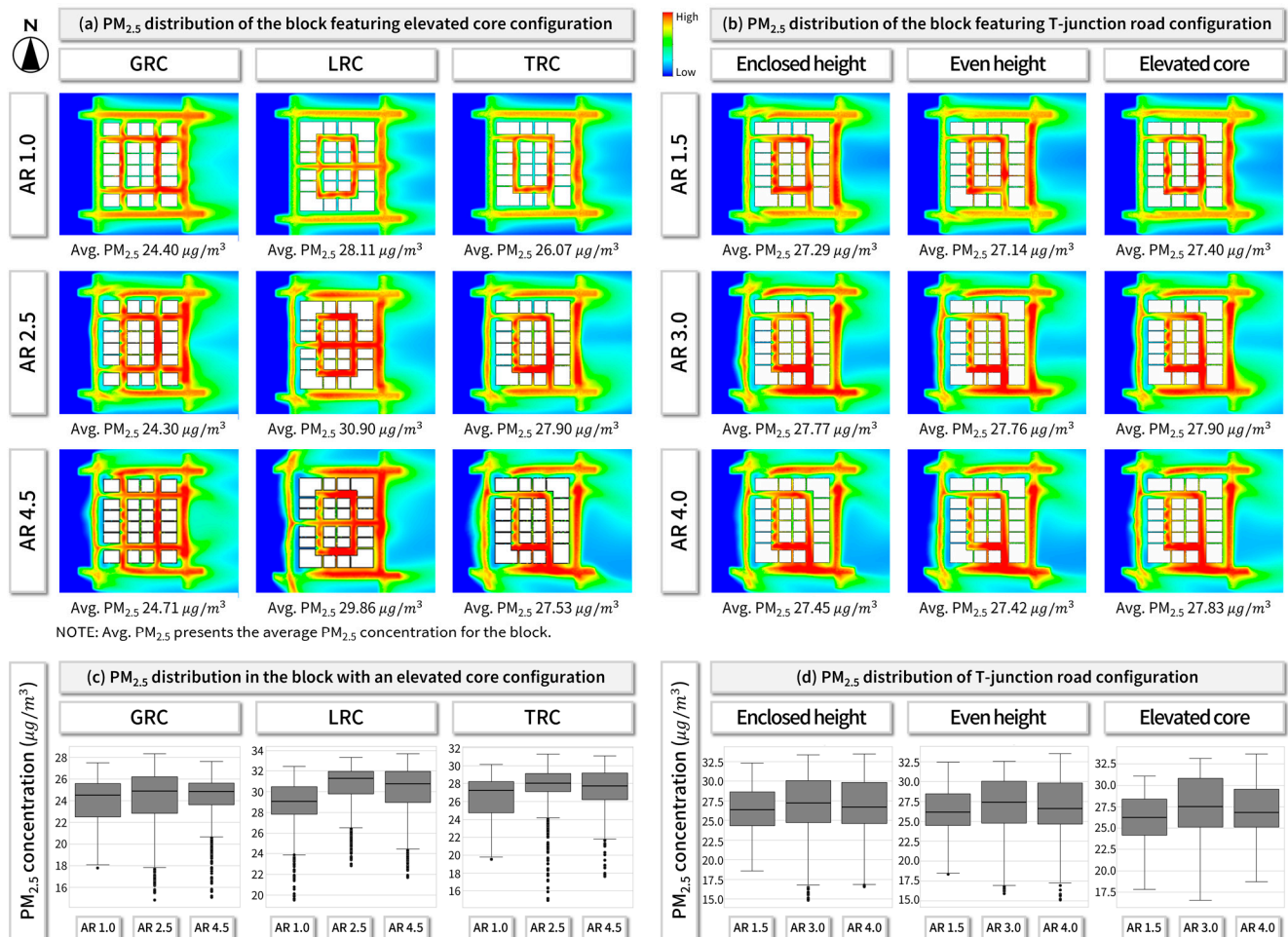


Figure 4. $PM_{2.5}$ distribution for each geometry model presented in the CFD simulation results: (a) $PM_{2.5}$ distribution in the block with an elevated core configuration, (b) $PM_{2.5}$ distribution in the block with TRC, (c) box plot of $PM_{2.5}$ distribution in the block with an elevated core configuration, and (d) box plot of $PM_{2.5}$ distribution of T-junction on road configuration.

The impact of block height configuration on $PM_{2.5}$ dispersion varies depending on road layout and AR. In a T-junction road layout, blocks with elevated core configuration exhibit the highest average $PM_{2.5}$ concentrations. However, the effects of enclosed height and even height configurations are inconsistent across different AR values, reflecting the nonlinear influence of AR on $PM_{2.5}$ concentration (Figure 4b).

In Figure 4c, the box plots depict $PM_{2.5}$ concentration distributions across different AR and road types, with the central line in each box representing the median $PM_{2.5}$ value. The median concentration peaks at AR 2.5 across all road types, while values at AR 1 and 4.5 are lower, indicating a nonlinear relationship between aspect ratio and pollutant levels. $PM_{2.5}$ distribution in GRC exhibits greater variability with a wider spread, whereas LRC and TRC show less variation, particularly at AR 2.5, where pollutant concentrations remain elevated. Similarly, Figure 4d reveals comparable $PM_{2.5}$ distribution patterns across block configurations, with the highest median concentration at AR 3 and the lowest at AR 1.5.

