

Article

Multi-Scale Validation of CFD Simulations for Pollutant Dispersion Around Buildings

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Abstract

This study establishes a multi-scale validation framework for Computational Fluid Dynamics (CFD) simulations of building-induced pollutant dispersion, integrating wind tunnel experiments, the CEDVAL benchmark dataset, and field measurements from a thermal power plant that serves as a proxy for nuclear facilities. The RNG k - ϵ and Large Eddy Simulation (LES) models were evaluated across these validation tiers. Results demonstrate that both models effectively capture key flow characteristics, with LES showing superior performance in predicting roof-level velocity and turbulence intensities. A systematic overestimation of rooftop and leeward concentrations was observed, though predictive accuracy improved with downwind distance (e.g., $FAC2 > 0.5$). The RNG k - ϵ model provided the best balance between accuracy and computational efficiency for engineering applications, while LES is recommended for high-fidelity near-field analysis. This work provides validated methodologies for environmental risk assessment in nuclear power planning and emission control strategy development.

Keywords: Computational Fluid Dynamics (CFD); atmospheric dispersion; building aerodynamics; model validation; RNG k - ϵ ; Large Eddy Simulation (LES)



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1. Introduction

The strategic expansion of China's nuclear power sector, particularly the development of inland plants, introduces complex challenges for environmental impact and safety assessments. These facilities typically employ large natural draft cooling towers, which significantly alter local airflow patterns through downdrafts, vortices, and flow recirculation, thereby critically influencing the dispersion of airborne effluents [1,2]. The accurate prediction of this dispersion is paramount, as evidenced by the 215 m cooling tower at the Jiangxi Pengze Nuclear Power Plant, which generates more complex wake dynamics and highly irregular dispersion patterns compared to the plant's chimney.

This challenge is inherent to pollutant dispersion in built environments. Pollutants released near buildings are significantly affected by complex airflow disturbances, which alter transport pathways and dispersion kinetics [3]. Traditionally, Gaussian models and empirical formulas have been used for prediction, but they often fail to capture the complex dynamics near structures, especially for non-simple geometries [4–10]. Computational Fluid Dynamics (CFD) has therefore emerged as an essential tool for simulating these atmospheric flows, bridging the gap between simplified models and physical experiments [11–13].

While best practice guidelines like COST 732 and AIJ have established standardized protocols for urban CFD applications [14,15], accurate prediction of near-field dispersion around complex industrial structures remains challenging. This is particularly true for nuclear facilities where traditional field tracer tests are often impractical [16,17]. The thermal power plant investigated in this study serves as a valid proxy for nuclear facilities in terms of geometric and aerodynamic complexity, enabling detailed dispersion analysis where direct nuclear plant data are unavailable.

The choice of turbulence model is pivotal to prediction accuracy. Reynolds-Averaged Navier–Stokes (RANS) models, including the RNG k - ϵ formulation, offer computational efficiency but often struggle to capture the complex separation and recirculation phenomena inherent in building wakes [18,19]. In contrast, Large Eddy Simulation (LES) explicitly resolves the energy-containing turbulent scales, providing superior accuracy for separated flows at a substantially higher computational cost [20–22]. This trade-off necessitates rigorous model validation.

Previous validation studies have predominantly focused on idealized building configurations or urban environments [23,24], revealing a critical research gap: the lack of a multi-scale validation framework for industrial applications. Specifically, there is an absence of integrated methodologies that systematically progress from canonical benchmarks to real-world industrial scenarios.

To bridge this gap, this study establishes a novel multi-scale validation framework that integrates three distinct tiers of validation within a unified methodology. The original contributions are:

- (1) A comprehensive validation methodology that coherently integrates standard building cases, the benchmark CEDVAL wind tunnel dataset, and full-scale field measurements.
- (2) A systematic evaluation of the RNG k - ϵ and LES turbulence models across these validation tiers, delivering new insights into their performance for industrial applications.
- (3) The development of practical validation protocols for complex industrial structures, with direct application to nuclear power plant geometries where experimental data are scarce.

Through this integrated approach, the study aims to: (1) quantify the performance of RNG k - ϵ and LES models in simulating flow and dispersion around buildings across different scales; (2) establish robust validation protocols using multi-fidelity datasets; and (3) demonstrate the predictive capability of CFD in real-world industrial settings with complex building clusters. The findings are expected to provide crucial insights for nuclear safety assessment, emergency response planning, and environmental impact evaluation [17].

2. Numerical Model and Methodology

2.1. Governing Equations and Turbulence Models

The numerical simulation of atmospheric flow and dispersion is governed by the fundamental principles of fluid dynamics, namely the conservation of mass and momentum. For incompressible flow, these are described by the Navier–Stokes equations. The inherent turbulence in atmospheric boundary layer flows necessitates the use of specialized modeling approaches to achieve computationally feasible solutions [25]. This study evaluates two prominent turbulence closure strategies: the Reynolds-Averaged Navier–Stokes (RANS)-based RNG k - ϵ model and the Large Eddy Simulation (LES) model [26].

(1) Governing Equations

The instantaneous flow field is described by the continuity and momentum equations [11,18]:

Continuity Equation:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1)$$

Navier–Stokes Momentum Equation:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad (2)$$

where u_i is the instantaneous velocity component, p is the pressure, ρ is the fluid density, and ν is the kinematic viscosity.

(2) RNG k - ε Turbulence Model

The RNG k - ε model is a widely used RANS-based closure [3,5]. The RANS methodology employs the Reynolds decomposition, splitting instantaneous variables into time-averaged and fluctuating components ($u_i = \bar{U}_i + u'_i$, $p = \bar{P} + p'$). Solving the time-averaged equations requires modeling the Reynolds stresses ($-\rho \overline{u'_i u'_j}$) to close the system.

This model uses the Boussinesq hypothesis, which relates the Reynolds stresses to the mean rate of strain via an isotropic eddy viscosity (ν_t):

$$-\overline{u'_i u'_j} = \nu_t \left(\frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) - \frac{2}{3} k \delta_{ij} \quad (3)$$

where k is the turbulent kinetic energy.

The eddy viscosity is modeled as $\nu_t = C_\mu \frac{k^2}{\varepsilon}$, where ε is the turbulent dissipation rate. The RNG k - ε model solves transport equations for k and ε :

Turbulent kinetic energy (k) Transport Equation:

$$\frac{\partial k}{\partial t} + \bar{U}_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \varepsilon \quad (4)$$

Turbulent dissipation Rate (ε) Transport Equation:

$$\frac{\partial \varepsilon}{\partial t} + \bar{U}_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \frac{\varepsilon^2}{k} \quad (5)$$

where P_k is the production term of turbulent kinetic energy. As an advanced variant derived from renormalization group theory, the RNG formulation incorporates an additional term in the ε -equation and analytically determined constants (e.g., $C_\mu = 0.0845$, $C_{\varepsilon 1} = 1.42$, $C_{\varepsilon 2} = 1.68$), which improve its capability for predicting complex flow features such as flow separation and vortex dynamics in building wakes, addressing key limitations of the standard model.

(3) Large Eddy Simulation (LES) Model

In contrast to RANS, the Large Eddy Simulation (LES) approach resolves the large, energy-carrying eddies in the turbulent flow directly, while modeling the effects of the smaller, universal scales [6]. This is achieved by applying a spatial filter to the Navier–Stokes equations, decomposing the flow variables into resolved (filtered) and subgrid-scale (SGS) components [9].

The filtered equations are:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} \quad (6)$$

where τ_{ij}^{sgs} is the Subgrid-Scale (SGS) stress tensor, representing the influence of the unresolved small scales on the resolved flow. The dominant transport of mass, momentum, and energy is governed by the dynamics of these resolved large-scale motions.

The SGS stresses are modeled using a closure hypothesis. A common approach is the Smagorinsky model, which defines an SGS eddy viscosity ν_{sgs} proportional to the filter width and the resolved strain rate tensor. The model then calculates the SGS stresses as $\tau_{ij}^{sgs} = -2\nu_{sgs}\bar{S}_{ij}$, analogous to the Boussinesq hypothesis.

(4) Model Selection Rationale

Studies indicate that RANS models like the RNG $k-\epsilon$ can exhibit significant uncertainties in predicting near-source concentration gradients within building wakes, primarily due to limitations in their turbulence closure schemes [27,28]. In contrast, LES offers improved predictive capability by directly resolving the large, energy-containing eddies responsible for convective transport [29,30]. The systematic validation conducted in this work against high-resolution experimental data is designed to quantitatively assess the performance of both approaches in simulating the building-induced flow structures that govern pollutant dispersion.

Accordingly, numerical simulations were performed using both the RNG $k-\epsilon$ model and the LES model. Since the tracer gas was released at ambient temperature, thermal buoyancy effects were neglected, corresponding to flow and dispersion under neutrally stratified atmospheric conditions.

2.2. Boundary Conditions and Computational Setup

A consistent strategy for defining the computational domain and boundary conditions was applied across all validation cases to ensure physical realism and comparability with experimental data. The general principle adhered to the “best practice guidelines” (e.g., COST 732, AIJ), ensuring minimal influence from domain boundaries on the flow around the structures of interest [14,15].

2.2.1. General Domain and Mesh Strategy

The computational domains were designed to be sufficiently large to avoid flow constriction and unrealistic pressure gradients. A structured, hexahedral-dominant mesh was employed in all cases, following a “near-dense-far-sparse” strategy. This approach ensures high resolution in regions of strong flow gradients (e.g., near building surfaces, in wake regions) while gradually coarsening the mesh in the far-field to optimize computational efficiency. Comprehensive grid independence tests, as detailed in subsequent validation sections, were conducted for each case to ensure the solution was independent of the mesh resolution.

2.2.2. Case-Specific Configurations

Case A: Standard Building Wind Tunnel Benchmark

(1) Computational Domain and Geometry

The computational domain replicated the dimensions of the wind tunnel test section: 17 m (length) $\times$ 1.5 m (width) $\times$ 1.0 m (height). A cubic building with a height of $H = 164$ mm was placed inside according to established best practices. A point emission source was positioned on the rooftop at $1.1H$ (180.5 mm).

