

Review

Synergising Physical Measurements, CFD Simulations, and Human Perception for Enhanced Indoor Air Quality: A Tripartite Review

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Abstract

Indoor air quality (IAQ) research remains divided across three separate streams: sensor-based monitoring, CFD simulation, and occupant-centered evaluation. This separation limits how readily technical measurements translate into actionable building guidance. To assess this divide, a systematic review and critical synthesis of 192 peer-reviewed studies was conducted, with each study categorized by which domain or domains it addressed. This categorization shows that fewer than 8% integrate all three—a figure derived directly from the classification rather than asserted independently of it. Accuracy itself proves uneven: under specific operational and environmental conditions reported in the literature, low-cost particulate sensors have been found to underestimate PM_{2.5} by as much as 50%, and wall-mounted placements often misrepresent breathing-zone exposure. These limitations carry into simulation, where the k - ω SST model persists as the practical standard despite Large Eddy Simulation's superior accuracy at two orders of magnitude greater computational cost. Building these findings, the review proposes a Tripartite IAQ Assessment Framework (TIAF) synchronizing sensor protocols, simulation outputs, and occupant surveys, addressing a regulatory tendency to privilege instrument metrics over lived experience. Implications extend to IAQ-responsive digital twins and post-pandemic governance, resolving the “stuffy-but-clean” paradox through validated, cross-domain integration.

Keywords: indoor air quality (IAQ); Tripartite IAQ Assessment Framework (TIAF); CFD simulation; low-cost sensors (LCS); occupant perception; thermal comfort; environmental governance



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1. Introduction

Indoor air quality (IAQ) is a major determinant of public health, cognitive performance, and sustainability of buildings. People in industrialized countries spend 85 to 90% of their time indoors, making indoor environments the primary source of exposure to airborne pollutants [1,2]. The WHO recognized indoor air pollution as a major global health threat in its 2021 Air Quality Guidelines (AQGs), which introduced substantially stricter limits for PM_{2.5}, NO₂, ozone, SO₂, and CO based on evidence that health effects occur below previous thresholds and that some pollutants have no safe exposure level [1,2]. Consequently, many indoor spaces that met earlier standards no longer comply with current recommendations [3]. However, efforts to address IAQ remain fragmented across

disciplines, limiting the translation of technical knowledge into meaningful reductions in exposure.

Urbanization, increasingly airtight buildings, and renewed attention to ventilation after COVID-19 have elevated IAQ to a central concern in sustainable design and public health policy [4,5]. The pandemic intensified research on airborne transmission and exposed limitations in existing ventilation and filtration strategies [4]. Despite this urgency, IAQ research remains divided among three independent domains: physical monitoring, CFD simulation, and occupant-centered assessment. This separation prevents the integrated understanding needed to advance IAQ management.

Advances in microelectronics and the Internet of Things (IoT) have transformed IAQ monitoring through affordable electrochemical and optical sensors. Wireless networks now provide continuous measurements of CO₂, particulate matter, VOCs, and formaldehyde with spatial and temporal coverage beyond traditional instruments [6,7]. Yasin et al. [2] demonstrated that low-cost IoT architectures can generate actionable IAQ data when supported by rigorous calibration, while Wang et al. [8] showed that year-long monitoring across multiple building types revealed seasonal and spatial variability that single-point measurements did not detect. Nevertheless, sensor accuracy remains limited by sensitivity, selectivity, cross-sensitivity, signal drift, and inconsistent calibration procedures [7,9]. Despite these challenges, integrating IoT platforms with cloud computing and machine learning has improved real-time pollutant classification, health-risk assessment, and adaptive ventilation control [10].

Machine learning models, particularly LSTM and GRU networks, outperform traditional methods in short-term prediction of CO₂ and PM_{2.5} concentrations. Taheri and Razban [11] reported that an LSTM-based demand-controlled ventilation strategy reduced HVAC energy use by up to 51% while maintaining acceptable IAQ. However, monitoring alone remains spatially discrete and retrospective. Although it quantifies pollutant concentrations, it cannot explain airflow patterns, pollutant transport pathways, or dispersion mechanisms, highlighting the need for numerical simulation.