The simulation model provides a simplified representation of a commercial urban block in Pangyo New Town, where $\text{PM}_{2.5}$ concentrations were previously analyzed through field measurements [53]. This high-density area, characterized by numerous tall buildings and surrounded by four-lane and eight-lane roads, experiences continuous accumulation of traffic-related air pollutants, with peak concentrations reaching up to $50 \mu\text{g}/\text{m}^3$.

To validate the CFD simulation results, we used field measurement data collected over six days in October. The dataset, which included $\text{PM}_{2.5}$ concentrations from seven monitoring points, was used to assess the model's accuracy (Figure 5). The monthly average $\text{PM}_{2.5}$ concentration recorded at an Automatic Weather Station 1.6 km from the site ranged from approximately 8 to $32 \mu\text{g}/\text{m}^3$, while CFD simulations estimated concentrations between 14 and $34 \mu\text{g}/\text{m}^3$. The validation process involved calculating correlation coefficients between the field measurements and CFD results, yielding R^2 values between 0.85 and 0.97 . This level of validation aligns with findings from other studies, reinforcing the reliability of the model [54–56].

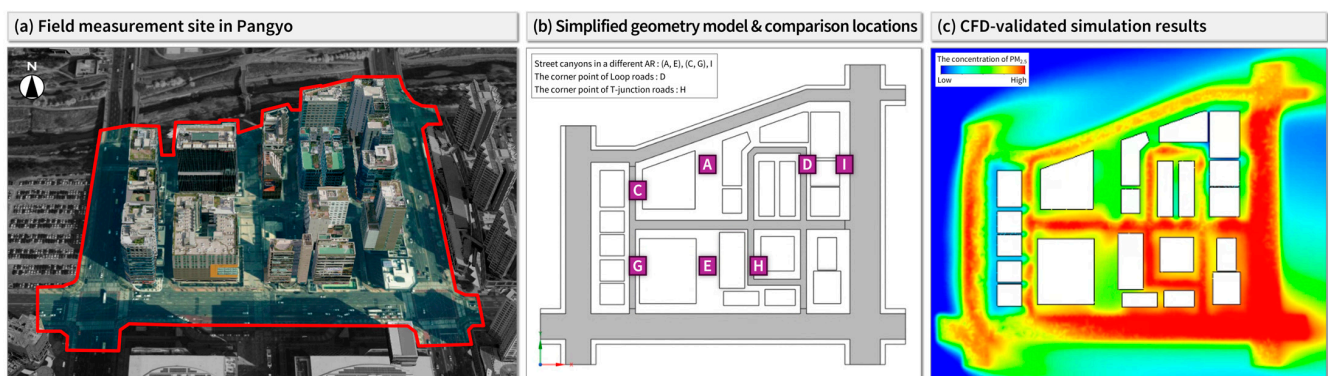


Figure 5. (a) Field measurement site in Pangyo. (b) Simplified geometry model and comparison locations, where (A, E), (C, G), and I are points within street canyons with different ARs, D is the corner point of Loop roads, and H is the corner point of T-junction roads. (c) CFD-validated simulation results for the field measurement site.

2.2.2. Data Processing for Machine Learning Integration

The CFD simulation dataset was used to train ML models, quantifying the impact of urban morphology and traffic-related factors on $\text{PM}_{2.5}$ dispersion. Point data samples were collected at 2 m intervals along back alleys, with a measurement height of 150 cm, representing the typical respiratory level for pedestrians based on the previous literature [57–59]. The number of samples per scenario varies by road configuration, with a total of 20,232 data samples: 348 from GRC, 273 from LRC, and 222 from TRC. Each sample includes meteorological conditions, traffic-related emissions, and urban morphology factors influencing $\text{PM}_{2.5}$ dispersion (Table 1).

To capture the impact of traffic-related emissions, each point data reflect the network distance from the centerline of arterial roads, assuming pedestrians travel along back alley sidewalks. Arterial roads and back alleys were assigned different levels of traffic-related emissions to reflect their varying pollutant contributions. Each road layout features distinct back alley intersections: GRCs have four-way intersections; LRCs include two-way and four-way intersections, and TRCs feature two-way and three-way intersections. Network distance from each intersection type was calculated for every point to account for indirect traffic-related emissions. When multiple intersections influenced a point, all distances were computed, and the closest value was selected for accuracy.

Table 1. Explanatory variables and their value range of the machine learning model.

	Variables	Variables' Value Range
Urban morphology factors	Road layout configuration	GRC, LRC, and TRC
	Aspect ratio configuration	1, 1.5, 2, 2.5, 3, 3.5, 4, and 4.5
	Block height configuration	Enclosed height configuration Even height configuration Elevated core configuration
	Side space between buildings	Existence (1) and absence (0)
Traffic-related factors	Distance from arterial roads	Network distance from a central line of arterial roads or the center of each intersection
	Distance from two-way intersection	
	Distance from three-way intersection	
	Distance from four-way intersection	
Meteorological factors	Wind velocity	Data Extracted from CFD simulation results
	Atmospheric pressure	

Additional consideration was given to the side space between buildings, a key factor in PM dispersion. Article 242 of the Korean Civil Act mandates a minimum 0.5 m setback from the property line to ensure fire safety. In this study, the side space was set at 2 m. Attributes were assigned to point data at the intersection of aligned side spaces in outer and inner blocks with the back alleys, providing a structured basis for analysis.