(2) Boundary Conditions and Pollutant Source

Inlet: A velocity inlet with a power-law wind profile $U(z) = U_{\text{ref}}(z/z_{\text{ref}})^\alpha$ was applied, simulating a neutrally stratified atmospheric boundary layer. The reference velocity U_{ref}

was 1.2 m/s at $z_{\text{ref}} = H$, with an exponent $\alpha = 0.16$. Turbulence parameters matched the experimental inflow conditions.

Outlet: A pressure outlet with zero static pressure.

Walls: No-slip conditions with surface roughness set to match the experimental setup.

Top and Side Boundaries: Symmetry (slip-wall) conditions were used to represent the wind tunnel confinement.

Pollutant Source: Carbon monoxide (CO) was released at the rooftop source at a constant rate of 120 mL/min (STP).

The boundary condition setup is illustrated in Figure 1.

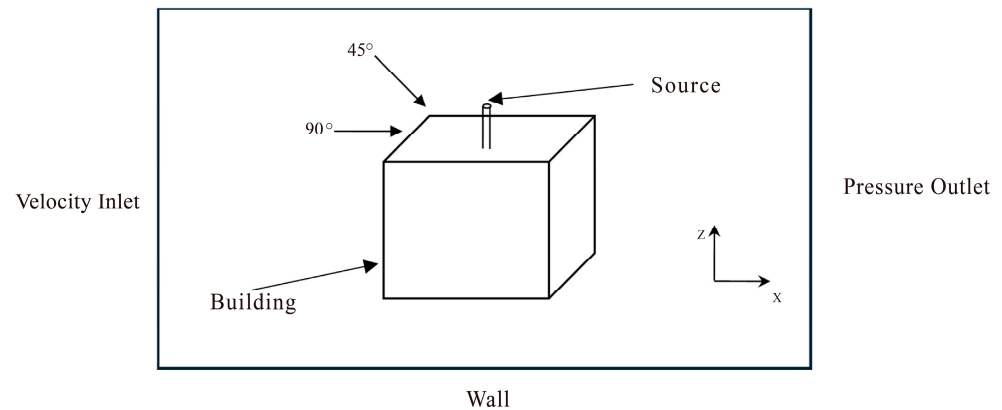


Figure 1. Schematic of the computational domain and boundary conditions for the standard building case.

Case B: CEDVAL A1–1 Benchmark

(1) Model Geometry and Scaling

The computational domain was built to contain the CEDVAL A1–1 building array at a geometric scale of 1:200. The central building had model-scale dimensions of 0.1 m × 0.15 m × 0.125 m (height), equipped with four rectangular exhaust vents (0.017 m × 0.007 m) on one side, as illustrated in Figure 2. The corresponding full-scale prototype dimensions are 20 m (width) × 30 m (length) × 25 m (height), as illustrated in Figure 3.

(2) Boundary Conditions

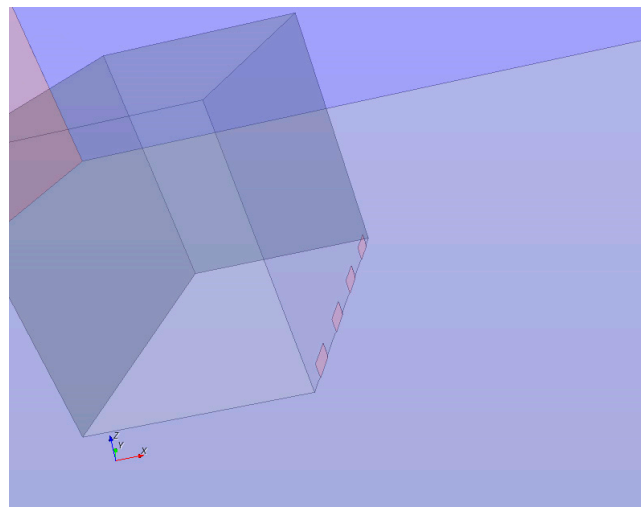


Figure 2. Configuration of the three-dimensional computational model. The four rectangular exhaust vents are highlighted in pink.

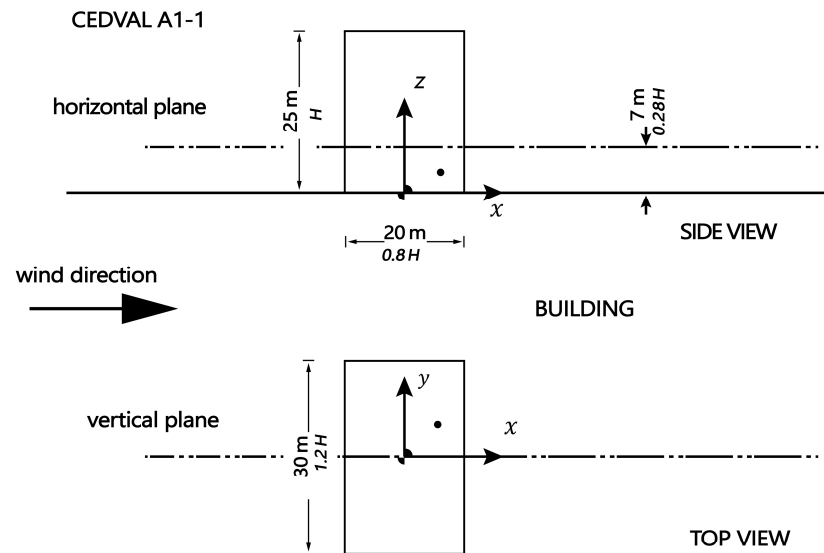


Figure 3. Dimensions of the building model used in the wind tunnel experiment.

Inlet: An exponential wind profile $U(z) = 6.0 \times (z/100.0)^{0.21}$ was prescribed, with the turbulence intensity profile given by $I = 0.811z^2 - 0.652z + 0.284$.

Outlet & Surfaces: A pressure outlet was used at the exit; all solid surfaces were treated as no-slip walls with a defined roughness height (0.14 in model scale).

Pollutant Source: Carbon monoxide (CO) was released from the four vents at a total volume flow rate of $0.033 \text{ m}^3/\text{s}$.

(3) Numerical Setup and Mesh

The steady-state RNG $k-\varepsilon$ model was employed for this simulation. A polyhedral mesh following the “near-dense-far-sparse” strategy was generated, resulting in approximately 78,000 cells (minimum size 1.25 m, average 2.5 m). The computational mesh is shown in Figure 4.

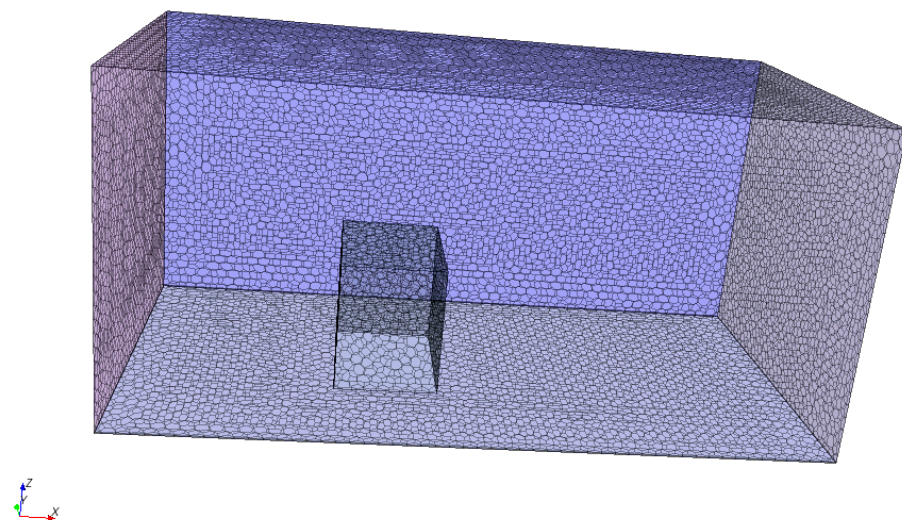


Figure 4. Computational mesh used in the CFD simulations.

Velocity and concentration fields were monitored at eight key points; their normalized coordinates (using $H = 25 \text{ m}$) are listed in Table 1.

Table 1. Coordinates of vertical wind speed monitoring points.

Monitoring Point Number	$X(H)$	$Y(H)$
1#	−1.66	0.00
2#	−1.30	0.00
3#	−0.70	0.00
4#	−0.08	0.00
5#	0.32	0.00
6#	0.72	0.00
7#	2.28	0.00
8#	3.20	0.00

Note: The “#” symbol denotes the monitoring point number (e.g., “1#” refers to monitoring point 1). Coordinates $X(H)$ and $Y(H)$ are normalized by the building height H .

Case C: Liaocheng Thermal Power Plant Field Case

(1) Site Description and Computational Domain

This case constitutes the third and final tier of the validation framework, designed to assess the CFD model’s predictive capability under real-world, industrial-scale conditions. The Liaocheng Thermal Power Plant site, featuring complex building clusters and a large natural-draft cooling tower (height: 145 m), serves as a geometric and aerodynamic proxy for nuclear facilities. A computational domain measuring $20 \text{ km} \times 20 \text{ km} \times 4 \text{ km}$ was centered on the plant to minimize boundary effects. Detailed 3D models of the main structures were created and imported into the CFD environment, with the surrounding terrain simplified as flat terrain.

(2) Boundary Conditions and Emission Sources

Inflow: A power-law wind profile representing Class D atmospheric stability was used, with an exponent of 0.25 and a reference speed of 3.4 m s^{-1} at 10 m height.

Other Boundaries: Settings followed the same principles as previous cases, scaled appropriately for the full-scale domain.

Pollutant Release: Passive tracer gas (sulfur hexafluoride, SF_6) was released from the rooftops of Boiler Rooms #3 and #4 at ambient temperature; thermal buoyancy effects were therefore neglected. The simulation thus focused solely on the dynamic dispersion induced by the building cluster under neutrally stratified conditions. The cooling tower’s key operational parameters (provided in Table 2 for context) were characterized, but its plume was not the active emission source in this validation.

Table 2. Key parameters of the cooling tower at the Liaocheng Thermal Power Plant.