CFD has become the leading method for analyzing indoor airflow, thermal stratification, and contaminant transport. By solving the Navier–Stokes equations with turbulence and particle-transport models, CFD predicts three-dimensional velocity, temperature, and concentration fields in complex indoor environments [12–15]. Obeidat et al. [12] identified Ansys Fluent 2023 R1 as the most widely used CFD platform due to its robust solver, extensive turbulence models, Discrete Phase Model (DPM), and support for user-defined functions. Model accuracy depends strongly on turbulence closure schemes. RANS approaches, especially Realizable $k-\epsilon$ and SST $k-\omega$ models, remain popular because they balance computational efficiency and predictive accuracy. Motamedi et al. [13] used the Realisable $k-\epsilon$ model and DPM to simulate the transport of SARS-CoV-2 droplets, showing that displacement ventilation reduced exposure to the breathing zone more effectively than mixing ventilation.

Higher-fidelity approaches such as LES and DES improve the representation of near-wall flows and turbulent anisotropy, although at a higher computational cost [14]. Askari et al. [15] demonstrated that furniture layout significantly affects pollutant removal efficiency, while Ozbakis and Erzincanli [16] reported an 8% improvement in contaminant capture using an optimized airflow-control valve. Emerging integration of CFD with BIM and digital twins offers new opportunities for continuous IAQ optimization, although computational demands still limit routine implementation.

Despite advances in monitoring and simulation, occupants determine whether indoor environments are acceptable. Buildings that meet regulatory limits can still be perceived as uncomfortable or unhealthy, affecting health, productivity, and behavior [17]. Consequently,

questionnaires, psychometric tools, and post-occupation evaluations (POEs) have become important methods for assessing the occupant experience. A review of 234 POE studies by Lolli et al. [17] found that IAQ and thermal comfort were the parameters most frequently evaluated and that subjective assessments often diverged from measured performance.

Occupant perception is shaped by sensory, cognitive, and emotional factors that cannot be fully represented by pollutant concentrations. Frontczak et al. [18] found that perceived freshness, odor intensity, and thermal comfort often predict IAQ satisfaction better than objective measurements. Similarly, studies by Young Ki Kim et al. [19] and Lolli et al. [17] reported cases of dissatisfaction under compliant conditions and satisfaction despite marginal exceedance of thresholds. These findings challenge the assumption that regulatory compliance guarantees occupant satisfaction.

Behavioral and social factors further complicate IAQ management. Hattori et al. [20] combined CO₂ monitoring with surveys in Japanese homes and found that occupants frequently underestimated poor ventilation despite elevated CO₂ levels. Parkinson et al. [21] analyzed data from more than 600 office buildings and identified poor air quality and inadequate ventilation as persistent complaints associated with reduced productivity and increased absenteeism. Novel approaches such as ecological momentary assessment (EMA) and experience sampling methods (ESM) provide richer insight into these subjective responses. Fissore et al. [22] concluded that relationships between objective IAQ metrics and perceived comfort remain weak, inconsistent, and context dependent.

A critical review of the literature reveals persistent separation among monitoring, CFD modeling, and occupant-centered assessment. Monitoring quantifies concentrations but rarely accounts for airflow mechanisms or occupant perceptions. CFD studies often lack validation against co-located sensor data and seldom include occupant feedback. Conversely, subjective investigations commonly omit concurrent physical measurements and simulations, preventing rigorous analysis of relationships among environmental conditions, predicted exposures, and human experience [23,24].

This fragmentation represents a major epistemological limitation. Without objective measurements, perceived poor air quality cannot be distinguished from psychosocial influences. Without CFD, spatial exposure patterns and source–receptor relationships remain unclear. Without an assessment of the occupant, technically optimal solutions may be rejected or discarded, reducing their effectiveness [21]. Therefore, the key research gap is not a lack of knowledge within individual domains but the absence of integrated frameworks that simultaneously combine measurement, simulation, and human-centered evaluation.

This review addresses this gap through a systematic and critical synthesis of contemporary IAQ research, complemented by foundational studies where essential, across three interconnected pillars: physical measurement, Ansys Fluent-based CFD simulation and occupancy-centered assessment.

2. Materials and Methods

2.1. Research Design and Systematic Mapping

This review critically integrates three IAQ research domains: physical monitoring, numerical modeling, and occupant-centered assessment. It identifies links and gaps between these approaches, addresses inconsistencies in performance evaluation, and highlights the need for multidisciplinary frameworks that connect measured and simulated conditions with occupant comfort and well-being.