Previous studies have established a strong correlation between building morphology and wind velocity, highlighting its critical role in shaping airflow patterns [60,61]. To further explore this relationship, this study extracted wind velocity and atmospheric pressure values from CFD simulation results. In CFD modeling, airflow dynamics are primarily dictated by urban morphology, with particle interactions and turbulence effects excluded to simplify the simulation process and improve computational efficiency.

2.2.3. Machine Learning Training and Hyperparameter Optimization

Processed CFD simulation data were used for ML and deep learning (DL) models to predict PM_{2.5} concentrations in the study area. Distinct regression techniques were applied and compared: RF, XGBoost, Support Vector Machine (SVM), Artificial Neural Network (ANN), and Convolutional Neural Network (CNN). These models were selected for their effectiveness in predicting continuous outcomes, with the primary objective of accurately modeling PM_{2.5} concentrations [62–64]. To ensure model reliability and mitigate overfitting, the dataset was randomly split into a training set (80%) and a testing set (20%), enabling the models to be trained on a substantial portion of the data while providing an independent evaluation on unseen data [65].

Hyperparameter tuning was conducted to enhance model performance, utilizing Gaussian Process-based optimization combined with 10-fold cross-validation. This approach models the performance of the algorithms as a probabilistic function, efficiently identifying optimal parameter settings [66]. This process minimizes the predefined loss function, resulting in improved predictive accuracy. Details of the hyperparameters, their search space, and the optimal values are summarized in Table 2.

Table 2. Hyperparameter tuning results using Gaussian process-based optimization.

ML Models	Parameters	IRCM *	GRCM *	LRCM *	TRCM *
RF	Max depth	12	10	12	12
	Max features	11	9	8	11
	Min sample split	10	10	10	10
	Min sample leaf	10	10	10	10
	N estimators	2000	1658	2000	1855
XGBoost	Max depth	12	12	15	12
	N estimators	234	899	988	997
	Learning rate	0.090	0.019	0.389	0.172
	Subsample ratio	0.923	0.203	0.865	0.462
	Subsampling ratio by tree	0.997	0.934	0.975	0.842
SVM	Regularization parameter	4.361	3.396	1.795	1.796
	Epsilon	0.002	0.001	0.001	0.000
	Kernel	rbf	rbf	rbf	rbf
ANN	Hidden layer sizes	500	199	378	477
	Alpha	0.0001	0.0001	0.0001	0.0247
	Activation	tanh	tanh	tanh	logistic
	Learning rate	0.001	0.001	0.001	0.001
CNN	Filters	16	16	128	128
	Kernel size	3	2	3	2
	Dropout rate	0.370	0.100	0.103	0.322
	Learning rate	0.009	0.010	0.003	0.008

* Note: IRCM is the Integrated Road Configuration Model; GRM is the Grid Road Configuration Model; LRCM is the Loop Road Configuration Model, and TRCM is the T-Junction Road Configuration Model.

2.2.4. Machine Learning Integrated with SHAP

Interpreting the results of ML models, particularly complex algorithms like XGBoost, remains a major challenge for researchers and practitioners. To address this, Lundberg and Lee introduced SHapley Additive exPlanations (SHAP), a game theory-based method for optimal credit allocation in ML models [67]. For tree-based ensemble models like XGBoost, TreeSHAP enhances computational efficiency and enables feature interaction analysis [68].

In this study, XGBoost outperformed other ML and DL models in analyzing PM_{2.5} concentrations. TreeSHAP improved interpretability by identifying key features and interactions, with analyses spanning overall trends and specific road typologies (GRC, LRC, and TRC), enabling the identification of the most critical determinants of PM_{2.5} concentrations. Interaction terms further captured synergies between variables, offering a nuanced understanding of how the built environment influences air quality.

The TreeSHAP equation used for this analysis is expressed as follows:

$$\phi_i = \sum_{S \subseteq N-i} \frac{|S|!(M - |S| - 1)!}{M!} [f_x(S \cup i) - f_x(S)] \quad (3)$$

here, ϕ_i represents the marginal contribution of feature i to the model's prediction; f_x is the prediction function of the XGBoost regressor, and M denotes the total number of features in the model. S refers to any subset of features excluding the i th feature, and $|S|$ indicates the size of the subset. By integrating SHAP with XGBoost, this study demonstrates the value of interpretable ML techniques in analyzing urban factors affecting PM_{2.5}, supporting data-driven urban planning and environmental management.

3. Results

3.1. Model Prediction Accuracy Comparison

This study evaluates the dispersion characteristics of PM based on road configurations, including the Grid Road Configuration Model (GRCM), Loop Road Configuration Model (LRCM), and T-junction Road Configuration Model (TRCM). Additionally, an Integrated Road Configuration Model (IRCM) was developed to encompass all road types, including grid, loop, and T-junction configuration.

Both R^2 and RMSE metrics were used to evaluate the predictive performance of the ML models (Table 3). Among these, XGBoost consistently delivered the best results across all geometry models, achieving the highest R^2 values (ranging from 0.91 to 0.95) and the lowest RMSE values (0.02). Figure 6 further illustrates this by presenting scatter plots of predicted versus measured $PM_{2.5}$ concentrations, which clearly demonstrate XGBoost's strong predictive capability for $PM_{2.5}$, followed by RF, while SVM, ANN, and CNN performed less effectively. Cross-validation using 10-fold K-fold validation on the same dataset showed consistent results, further confirming the reliability and robustness of the model's findings (Figure in Appendix B).