Parameter	Unit	Numerical Value
Base diameter (inner)	m	116.334
Total height	m	145
Outlet diameter (inner)	m	66.970
Throat diameter	m	62.342
Throat height (above ground)	m	108.75
Air inlet height	m	10.034
Cold air inlet velocity	m/s	3.67
Cold air volumetric flow rate	m^3/s	12,662.77

(3) Numerical Setup and Mesh

The RNG $k\text{-}\epsilon$ turbulence model was selected for this large-scale application, balancing accuracy and computational efficiency as indicated by preceding validation tiers. A polyhedral mesh was generated with local refinement: surface resolution on major structures

was 4 m, coarsening to 50–100 m in the far-field. The final grid contained approximately 2.89 million cells (see Figure 5).

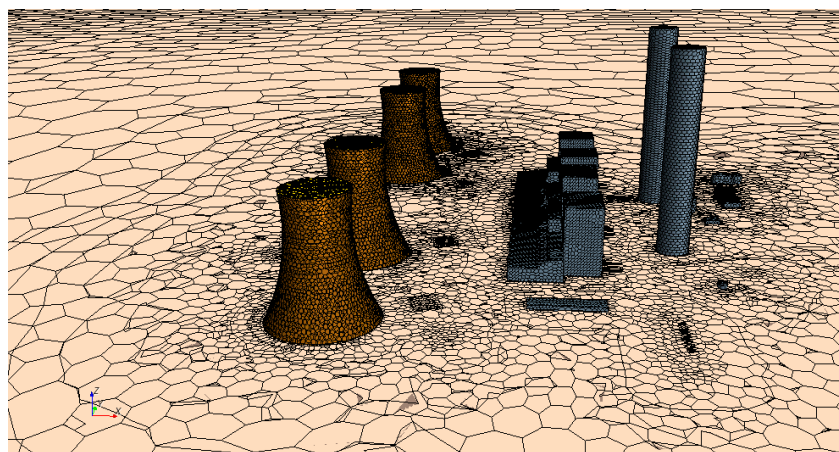


Figure 5. Computational grid for the Liaocheng thermal power plant case.

The completed model was imported into the CFD software STAR-CCM+ 5.0 (Siemens Digital Industries Software, Plano, TX, USA), as shown in Figure 6.

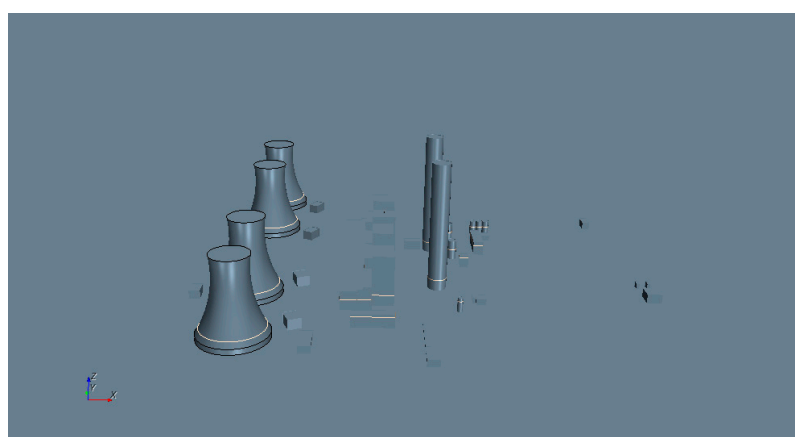


Figure 6. Three-dimensional Model of Liaocheng Thermal Power Plant Area.

The key boundary conditions and model constants for the three primary validation cases are summarized in Table 3.

Table 3. Summary of key boundary conditions and model constants.

Parameter/Case	Standard Building	CEDVAL Benchmark	Liaocheng Plant
Wind Profile Exponent (α)	0.16	0.21	0.25
Reference Velocity	1.2 m/s at H	6.0 m/s at 100 m (full-scale)	3.4 m/s at 10 m
Surface Roughness	Matched to experiment	0.0007 m (model scale)	Matched to site
Turbulence Model Constants	$C_{1\epsilon} = 1.44$, $C_{2\epsilon} = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\epsilon = 1.3$	(Same as Standard Building)	(Same as Standard Building)

2.3. Grid Independence and Validation Strategy

A rigorous, multi-tiered approach was employed to ensure the reliability and accuracy of the Computational Fluid Dynamics (CFD) simulations. This strategy encompassed two critical components: first, establishing mesh-independent solutions for each case through systematic grid sensitivity analysis; second, validating the models against experimental data across three distinct scales of complexity.

2.3.1. Grid Independence Analysis

A consistent “near-dense-far-sparse” meshing strategy was applied across all cases. This approach ensures high resolution in regions with strong flow gradients, such as near building surfaces and in wake regions, while gradually coarsening the mesh in the far-field to optimize computational efficiency without sacrificing accuracy. The determination of the final grid for each case was based on a grid convergence study, where key flow or concentration parameters were monitored across systematically refined mesh systems.

The results of the grid independence studies for the three primary validation cases are summarized in Table 4. For each case, the solution was deemed mesh-independent when further grid refinement led to negligible changes (typically <2%) in the monitored parameters. The final selected grid size for each case provided an optimal balance between computational accuracy and cost.

Table 4. Summary of grid independence analysis results.

Case Description	Number of Grid Systems Tested	Key Monitoring Parameter	Final Selected Grid Size	Justification
Standard Building	4	Wind Speed Magnification Factor at 2 points	381,542 cells	Results converged to within 1% of experimental values; further refinement yielded negligible improvement (<0.5%).
CEDVAL Benchmark	4	Normalized Concentration (K) at 2 points	323,560 cells	Solution converged at this level; additional cells (665,120) changed results by <0.3%.
Liaocheng Plant	4	Ground-level Concentration at 2 points	~2.89 million cells	Concentrations changed by <0.2% with further refinement to ~4.00 million cells.

2.3.2. Multi-Scale Validation Strategy

To ensure a rigorous and systematic evaluation, the CFD methodology was validated through a novel multi-scale framework. This framework progresses through three distinct yet interconnected tiers, moving from canonical flows to real-world industrial complexity. This structured approach ensures that the models are tested and their reliability established across a spectrum of geometric complexity and scale, thereby building confidence in their predictive capabilities for practical engineering applications. The detailed workflow of this framework, including the specific models and validation metrics employed at each stage, is visually summarized in Figure 7 and elaborated in the following section.

This integrated methodology progresses through three distinct yet interconnected tiers of validation, ensuring the CFD models’ reliability across a spectrum of geometric complexity and scale.

The process begins with Stage 1: Standard Building Case, which establishes fundamental model reliability using a canonical cubic building geometry. Here, both the RNG k - ϵ and LES models are evaluated against high-fidelity wind tunnel data for flow and dispersion, providing a baseline performance assessment and a direct comparison of the turbulence closure schemes [31–35].

The framework then advances to Stage 2: CEDVAL Benchmark validation. This tier utilizes the well-established CEDVAL wind tunnel dataset for a standardized building array, testing the model’s performance in a more complex, yet still controlled, aerodynamic environment [36]. The RNG k - ϵ model is primarily employed in this stage to assess its suitability for engineering applications involving building clusters [37,38].

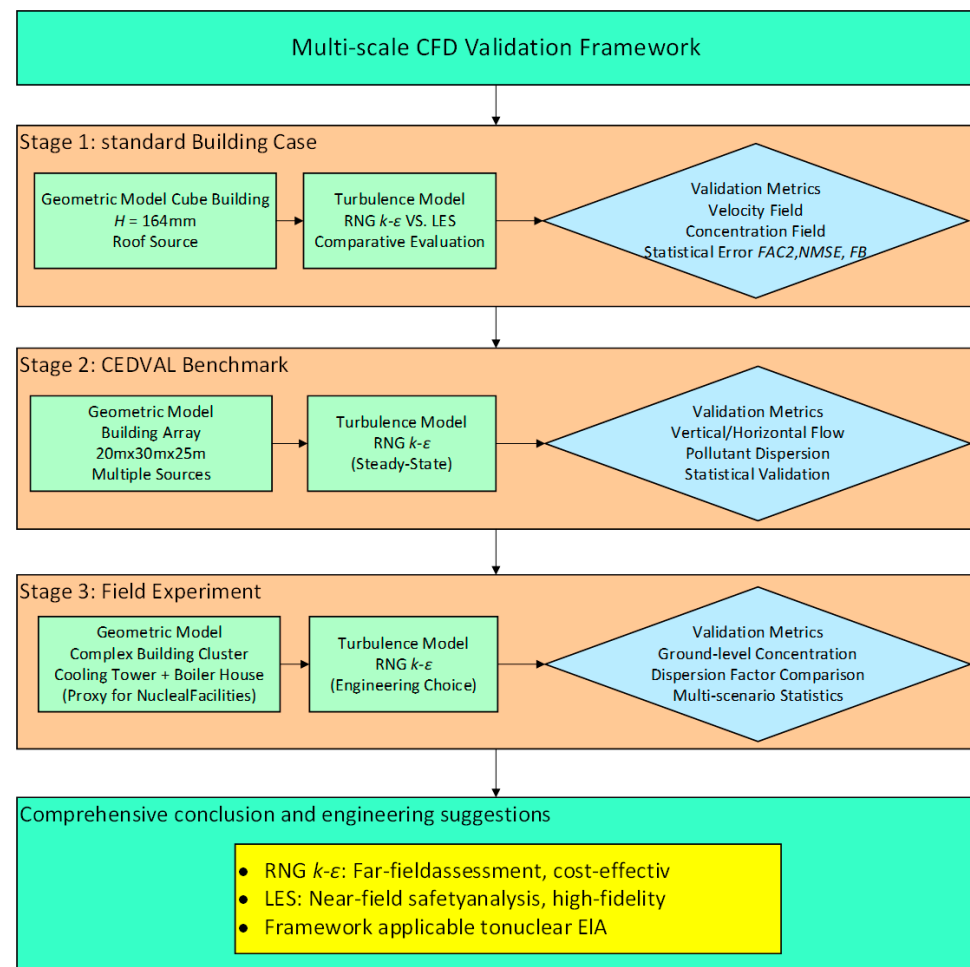


Figure 7. Multi-scale validation framework methodology workflow.