2.2. Search Strategy, Timeframe, and Bibliometric Identification

A systematic review was conducted on Scopus, Web of Science and Google Scholar, covering January 2004 to December 2025. The literature from 2020 to 2025 formed the

core evidence base, while older studies were retained when essential for mathematical foundations or to track the evolution of IoT monitoring, advanced CFD methods, and post-pandemic ventilation research. The search strategies prioritized high-impact peer-reviewed journals and conference proceedings to capture current technological and social developments.

- Pillar 1 (Physical): (“Indoor Air Quality” OR “IAQ”) AND (“Low-cost sensors” OR “IoT” OR “Real-time monitoring”).
- Pillar 2 (Numerical): (“Ansys Fluent” OR “CFD”) AND (“Turbulence Modelling” OR “Contaminant Transport” OR “Validation”).
- Pillar 3 (Human): (“Occupant Perception” OR “Subjective Assessment” OR “Knowledge-Action Gap” OR “Acceptability”).

2.3. Systematic Screening and Study Selection Process

A final set of 192 studies was selected through a multi-stage screening process. Title and abstract reviews exclude irrelevant studies, non-built-environment research, and work lacking empirical or numerical rigor. Full-text assessment then verified methodological relevance to the review scope, while consensus-based decisions resolved uncertainties and reduced selection bias.

2.4. Inclusion, Exclusion, and Quality Assessment Criteria

Scholarly quality was maintained through a dual layer framework that combined explicit eligibility thresholds with a qualitative scoring matrix.

2.4.1. Inclusion and Exclusion Protocols

Inclusion: studies that integrate at least two of the three research pillars; research using verified numerical solvers (e.g., Ansys Fluent) for enclosed, occupied indoor environments; papers that address metrological reliability, calibration or field-deployment uncertainties of low-cost sensors; and studies that evaluate human factors, occupant satisfaction surveys, or behavioral feedback loops in IAQ governance.

Exclusion: papers on outdoor atmospheric pollution or regional macro-meteorology alone; studies using obsolete, unvalidated, or generic CFD codes; and non-peer-reviewed gray literature, commercial brochures, or unsubstantiated white papers.

2.4.2. Quality Assessment Criteria

Every full-text article was scored against four academic benchmarks:

- **Methodological Transparency:** explicit declaration of experimental boundary conditions, sensor calibrations, or mathematical formulations.
- **Validation Rigor:** formal validation of numerical models against experimental measurements or established benchmark data.
- **Metrological Integrity:** account for spatial representativeness, sensor drift mitigation, or baseline error in physical data acquisition.
- **Statistical Validity:** validated statistical structures, sufficient sample sizes, or standardized protocols (e.g., post-occupancy evaluation) in human-centric surveys.

Studies that met fewer than three quality criteria were excluded to avoid low-reliability conclusions. This process revealed a recurring limitation in IAQ research: poor spatial representativeness caused by differences between wall-mounted measurements and actual breathing-zone conditions. The gap highlights the need for CFD modeling to improve exposure assessment and environmental optimization.

2.5. Quality Assessment and Epistemological Triangulation

To address the fragmentation identified in the IAQ research, this review applies epistemological triangulation by integrating physical measurements, numerical simulations, and occupant feedback. This approach supports the proposed Tripartite IAQ Assessment Framework (TIAF), ensuring consistency between empirical evidence and theoretical interpretation while supporting sustainable building design. The study framework is presented in Figure 1.