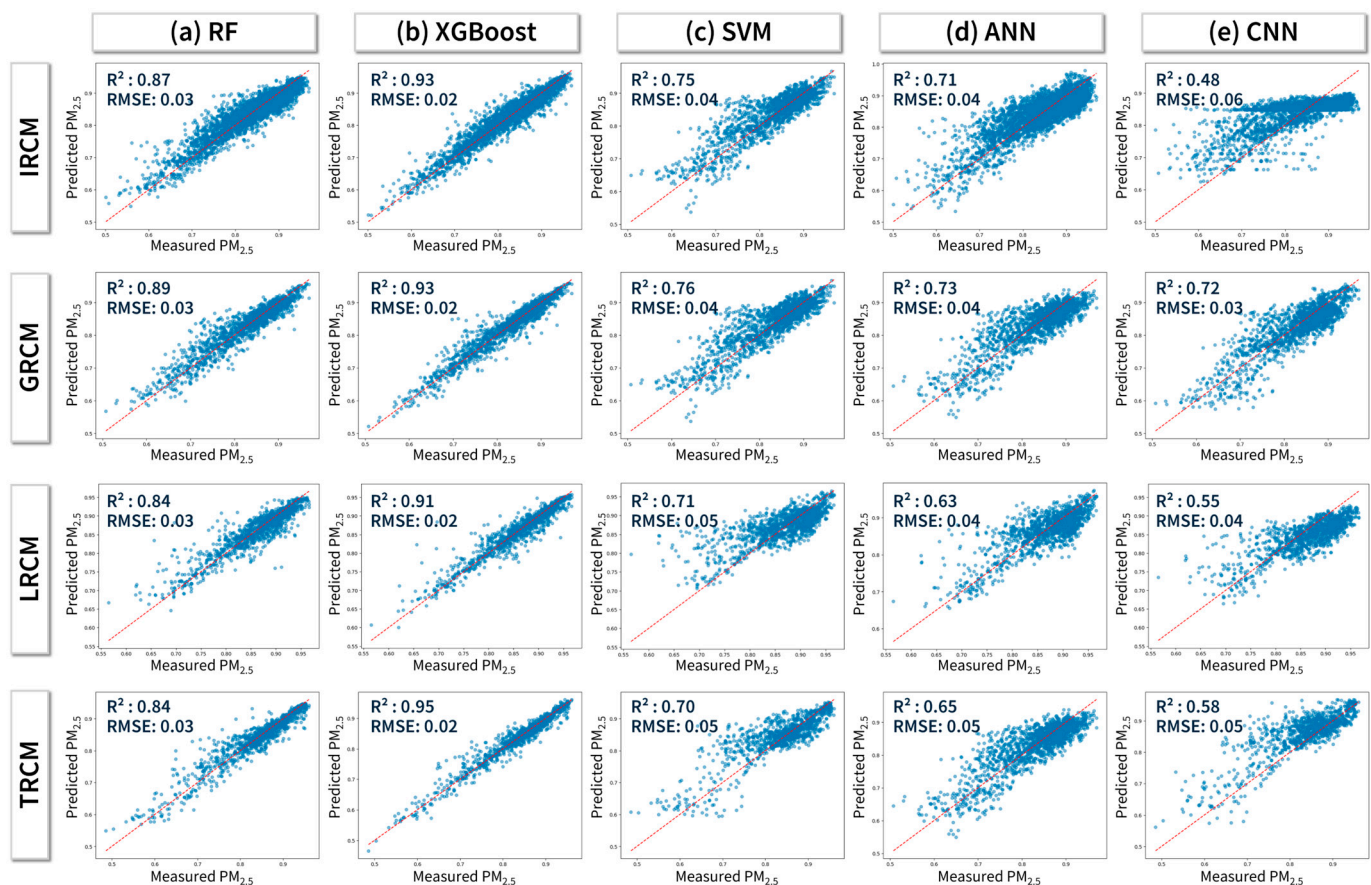


Figure 6. $PM_{2.5}$ prediction model performance results for (a) RF, (b) XGBoost, (c) SVM, (d) ANN, and (e) CNN models.

Table 3. Model performance comparison.

ML Models	IRCM		GRCM		LRCM		TRCM	
	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE
RF	0.87	0.03	0.89	0.03	0.84	0.03	0.84	0.03
XGBoost	0.93	0.02	0.93	0.02	0.91	0.02	0.95	0.02
SVM	0.75	0.04	0.76	0.04	0.71	0.05	0.70	0.05
ANN	0.71	0.04	0.73	0.04	0.63	0.04	0.65	0.05
CNN	0.48	0.06	0.72	0.03	0.55	0.04	0.58	0.05

Notably, within the XGBoost model, the TRCM geometry achieved the highest R² values, emphasizing its suitability for accurately predicting PM_{2.5} concentrations. This was followed by GRCM, IRCM, and LRCM. These differences across geometry models underscore the critical role of urban morphology in determining model accuracy, with TRCM emerging as the most predictable geometry.

3.2. Factors Affecting Particulate Matter Dispersion in High-Density Urban Blocks

Figure 7 presents the results of the XGB model with SHAP interpretation. The findings indicate that the key factors influencing pollutant dispersion in high-density urban areas are wind velocity, distance from arterial roads, atmospheric pressure, and AR, which consistently ranked as the top four determinants.