Finally, the framework culminates in Stage 3: Field Experiment at the Liaocheng Thermal Power Plant, serving as a proxy for nuclear facilities. This stage validates the model's predictive capability under real-world atmospheric conditions and complex industrial geometry, directly addressing the research gap in applications beyond idealized configurations. The RNG $k-\epsilon$ model was selected for this large-scale simulation based on its balance of accuracy and computational efficiency, as informed by the previous stages.

This tiered approach ensures that the model is rigorously tested at each step, from fundamental dynamics to full-scale industrial application, thereby providing a robust foundation for the environmental impact and safety assessments discussed in this work (see also Supplementary Video S1 for a visual summary of the framework).

3. Results for a Standard Building Case

This section presents the simulation results for the standard cubic building case, which serves as the foundational tier of the multi-scale validation framework. The objective is to establish baseline performance metrics for the RNG $k-\epsilon$ and LES models in predicting flow and dispersion around an isolated structure. The CFD simulations were conducted using the configuration detailed in subsection of Section 2.2.2 (Case A), and the results are compared against high-fidelity wind tunnel data for velocity and concentration fields under varying wind incidence angles ($\theta = 0^\circ$ to 90°).

3.1. Influence of the Building on the Flow Field

The performance of the RNG $k-\epsilon$ and LES models in simulating the building-induced flow field was evaluated by comparing the predicted normalized velocity and turbulence intensity profiles with the benchmark wind tunnel data from Castro and Robins [35] under 90° and 45° wind incidence angles.

Figures 8 and 9 compare the normalized velocity (U/U_{ref}) distributions at various downwind locations [39]. The results demonstrate that both turbulence models successfully capture the key flow features, including the velocity acceleration at the building sides, the pronounced velocity deficit in the near-wake, and the subsequent flow recovery in the far-wake. The predictions from both models show general consistency with the experimental data in replicating the overall pattern of the mean velocity distribution.

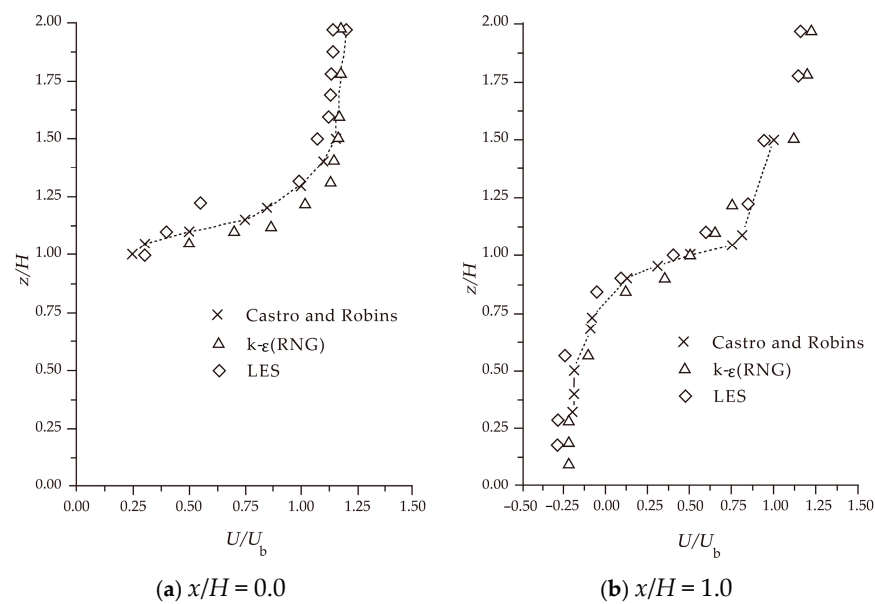


Figure 8. Normalized velocity versus height (z/H) for different models under a 90° wind incidence angle.

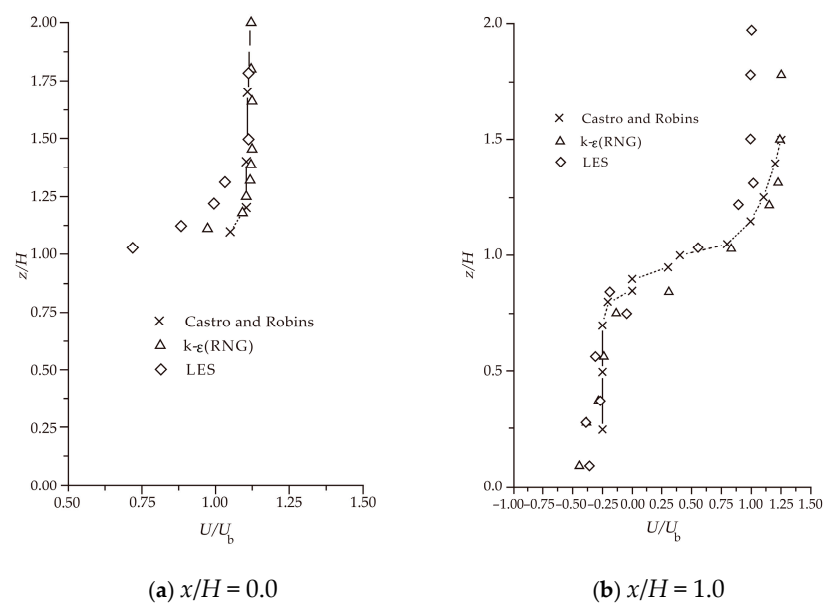


Figure 9. Normalized velocity versus height (z/H) for different models under a 45° wind incidence angle.

However, significant differences between the models emerge in the prediction of turbulence, as quantified in Figure 10. The RNG k - ε model exhibits a systematic underestimation of turbulence intensity in critical regions. Specifically, it underpredicts the peak turbulence intensity near the roof edge ($z/H \approx 1.0$ – 1.25) and within the near-wake core ($x/H \approx 1$). This discrepancy stems from the model's isotropic eddy-viscosity assumption, which struggles to represent the strongly anisotropic and non-equilibrium turbulence generated by flow separation. The underestimation of turbulent kinetic energy (TKE) production leads to an overly slow velocity recovery and an overestimation of the recirculation zone size.

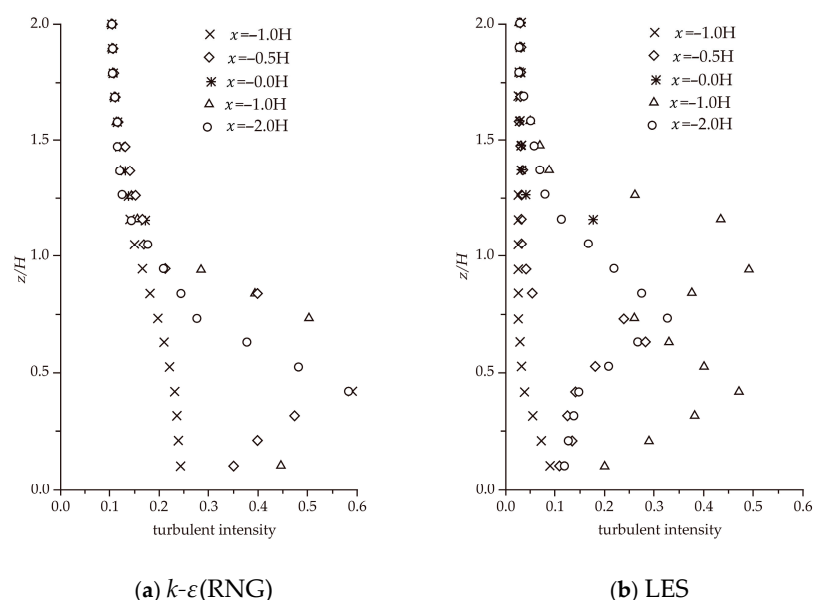


Figure 10. Turbulence intensity versus height (z/H) for different models under a 90° wind incidence angle.

In contrast, the LES model shows superior agreement with the experimental data in these critical regions. By directly resolving the energy-containing turbulent eddies, LES accurately captures the sharp rise in turbulence intensity at the roof shear layer and the magnitude and distribution of the peak turbulence in the wake core. This results in a more physically realistic simulation of the flow reattachment process and the size of the recirculation zone.

In summary, while the RNG k - ε model provides an acceptable prediction of the mean flow for general engineering applications, its limitations in simulating separation-induced turbulence are evident. LES is necessary for high-fidelity analysis of near-wake flow dynamics, which has direct implications for accurately predicting subsequent pollutant dispersion.

3.2. Influence of the Building on the Concentration Field

The performance of the RNG k - ε and LES models in simulating contaminant dispersion was evaluated by comparing the predicted normalized concentration, $K = C^* \cdot U \cdot H^2 / Q$, against wind tunnel measurements for 90° and 45° wind incidence angles.

Figure 11 compares the normalized concentration distributions for the 90° wind incidence case. A key observation is the consistent over-prediction of concentrations within $1.0H$ downwind of the rooftop and leeward side by both CFD models. This discrepancy is directly linked to the flow field analysis in Section 3.1, where both models, particularly RNG k - ε , simulated an enlarged recirculation zone, leading to enhanced pollutant trapping. This over-prediction diminishes with downwind distance as the building's influence weakens.