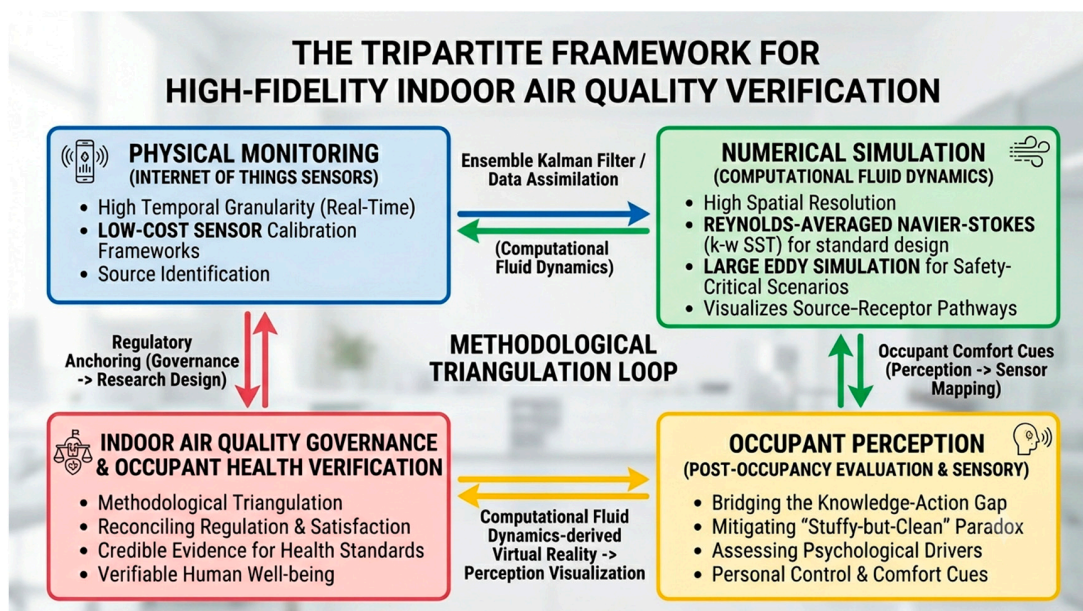


Figure 1. The tripartite approach to high-fidelity indoor air quality verification.

3. Results

3.1. Direction 1: Real-World Physical Measurements

3.1.1. Monitoring of Key Physical and Chemical Parameters

Physical monitoring provides an empirical basis for both CFD modeling and occupant-centered IAQ assessment. Although low-cost electrochemical and optical sensors have improved monitoring coverage and resolution, concerns about measurement accuracy remain. Therefore, physical data must meet strict quality requirements before being used as CFD boundary conditions.

Table 1 highlights the mismatch between ventilation indicators and source-related pollutants. Measurement of PM_{2.5} and VOCs alongside CO₂ shows that carbon dioxide alone cannot represent overall IAQ; acceptable ventilation rates do not necessarily ensure low exposure to pollutants. Consequently, IAQ assessment requires multi-parameter monitoring, supported by CFD, to capture spatial variations that fixed sensors cannot detect.

Table 1. Comparative effectiveness of primary IAQ pollutants as monitoring proxies.

Pollutant	Primary Role in IAQ Assessment	Effectiveness as an Indicator	Critical Limitations and Technical Gaps	Citations
CO ₂ (Carbon Dioxide)	Ventilation and Occupancy Proxy	Highly effective in inferring the adequacy of ventilation and human-related metabolic emissions.	Often, it does not detect non-occupancy pollutants (VOCs/PM). Elevated levels (>1000 ppm) may occur even when other metrics are acceptable.	[25–29]

Table 1. Cont.

Pollutant	Primary Role in IAQ Assessment	Effectiveness as an Indicator	Critical Limitations and Technical Gaps	Citations
PM (Particulate Matter)	Direct Health Exposure Metric	Most effective in identifying physical hazards from indoor sources (cooking, combustion, movement).	Highly dependent on localized activity; may exceed guidelines in offices/classrooms even with adequate CO ₂ ventilation.	[25,28,30–33]
Volatile Organic Compounds (VOCs)	Material and Chemical Source Indicator	Essential for detecting emissions from building materials, cleaning products, and furniture.	Unrelated to CO ₂ peaks. Spikes can occur during cleaning or social events without the corresponding changes in CO ₂ .	[26,29–31,34]

Comparison of CO₂, PM_{2.5}, and VOCs shows that selecting a monitoring proxy is also a regulatory and public health decision. Because it is inexpensive, stable, and easy to interpret, CO₂ has become the primary indicator of ventilation adequacy in frameworks such as ASHRAE Standard 62.1 [35] and EN 16798-1 [36]. However, evidence indicates that CO₂ often correlates poorly with particulate and chemical pollutants, allowing buildings to meet ventilation requirements while exposing occupants to harmful emissions. This limitation has become more significant following the WHO 2021 guidelines, as many buildings compliant with earlier CO₂-based standards fail the current PM_{2.5} recommendations [3]. These findings support the transition from single proxy to multi-pollutant monitoring despite cost and implementation barriers.