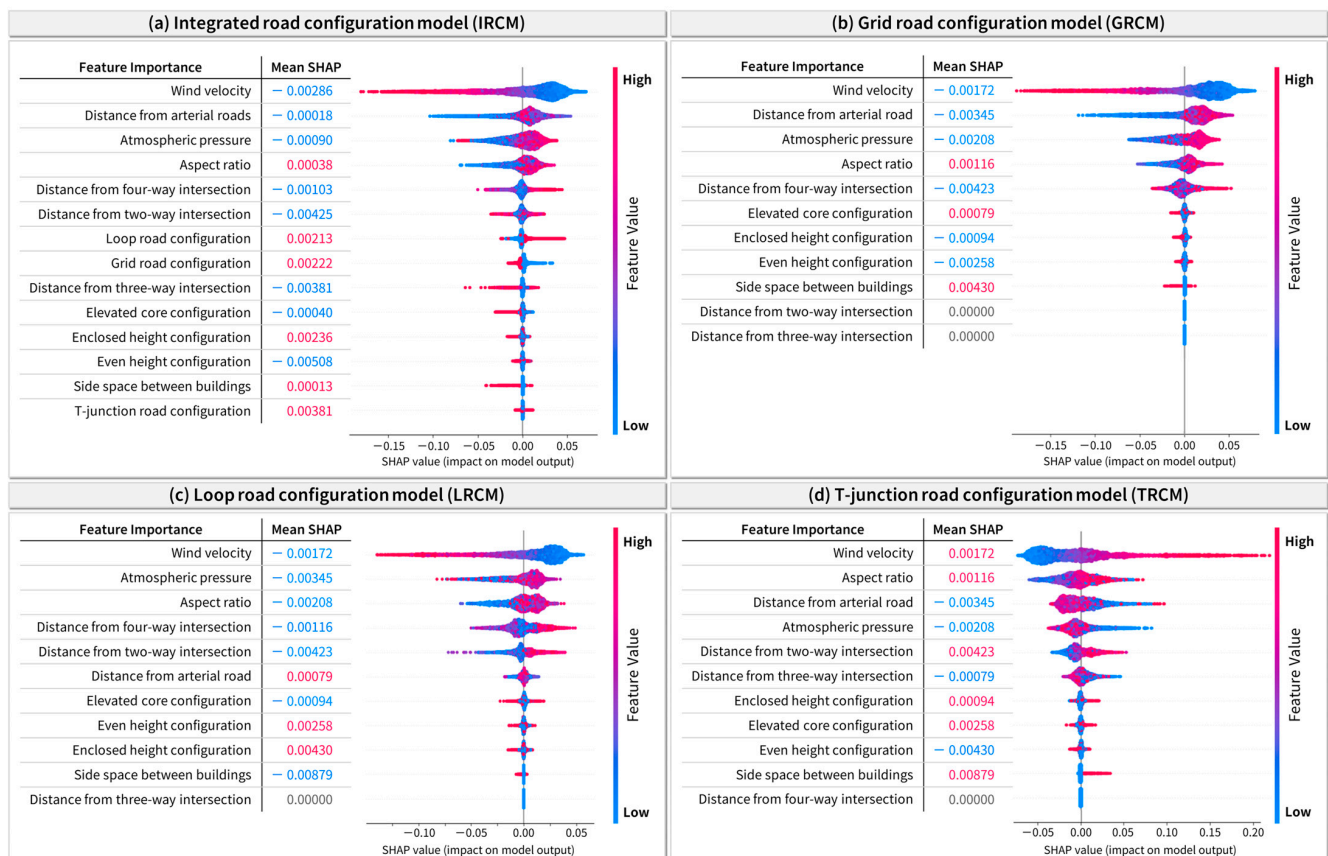


Figure 7. Variable importance and SHAP analysis results for (a) integrated road configuration model (IRCM), (b) grid road configuration Model (GRCM), (c) loop-road configuration model (LRCM), and (d) T-junction road configuration model (TRCM).

In IRCM, which considers all road types, distance from arterial roads was the second most influential factor after wind velocity, followed by atmospheric pressure and AR. The

analysis also highlights the significant impact of road type on pollutant concentration levels. Additionally, variables related to the configuration of block height and side-lot spacing influenced PM_{2.5} levels, though their impact was relatively less significant compared to meteorological conditions and road layout configuration.

Across all road configuration models, meteorological conditions, particularly wind velocity, consistently emerged as the most influential factor. Wind velocity generally exhibited a negative relationship with pollutant concentration, indicating that higher wind speeds contributed to lower PM_{2.5} levels. Similarly, atmospheric pressure was consistently identified as a significant factor across all models, also showing a negative correlation with pollutant concentration, further highlighting the role of meteorological conditions in pollutant dispersion.

Beyond meteorological factors, the impact of traffic emissions on pollutant concentration was analyzed using the network distance from emission sources, such as arterial roads and major intersections, where high levels of pollutants are typically generated. The results from the GRCM and TRCM show that pollutant concentrations decreased as the distance from arterial roads increased. Similarly, concentrations also declined with greater distance from three- or four-way intersections, suggesting that proximity to arterial roads and major intersections may contribute to pollutant accumulation. However, the LRCM showed the opposite trend, where the enclosed structure of loop roads restricted airflow and dispersion, causing higher pollutant concentrations as the distance from arterial roads increased.

The influence of urban morphology on PM dispersion varies across different road configuration models. In the GRCM, pollutant concentrations were higher in blocks with an elevated core configuration, where inner buildings were taller than outer buildings. In contrast, the LRCM exhibited the opposite trend, with higher pollutant concentrations observed in blocks with an enclosed height configuration, where perimeter buildings were taller than inner buildings.