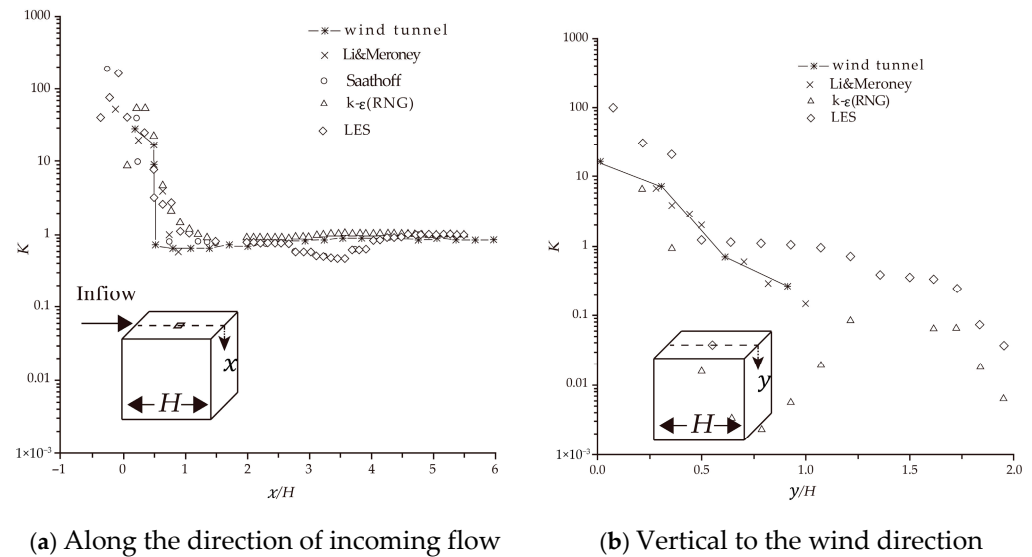


Figure 11. Normalized concentration distribution along the downwind and crosswind axes under a 90° wind incidence angle.

The models exhibited divergent performance at the building's sidewall. The RNG $k-\epsilon$ model underestimated the lateral concentration spread, while the LES prediction aligned more closely with the measurements (Figure 11b). This highlights a fundamental limitation of the RNG $k-\epsilon$ approach in accurately simulating complex lateral dispersion processes.

Under the 45° oblique wind incidence (Figure 12), the simulations showed a slight underestimation of roof-level concentrations, indicating a shared challenge in capturing rooftop flow dynamics for oblique winds. Across the entire domain, the LES model demonstrated superior alignment with the measured dispersion pattern compared to the RNG $k-\epsilon$ model.

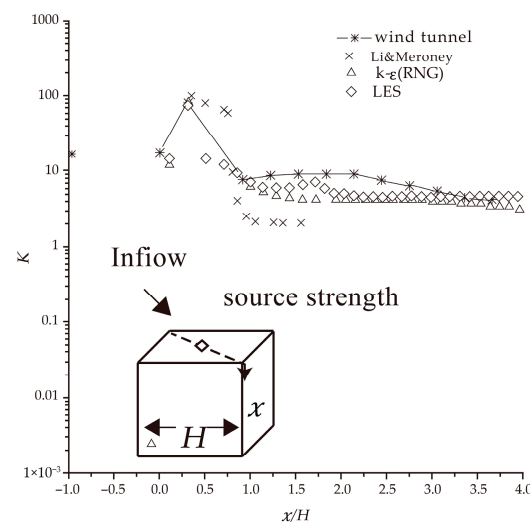


Figure 12. Normalized concentration distribution along the downwind axis under a 45° wind incidence angle.

In summary, the concentration field simulations align with the flow patterns identified in the preceding analysis. The fidelity of dispersion predictions is closely tied to the representation of turbulence in the underlying model. For near-field concentration gradients, the LES results align more closely with the experimental data. The RNG $k-\epsilon$ model reproduces the overall trends in concentration distribution; however, in the critical near-wake region,

discrepancies remain evident in its prediction of peak concentrations and the lateral spread of pollutants compared to measurements.

4. Results for the CEDVAL Benchmark Case

This section presents the simulation results for the CEDVAL A1–1 building array benchmark, which serves as the second tier of the validation framework. The objective is to evaluate the model's performance in a standardized, complex urban-like environment. The CFD simulations were conducted using the configuration detailed in subsection of Section 2.2.2 (Case B), and the results are compared against the high-quality experimental dataset from the University of Hamburg's Environmental Wind Tunnel Laboratory.

4.1. Flow Field Results and Comparison

The simulated flow field around the CEDVAL building array demonstrates the model's capability to capture complex urban airflow phenomena. Figure 13 illustrates the vertical wind velocity contours at a height of 7 m ($0.28H$), revealing the acceleration of flow over the building roof and the formation of a recirculation cavity in the immediate leeward region. This pattern is further elaborated in Figure 14, which shows the horizontal wind field at the same height, clearly depicting the windward stagnation zone and the leeward cavity with significantly reduced wind speeds.

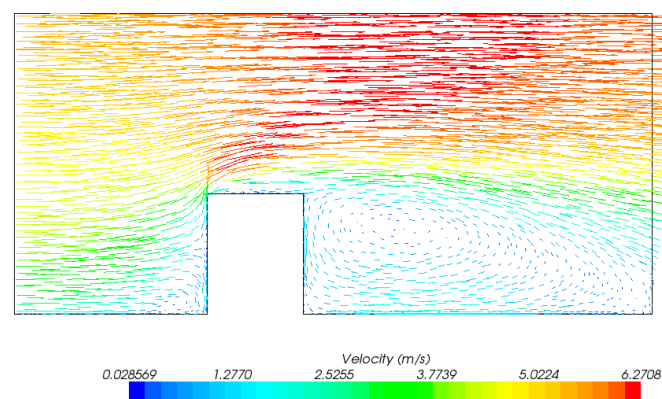


Figure 13. Contours of the vertical wind velocity component.

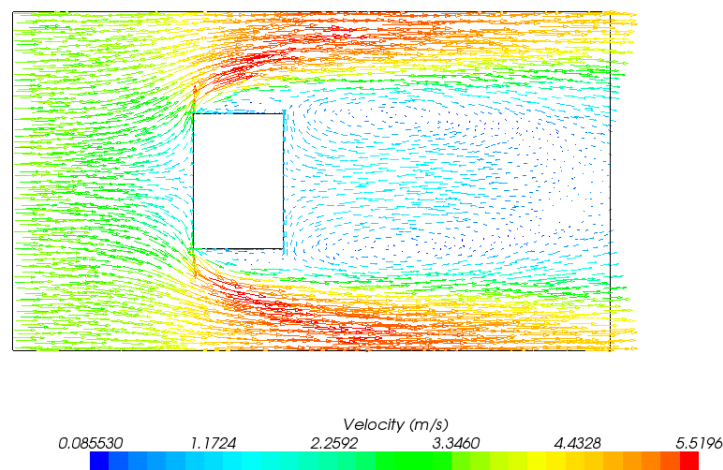


Figure 14. Horizontal wind field at a height of 7 m ($0.28H$).

Quantitative comparisons with wind tunnel measurements were conducted at eight monitoring points (Table 1). Figure 15 displays vertical profiles of wind speed at four

representative locations, where the CFD predictions show consistent alignment with the experimental data. The simulations reproduce the following key flow features:

- (1) acceleration of wind speed near the building top,
- (2) velocity deficits in the immediate leeward region (Points 3# and 4#), and
- (3) gradual recovery of the wind profile with increasing downwind distance (Points 7# and 8#).

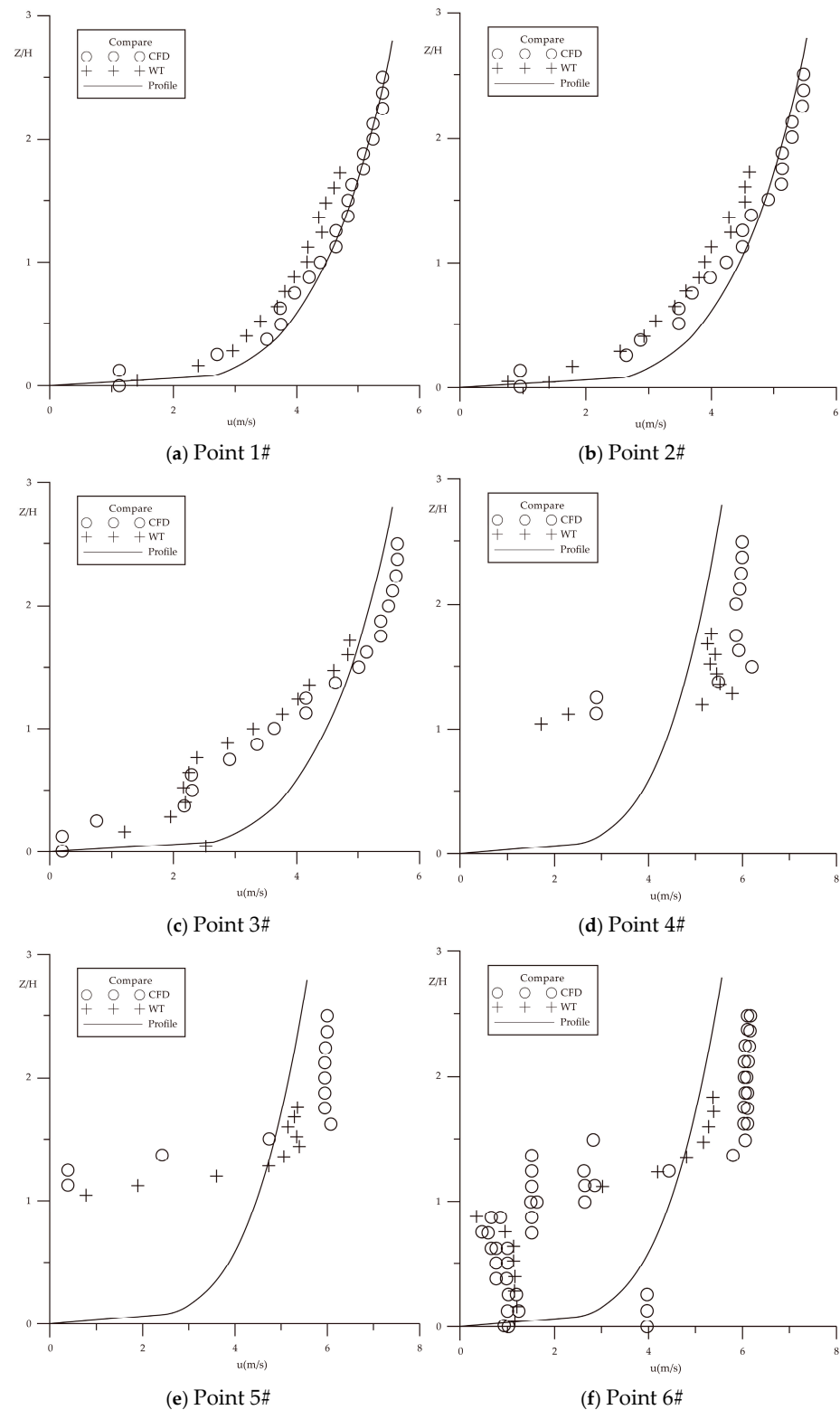


Figure 15. Cont.

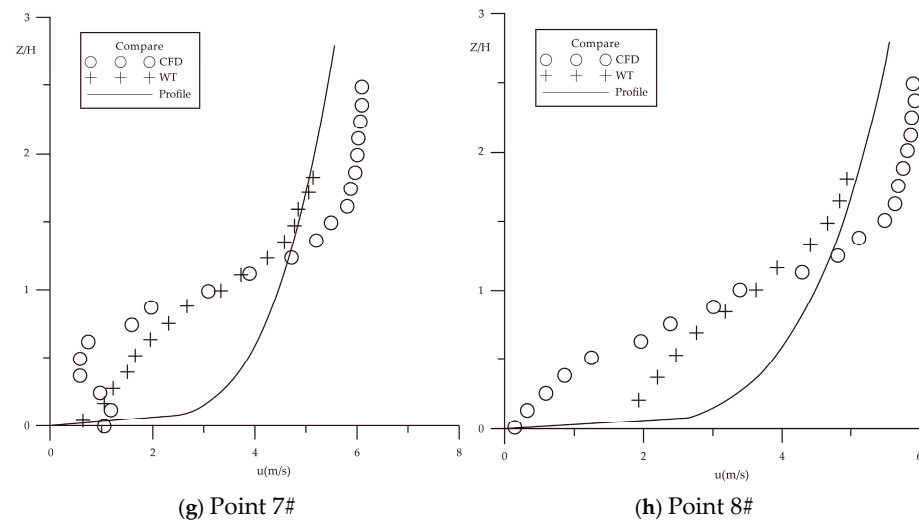


Figure 15. Vertical profiles of wind speed at selected monitoring points.

Across all monitored locations, the simulated values correspond closely to the measurements, reflecting the model's ability to capture the mean flow characteristics of the building array configuration.

4.2. Concentration Field Results and Comparison

The pollutant dispersion pattern predicted by the CFD model is presented in Figure 16, showing the typical behavior of plume development and transport around the building array. To quantitatively assess the model performance, concentration measurements were compared along nine monitoring lines as specified in Table 5, which includes both vertical profiles at fixed downwind distances and horizontal profiles at ground level.

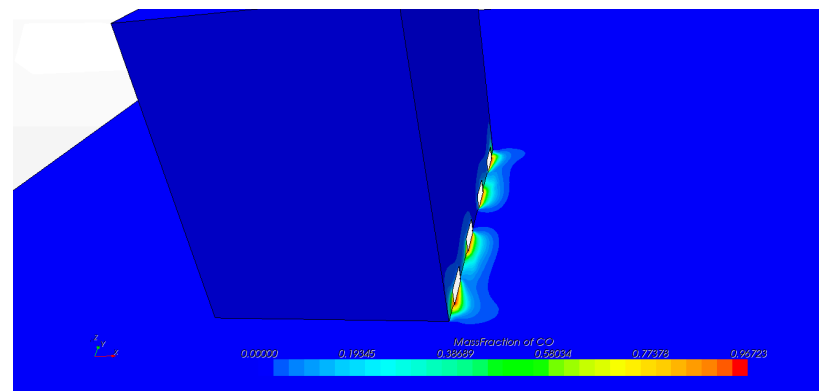


Figure 16. Simulated pollutant dispersion pattern (volume concentration).

Table 5. Coordinates of the monitoring points.

No.	$X(H)$	$Y(H)$	$Z(H)$
1	0.92	—	0.28
2	1.52	—	0.28
3	2.0	—	0.28
4	2.8	—	0.28
5	3.6	—	0.28
6	0.96	0.0	—
7	1.52	0.0	—
8	2.0	0.0	—
9	2.96	0.0	—

Figure 17 presents a side-by-side comparison of CFD-predicted and wind-tunnel-measured normalized concentration (K) values across all nine monitoring locations. The simulated results align with the measurements in both trend and order of magnitude. Key features reflected in the comparison include:

- (1) The vertical stratification of concentration at different downwind distances (Points 1–5) is reproduced by the simulation.
- (2) The distribution of ground-level concentrations (Points 6–9) closely follows the measured profiles.
- (3) Slight deviations between simulation and experiment appear mainly in zones with steep concentration gradients.
- (4) The overall dispersion pattern, including the locations of peak concentrations, is consistent with the experimental data.

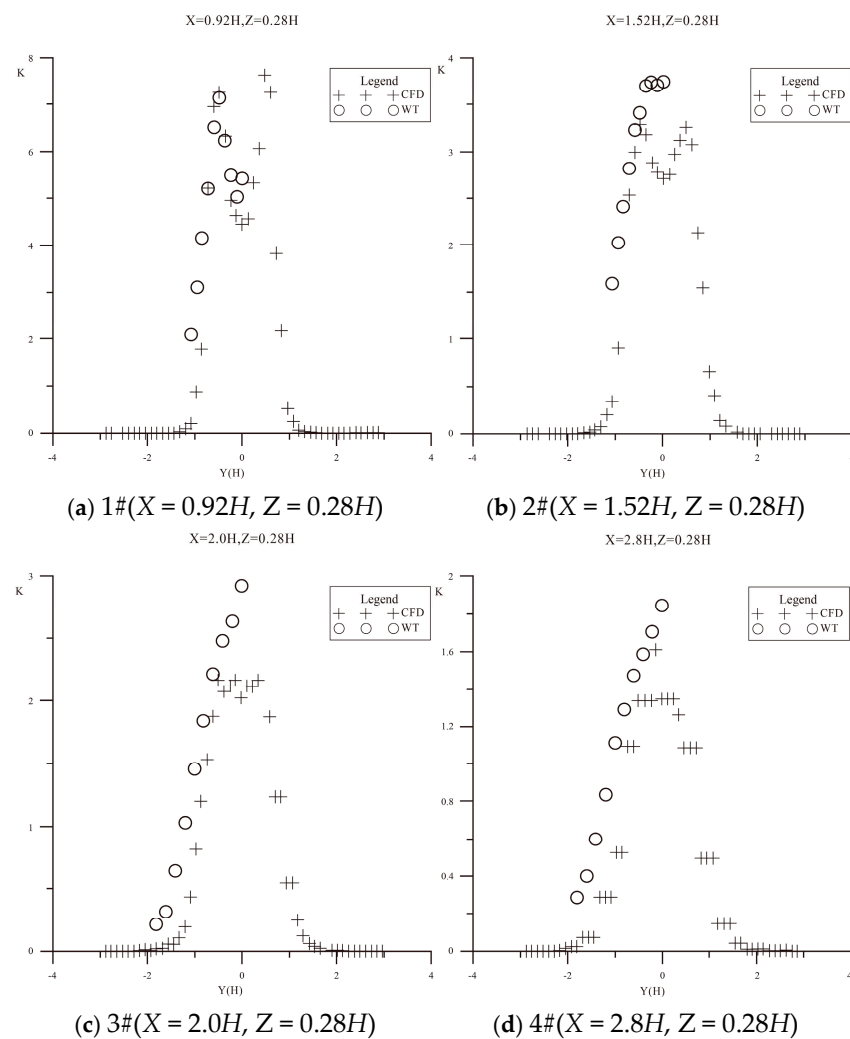


Figure 17. Cont.