In addition to block height configurations, side spaces between buildings also affect pollution levels, though their impact varies by model. In the LRCM, side spaces help reduce pollution levels, indicating improved ventilation in the enclosed loop-road environment. However, in the GRCM and TRCM, where grid and T-junction road layouts provide more open connections to arterial roads, side spaces tend to increase pollution levels within the block.

Furthermore, AR—defined as the ratio of average building height to road width—shows a positive relationship with pollutant concentration, indicating that higher AR values are associated with greater pollutant accumulation. Notably, AR plays a particularly significant role in determining pollutant concentration in the TRCM, where road geometry and airflow patterns may exacerbate pollutant retention more than in other models. These findings highlight the complex interplay of urban morphology factors, emphasizing the need for tailored design strategies that account for building height distribution, side spacing, and AR to optimize airflow dynamics and pollutant dispersion across different road configurations.

3.3. Interaction Effects Between Factors on Particulate Matter Concentration

This study also reveals the interaction between urban morphology and meteorological factors influencing PM concentration. While the findings from the GRCM and TRCM consistently show that lower AR values enhance particulate dispersion, the interaction analysis in the LRCM reveals a critical threshold effect. Specifically, when AR exceeds 2.5, high wind velocity counteracts PM_{2.5} accumulation, leading to lower concentrations despite the increased AR (Figure 8a). A similar interaction effect was observed in the TRCM. Specifically, in a T-junction road network with a uniform building height configuration,

high wind velocity led to increased $\text{PM}_{2.5}$ accumulation, resulting in higher pollutant concentrations (Figure 8b). This suggests that uniform building heights in T-junction road layouts may disrupt airflow patterns, leading to localized pollutant trapping under strong wind conditions.

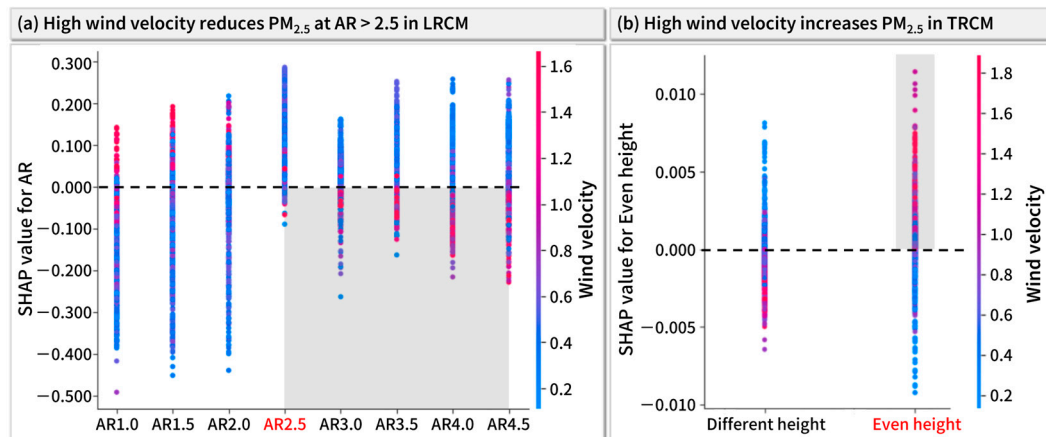


Figure 8. Effect of wind velocity on $\text{PM}_{2.5}$ concentration. (a) High wind velocity reduces $\text{PM}_{2.5}$ at $\text{AR} > 2.5$. (b) In a T-junction network, it increases $\text{PM}_{2.5}$ accumulation.

4. Discussion

The findings of this study provide critical insights into how road configurations, building layouts, and urban geometry influence $\text{PM}_{2.5}$ concentrations, contributing to urban planning and air quality management discussions. While previous studies have extensively examined pollutant dispersion within individual street canyons [69–71], there has been limited focus on $\text{PM}_{2.5}$ distribution at the block level. This study addresses this gap by taking a holistic approach, demonstrating that the balance of building arrangement and height within a block plays a crucial role in shaping air quality. The findings highlight that in densely built environments, airflow dynamics and pollutant removal mechanisms vary largely based on road network type, underscoring the need for block-scale urban design strategies.

A key finding of the CFD simulation is that road configuration considerably determines $\text{PM}_{2.5}$ concentration and dispersion. Among the road types examined, grid-road networks demonstrate the highest efficiency in pollutant dispersion, followed by T-junction roads, while loop-road networks are the least effective in pollutant removal. The open and interconnected nature of the grid layout enhances airflow, facilitating faster pollutant removal. In contrast, the enclosed structure of loop roads traps pollutants, leading to higher $\text{PM}_{2.5}$ concentrations. These findings emphasize the need to incorporate road configuration strategies into urban planning policies, particularly in high-density areas, to improve air quality. The policy implications of these findings suggest that loop-road networks require interventions that enhance internal ventilation, while grid-road networks should focus on blocking emissions from external sources rather than relying solely on internal pollutant removal.

This study highlights the necessity of tailoring $\text{PM}_{2.5}$ mitigation strategies to specific road configurations through building design interventions. The findings suggest that high-density urban planning should prioritize strategic building arrangements to balance pollutant dispersion and ventilation efficiency. In loop-road networks, a block configuration with taller central buildings can enhance pollutant removal, playing a role as crucial as wind velocity in air circulation. Policy strategies should promote centrally elevated buildings with side spaces functioning as pedestrian passages that connect the interior and exterior of the block, facilitating air exchange and reducing pollutant stagnation in the enclosed

loop-road environment. In grid-road networks, the focus shifts from mitigating pollutant accumulation within the canyon to blocking emissions from arterial roads. Increasing perimeter building height while keeping inner buildings lower helps shield inner block areas from traffic emissions originating from arterial roads. Additionally, maintaining a lower AR and minimizing side spaces between buildings further support pollution mitigation in grid-road environments.