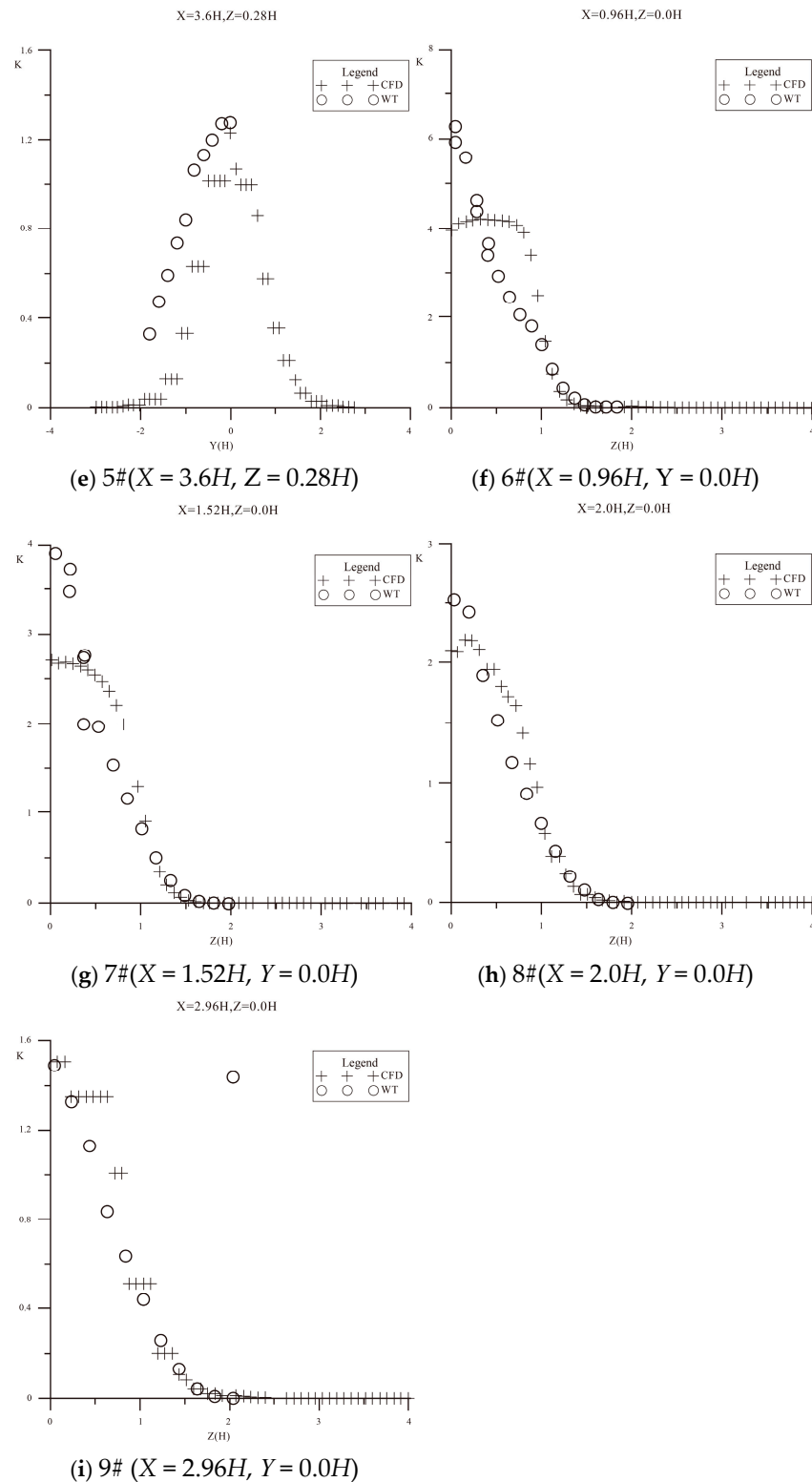


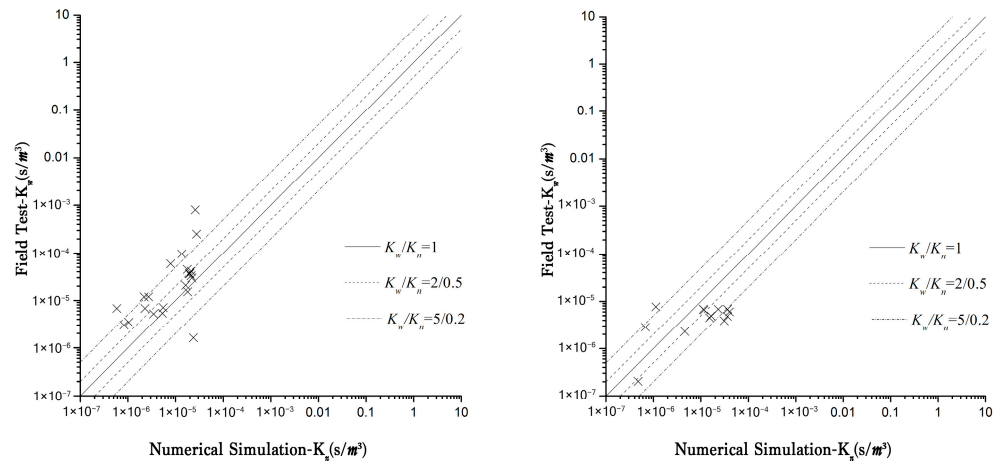
Figure 17. Comparison of CFD simulations and experimental data showing close agreement.

5. Results from the Field Experiment at Liaocheng Thermal Power Plant

This section presents the results from the final validation tier, which assesses the model's predictive capability under real-world atmospheric conditions at a full-scale industrial site. The simulation setup for the Liaocheng plant, as described in subsection of Section 2.2.2 (Case C), was validated against field tracer measurements.

5.1. Ground-Level Concentration Comparison

Field experiments involved pollutant releases from the roofs of Boiler Houses #3 and #4 under northeast wind conditions. Figure 18 compares the normalized ground-level concentrations from CFD simulations and field measurements at various downwind distances for both release scenarios.



(a) Release from Boiler Room #3 Roof

(b) Release from Boiler Room #4 Roof

Figure 18. Comparison of normalized ground-level concentrations from field experiments and CFD simulations.

The simulated downwind concentrations near the buildings are generally higher than the field measurements. This systematic overprediction diminishes with downwind distance, as the simulated results gradually converge with the measured values. The larger leeward recirculation zone predicted in the simulations correlates with these concentration differences. Characteristic wake patterns—including reduced wind speed and elevated turbulence intensity behind the structures—are evident in both datasets.

5.2. Spatial Distribution of Dispersion Factors

Figure 19 provides a more detailed comparison of the dispersion factors obtained from field experiments and CFD simulations for a release from Boiler Room #3 under identical conditions, showing the plume development at specific downwind distances.

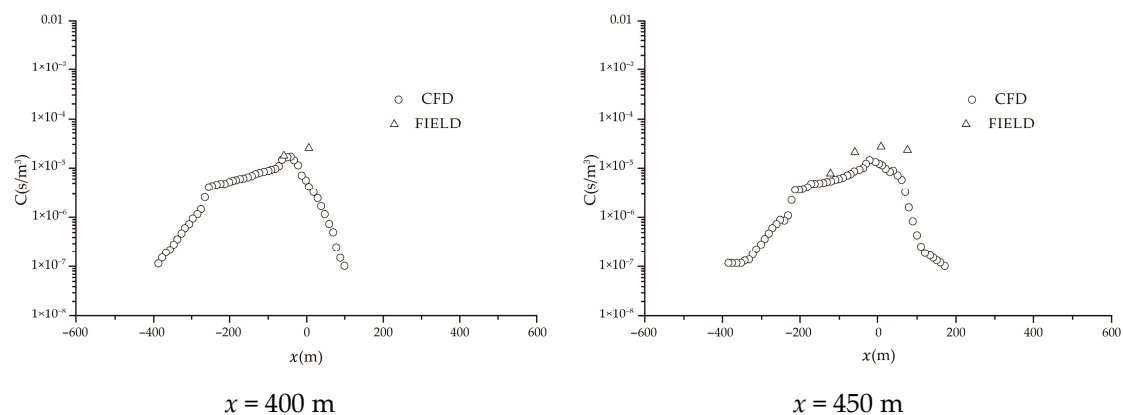


Figure 19. Cont.

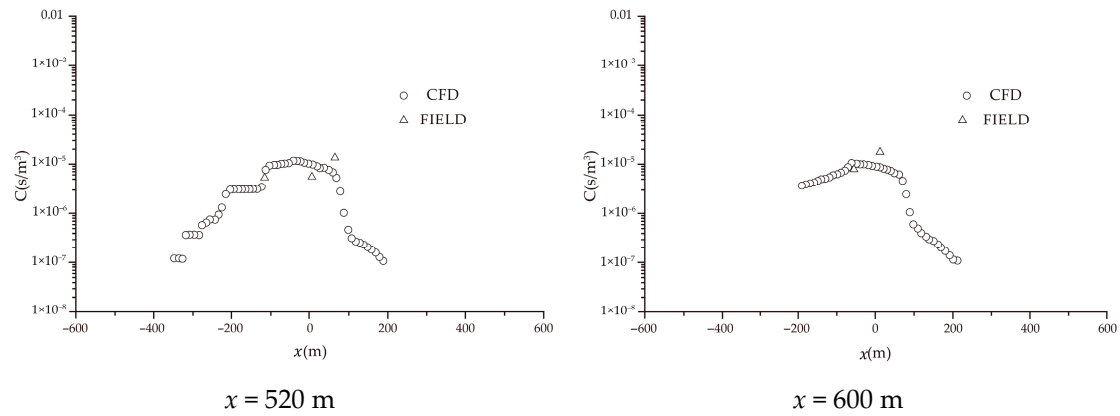


Figure 19. Comparison of ground-level dispersion factors from field experiments and CFD simulations for a rooftop release from Boiler Room #3 under NE wind conditions.

The simulation results generally follow the same trend as the experimental data, successfully capturing the evolution of the plume's cross-sectional distribution. While minor discrepancies appear at closer distances, the results show convergence with increasing downwind distance. The comprehensive analysis indicates that the plume distribution increasingly approximates a Gaussian profile with negligible skewness, aligning with typical atmospheric dispersion behavior. The simulated concentrations show a slight underestimation compared to field measurements in some areas, which can be attributed to the model's stronger emphasis on convective transport relative to diffusive processes.

6. Comprehensive Model Validation and Performance Assessment

6.1. Quantitative Validation Metrics and Criteria

To quantitatively evaluate the agreement between CFD predictions and wind tunnel measurements for the standard building case, a statistical analysis was performed using established metrics: the Factor of Two (FAC2), Normalized Mean Square Error (NMSE), and Fractional Bias (FB). These metrics were calculated based on the normalized concentration (K) at all measurement points for both 45° and 90° wind incidence angles.

The statistical metrics are defined as follows:

FAC2: The fraction of predicted concentrations (C_n) within a factor of two of the observed values (C_m). A value greater than 0.5 (50%) is generally considered acceptable.

Fractional Bias (FB): Measures the systematic bias between predictions and measurements:

$$FB = \frac{\overline{C_n} - \overline{C_m}}{0.5(\overline{C_n} + \overline{C_m})} \quad (7)$$

where $\overline{C_n}$ and $\overline{C_m}$ are the mean predicted and measured concentrations, respectively.

A value of $|FB| < 0.3$ indicates acceptable bias.

Normalized Mean Square Error (NMSE): Quantifies the overall scatter of the predictions:

$$NMSE = \frac{\overline{(C_n - C_m)^2}}{\overline{C_n} \cdot \overline{C_m}} \quad (8)$$

An NMSE value below 4.0 is typically considered indicative of good agreement.

6.2. Validation Results Across Tiers

6.2.1. Standard Building Case

This tier validated the fundamental capability of the CFD models to simulate flow and dispersion around an isolated cubic building, using high-fidelity wind tunnel data under 45° and 90° wind incidences. The statistical results are summarized in Table 6.

Table 6. Statistical comparison of concentration values between CFD simulations and wind tunnel tests for the standard building case.

Statistical Metric	45° Wind Incidence	90° Wind Incidence
<i>FAC2</i>	0.63	1.5
<i>NMSE</i>	3.56	2.12
<i>FB</i>	−0.13	0.25

As shown in Table 6, all metrics (*FAC2*, *NMSE*, and $|FB|$) for both incidence angles satisfy the acceptance criteria defined in Section 6.1. This confirms that the CFD methodology provides reliable predictions for the flow and pollutant dispersion around a standard, isolated building.

6.2.2. CEDVAL Benchmark Case

This tier assessed the model's performance for a more complex, standardized building array using the benchmark CEDVAL A1–1 wind tunnel dataset. The statistical results against this benchmark are summarized in Table 7.

Table 7. Statistical comparison of concentration values between CFD simulations and CEDVAL wind tunnel tests.

Statistical Metric	CFD Result
<i>FAC2</i>	0.85
<i>NMSE</i>	2.54
<i>FB</i>	−0.16

The values in Table 7 (*FAC2* = 0.85, *NMSE* = 2.54, *FB* = −0.16) all meet the acceptance thresholds established in Section 6.1. This demonstrates that the CFD model, primarily employing the RNG *k*– ϵ closure, reliably simulates both airflow and dispersion in a complex building cluster environment.

6.2.3. Field Experiment Case

The final tier evaluated the model's predictive accuracy under real-world, industrial-scale conditions using field measurements from the Liaocheng Thermal Power Plant, which serves as a proxy for nuclear facilities. The statistical results for releases from two boiler room roofs are consolidated in Table 8.

Table 8. Statistical comparison of ground-level concentrations between numerical simulations and field experiments.

Statistical Metric	Scenario 1: Release from Boiler Room #3 Roof	Scenario 2: Release from Boiler Room #4 Roof
<i>FAC2</i>	0.51	0.53
<i>NMSE</i>	3.27	1.31
<i>FB</i>	−0.24	0.12

The acceptance criteria defined in Section 6.1 ($FAC2 > 0.5$, $NMSE < 4$, $|FB| < 0.3$). This successful validation confirms the practical reliability of the CFD methodology for simulating pollutant dispersion in full-scale, complex industrial settings.

6.3. Synthesis of Model Performance and Selection Guidelines

Building upon the quantitative validation results presented in Section 6.2, this section synthesizes the performance of the RNG $k-\epsilon$ and LES models across the multi-scale framework and translates the findings into clear, actionable guidelines for engineering practice.

6.3.1. Consolidated Model Performance and Trade-Offs

The validation across three distinct tiers—isolated building, building array, and full-scale industrial site—provides a comprehensive performance profile for each turbulence closure scheme.

The RNG $k-\epsilon$ model demonstrated consistent robustness and computational efficiency. It met all statistical acceptance criteria ($FAC2 > 0.5$, $NMSE < 4$, $|FB| < 0.3$) across every case, proving its reliability for predicting overall flow patterns and far-field dispersion in scenarios ranging from canonical to real-world complexity. Its principal advantage lies in its computational practicality, being approximately 20–30 times faster than LES in comparable setups, making it feasible for large-domain simulations and multi-scenario analyses.

However, the validation systematically quantified its key limitation: the underestimation of peak turbulence in critical separation zones (e.g., roof shear layer, near-wake core), leading to an over-prediction of the recirculation zone size and near-field concentrations. This is an inherent constraint of its isotropic eddy-viscosity assumption when modeling strongly anisotropic, separated flows.

Conversely, the LES model delivered superior accuracy in resolving near-field physics. It excelled in capturing the high-gradient turbulence and transient structures in separation regions, yielding predictions of velocity recovery and concentration decay that were in markedly better agreement with high-fidelity experimental data. This high-fidelity capability comes at the aforementioned substantial computational cost.

6.3.2. Application-Driven Model Selection Guidelines

The choice between models is therefore not a question of overall superiority but of selecting the appropriate tool based on the specific objective and required fidelity of the analysis. The following guidelines (Table 9) are derived directly from the validated performance trade-offs:

Table 9. Model selection guidelines based on analysis priority and fidelity requirement.

Analysis Objective & Priority	Recommended Model	Primary Justification
System-level, Far-field Assessment	RNG $k-\epsilon$	Provides the optimal balance of accuracy and computational efficiency for simulating large domains and ensemble meteorological conditions, where capturing long-range transport is key.
- Plant-wide environmental impact (EIA) - Long-range emergency planning - Urban-scale pollutant mapping		
Component-level, Near-field Analysis		
- Rooftop/acute exposure risk assessment - Ventilation system or air intake design - Detailed study of flow separation/reattachment	LES	Accuracy is paramount for predicting high-concentration gradients and complex turbulence dynamics that dictate local safety and design performance.

6.3.3. Implications for the Validated Framework

The successful validation of the RNG $k-\epsilon$ model across all scales, culminating in its reliable performance at the full-scale industrial site, provides high confidence in its use for engineering applications where regulatory concern often focuses on far-field impact. The multi-scale framework itself is validated as an effective methodology for progressively building this confidence, from fundamental research to industrial application. This structured approach offers a template for developing and benchmarking simulation tools for other complex environmental flow problems.

7. Discussion

This study has developed and demonstrated a robust multi-scale validation framework for CFD simulations of building-induced dispersion. While Section 6 provided a comprehensive, quantitative assessment of model performance and clear selection guidelines, the following discussion interprets these outcomes within a broader scientific and practical context, elucidating the study's wider implications.

7.1. Advancing Validation Methodologies for Industrial CFD

The core methodological contribution of this work lies in its structured, tiered validation approach. Moving beyond single-case or single-fidelity validation, this framework provides a blueprint for establishing credibility in complex application domains where direct experimentation is challenging, such as nuclear safety. By systematically progressing from controlled, high-fidelity benchmarks (wind tunnel) to uncontrolled, real-world complexity (field site), it builds a chain of evidence that is more resilient to criticism than isolated validations. This approach directly addresses a key barrier to the adoption of high-fidelity simulations in regulatory contexts: the need for transparent, traceable, and multi-faceted proof of predictive capability. Future studies on other complex geometries (e.g., chemical plants, urban data centers) can adopt and adapt this framework, enhancing the overall rigor of industrial environmental assessments.

7.2. The Proxy Site Strategy and Its Role in Nuclear Safety

The use of an operational thermal power plant as a proxy for a nuclear facility proved to be a pivotal strategy. It circumvented the fundamental limitation of being unable to conduct tracer tests at nuclear sites, thereby enabling a crucial full-scale validation under realistic atmospheric conditions. This demonstrates that carefully selected proxy sites, sharing key geometric and aerodynamic attributes with critical infrastructure, can serve as invaluable open-air laboratories. This strategy can de-risk the safety certification of new facilities, particularly novel designs like small modular reactors (SMRs) or inland plants, by allowing for pre-operational model validation and scenario testing. It establishes a pragmatic pathway for applying advanced CFD where it is needed most but direct data is scarce.

7.3. Beyond Model Choice: Implications for Simulation Practice and Knowledge Gaps

The clear delineation between RNG $k-\epsilon$ and LES applications reinforces that “fitness for purpose” must guide CFD practice. However, it also highlights a persistent knowledge gap: the lack of equally robust, validated guidance for the emerging class of hybrid RANS/LES models. These models aim to bridge the efficiency-accuracy gap identified in this study. Our work provides the essential high-fidelity benchmark data against which such hybrid models should be tested. Furthermore, the documented limitations of RANS models in separating flows underscore that improving dispersion predictions may rely less on refining RANS constants and more on strategically deploying scale-resolving methods (like LES) in

critical regions, potentially through embedded or zonal approaches—a direction signposted by our findings for future numerical development.

7.4. From Validation to Integration: A Pathway for Urban Environmental Design

The validated capability to simulate flow and dispersion around complex clusters transcends the nuclear context. For urban planning, it signifies a shift from reliance on simplified empirical correlations to the potential for physics-based, site-specific virtual prototyping. Planners and architects could use such validated tools to assess not just pollutant hotspots but also pedestrian wind comfort, natural ventilation potential, and the dispersion of pathogens or heat. This moves environmental consideration from a post-design compliance check to an integral driver of sustainable urban form. The challenge ahead lies not in the simulation capability itself but in integrating these high-fidelity tools into streamlined, stakeholder-accessible workflows for decision support.

8. Conclusions

This research successfully conceived, implemented, and demonstrated a novel multi-scale validation framework, rigorously testing Computational Fluid Dynamics (CFD) models for pollutant dispersion from the laboratory scale to the industrial field scale. The study's primary outcomes are threefold, culminating in a significant advancement for engineering simulation practice.

First, it delivers a validated and ready-to-apply methodology. The framework itself—integrating wind tunnel benchmarks, standardized databases, and strategic full-scale proxy site testing—has been proven effective. It provides a structured, defensible process for establishing the credibility of CFD simulations in safety-critical and environmentally sensitive applications.

Second, it generates decisive, evidence-based guidance for practitioners. By rigorously quantifying the performance of two principal turbulence modeling approaches across multiple scales, the study moves beyond general advice to provide clear, context-specific recommendations. Engineers are now equipped with a justified rationale for selecting between computationally efficient RANS models for system-level assessments and high-fidelity LES for detailed, component-level analyses.

Third, it bridges a critical gap between high-fidelity research and industrial application. By validating models against real-world, complex industrial geometry, the work translates advanced CFD from a research tool into a reliable asset for practical engineering challenges, particularly in the field of nuclear facility safety and environmental impact assessment.

While this study provides a robust foundation, its boundaries point toward valuable future work. The present validation was conducted under neutrally stratified atmospheric conditions, neglecting thermal buoyancy effects which can dominate dispersion from major heat sources like cooling towers. Subsequent research should incorporate these effects and explore a wider range of atmospheric stabilities. Furthermore, the validated trade-off between RNG $k-\epsilon$ and LES underscores the need to develop and benchmark advanced hybrid RANS/LES models that could offer a superior compromise for specific scenarios. Finally, extending the demonstrated multi-scale framework to encompass more complex urban morphologies and diverse pollutant source types would significantly enhance its generality and utility for broader environmental planning.

In essence, this work provides more than a set of simulation results; it offers a validated pathway and a trusted toolkit. It empowers engineers, informs regulators, and contributes to the foundational knowledge required to design safer industrial facilities and more resilient urban environments, using simulation not just as a design tool but as a cornerstone of confident environmental stewardship. The established framework and clear

findings both resolve immediate practical questions and chart a clear course for ongoing methodological refinement.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/pr13124076/s1>, Video S1: Multi-Scale_CFD_Validation_end_pptx_output.

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