This study uncovers the interaction effects between urban morphology factors and meteorological conditions, expanding the understanding of how urban design strategies influence air quality. While existing research has examined the individual impacts of wind velocity and street canyon geometry [72,73], this study demonstrates that their effects are not independent. Instead, the interplay between morphological characteristics and meteorological factors shapes the effectiveness of urban design interventions, emphasizing the need for context-specific approaches to air pollution mitigation. A key finding from the interaction analysis is the threshold effect of AR: when AR exceeds 2.5, high wind velocity helps disperse PM_{2.5} accumulation, leading to lower pollution levels even in dense urban environments. While higher AR is generally linked to pollutant accumulation due to reduced ventilation [74], it also intensifies turbulence, influencing pollutant transport and dispersion [75]. Turbulent transport enhances vertical mixing, facilitating pollutant exchange between primary recirculation and the outer flow, which helps reduce buildup at pedestrian levels, particularly where strong turbulence disrupts stagnant air pockets [76]. Our findings align with previous field studies highlighting wind velocity as a key factor in PM_{2.5} dispersion [77,78]. Yin's study identified a U-shaped relationship between wind speed and PM concentrations, showing that both low and high wind speeds contribute to higher PM levels compared to moderate speeds, underscoring the complexity of wind-PM interactions [77].

This suggests that optimizing wind corridors and building alignments in high-AR areas can largely improve pollutant dispersion. The implications are particularly relevant for high-density urban settings, such as Korea's commercial districts, where most street canyons surpass this threshold. However, we acknowledge that dispersion mechanisms depend on the urban arrangement, core size, and local wind interactions, and the threshold effect at AR = 2.5 observed in our study may not be universally applicable across different urban layouts. Given these variations, policy interventions should prioritize aerodynamic considerations, such as creating ventilation corridors and minimizing excessive block enclosures that trap pollutants. To further refine these strategies, future studies should explore concentration decrease trends across diverse urban configurations [70,79,80].

These findings collectively demonstrate that integrating ML with CFD is a powerful approach to advancing urban air quality analysis. By dynamically refining predictions and improving simulations of complex fluid dynamics, this integration enhances the adaptability of pollutant dispersion models to evolving urban conditions [64]. Unlike traditional numerical models, which may have limited capacity to adjust to real-time data variations, ML-driven CFD analysis processes new information more efficiently [37,63,64,81], capturing the intricate interactions between urban morphology, road configurations, and meteorological factors.

This integration is crucial for urban areas, where proactive measures informed by high-accuracy predictions can largely improve air quality [63,64]. For example, ML-enhanced CFD simulations can support zoning regulations by identifying areas where building height and density adjustments can improve ventilation and pollutant dispersion. Furthermore, integrating ML-driven CFD analysis into early-stage urban planning processes can help optimize road network layouts, ensuring that new developments incorporate aerodynamic considerations to minimize pollution accumulation.

Despite the valuable insights gained from this study, certain limitations should be acknowledged. First, the CFD simulations were conducted under steady-state conditions, based on the prevailing westerlies in South Korea, which do not account for temporal variations in pollutant concentrations due to changing meteorological conditions, such as wind direction shifts. Additionally, microclimatic factors can influence airflow and pollutant dispersion in high-density urban areas. Urban morphological elements, including building height, volume, form, and layout, can modify wind flow, creating corner wind zones, stagnation areas, and pollutant accumulation [82]. Future studies should emphasize the importance of integrating both urban morphology and large-scale topographical influences to develop more effective air quality and airflow management strategies in cities.

Future research should incorporate simulations with diverse wind directions to better capture the dynamic nature of PM_{2.5} dispersion in urban environments [83–85]. Second, while this study incorporates urban morphology and meteorological factors, other aspects, such as pollutant emission levels and land-use patterns, were not explicitly examined. Broadening the analysis to include spatial variations in land use, emission source estimations, and validation with extended field data would enhance the robustness and applicability of the findings [86–88]. Moreover, advancing simulation methodologies to better reflect the complexities of real-world urban environments remains an important area for future research.

5. Conclusions

This study advances the understanding of PM_{2.5} dispersion in high-density urban environments by integrating CFD simulations with interpretable ML models, offering a data-driven approach to analyzing pollutant accumulation at the block scale. While traditional studies focus on individual street canyons, this research demonstrates that road configurations, building arrangements, and AR interact with meteorological conditions to shape air quality at a broader urban block level. The findings emphasize that pollutant dispersion efficiency varies greatly depending on road network type, with grid-road configurations facilitating better airflow and loop-road layouts contributing to pollutant stagnation. Furthermore, building height distribution and side spacing must be carefully considered within different road structures to optimize ventilation and mitigate PM_{2.5} concentrations. This highlights the need for context-specific interventions, as strategies effective for one road type may be counterproductive for another.

These findings offer practical guidance for urban planners and policymakers, highlighting the need for tailored urban design strategies to mitigate PM_{2.5} pollution effectively. Successful interventions must account for the interactions between road configurations, building layouts, and meteorological factors, ensuring that urban design enhances airflow dynamics while limiting pollutant accumulation. The relationship between AR and wind velocity further emphasizes the importance of aerodynamic design considerations, such as wind corridors and strategic building alignments, in improving urban air quality. By providing an evidence-based framework, this research offers urban planners and policymakers practical strategies to foster healthier, more resilient cities capable of addressing air pollution challenges in high-density environments.

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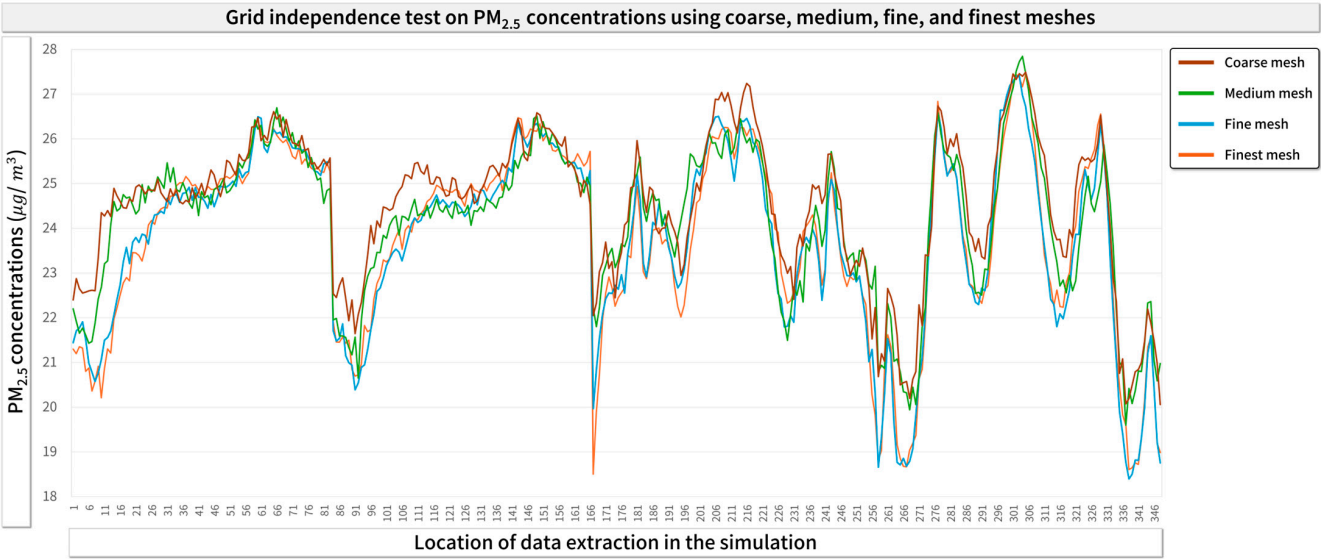
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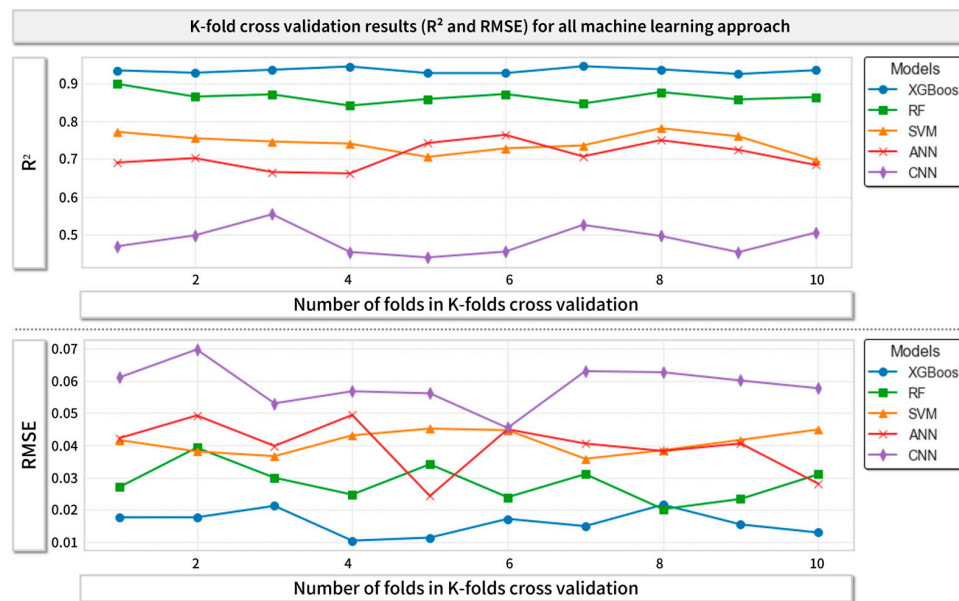
Abbreviations

PM _{2.5}	Fine particulate matter
CFD	Computational Fluid Dynamics
PM	Particulate matter
ML	Machine learning
RF	Random Forest
XGBoost	Extreme Gradient Boosting
AR	Aspect ratio
SST k-ω	Shear-Stress Transport k-ω
GRC	Grid road configuration
LRC	Loop road configuration
TRC	T-junction road configuration
DL	Deep learning
SVM	Support Vector Machine
ANN	Artificial Neural Network
CNN	Convolutional Neural Network
IRCM	Integrated road configuration model
GRCM	Grid road configuration model
LRCM	Loop road configuration model
TRCM	T-junction road configuration model
SHAP	SHapley Additive exPlanations

Appendix A. Grid Independence Test on PM_{2.5} Using Four Types of Meshes



Appendix B. K-Fold Cross Validation Results (R^2 and RMSE) for All Machine Learning Approach



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