Table 2 illustrates the uncertainty of low-cost sensors. PM_{2.5} sensors frequently underestimate concentrations, while VOC sensors are affected by cross-sensitivity and signal drift. Although suitable for identifying temporal trends, these limitations reduce their regulatory reliability. Therefore, sensor data used in Ansys Fluent simulations require rigorous calibration and error correction to ensure that CFD predictions accurately represent indoor conditions.

Table 2. Metrological characteristics and performance limitations of low-cost IAQ sensors.

Pollutant	Typical Performance Pattern	Citations
CO ₂ (NDIR Sensors)	Often within ~10–15% of reference; small drift; robust to normal T/RH ranges but some dependence	[29,37–40]
PM _{2.5}	Good trend detection; often underreports mass; (up to ~50%); size resolution (PM _{1/2.5/10}) unreliable	[33,38–42]
TVOC	Detects events and trends; high cross-sensitivity, poor quantitative agreement; limited calibration range	[29,37,38,40,43,44]

Combining calibrated CO₂, PM_{2.5} and VOC detection provides a more effective representation of total indoor air quality than any pollutant alone.

3.1.2. The IoT Revolution: Reference Grade vs. Low-Cost Sensors

- **Metrological Reliability: Reference vs. LCS.** Reference and research-grade instruments offer high accuracy, low noise, and documented uncertainty, serving as ground truth in all LCS calibration and validation work [45–49]. Indoor and chamber evaluations show that LCS typically underestimates or overestimates PM by up to ~50%, give acceptable CO₂ ($\pm 15\%$), and often poor VOC/gas accuracy without correction [7,38,47,49,50]. Reviews find only moderate correlations against comparison instruments—sufficient for qualitative trends and non-critical building management, but not a replacement for reference instruments [49,51].
- **Calibration Challenges and Signal Drift.** IAQ data is strongly dependent on IAQ calibration context. Laboratory calibrations are unreliable in the field, making on-site reference devices a fundamental recommendation for data integrity [46,49,51–53]. Temperature, relative humidity, and type of aerosol complicate matters further; incorporating these into compensation models improves accuracy but often reduces stability under varying conditions [46–49,54]. Drift and obsolescence pose long-term challenges: longitudinal studies consistently report sensor drift and defective modules over time, implying the need for periodic or continuous recalibration, particularly for gaseous pollutants and certain CO₂ sensors [45,49,52,53,55]. Even machine learning introduces “concept or model drift”; a decline in accuracy over time partially addressed by batch updates that extend validity by a few weeks without resolving the underlying problem [55].

A fundamental contradiction in the machine learning (ML)-correction literature remains unresolved. Reference-grade instruments remain essential for calibrating and validating low-cost sensors (LCS) [45–49]. Although ML approaches can improve the accuracy of LCS to near-reference levels in controlled environments, with $R^2 > 0.90$ for PM_{2.5} and CO₂ [48,52,53], these gains often decrease in real buildings due to environmental variability, sensor aging, and changing aerosol composition [55]. Studies show that, when reference measurements are limited, simple linear models may generalize better than complex algorithms [49]. Consequently, the main challenge is not algorithm development but robust long-term field validation, including periodic reference measurements, drift monitoring, and transparent reporting of accuracy degradation. Until such practices become standard, claims of near-reference LCS performance should be treated cautiously, particularly when sensor data are used as boundary conditions for high-resolution CFD.

- **Advanced Error Correction: Machine Learning Frameworks.** ML is widely used to improve the accuracy of low-cost sensor networks. Methods ranging from k-Nearest Neighbors and Random Forest to deep neural networks can enhance sensor performance [53,56,57]. However, simpler linear models often provide better robustness and cross-environment generalization, particularly for the monitoring of particles [46,49,54,58]. Beyond calibration, ML helps compensate for non-linear sensor responses, cross-sensitivities, and temperature-related drift [48,52,53,55,59]. It also enables virtual sensing and supports large-scale network calibration using a limited number of reference instruments [48,52,53,57,58]. By converting noisy measurements into more reliable data streams, ML facilitates the integration of physical monitoring with CFD-based numerical simulation.

3.1.3. Spatial Granularity and Sensor Placement Strategies

Atmospheric sensors are typically sparse and fixed, while exposure occurs in localized breathing zones with uneven pollutant distributions. Recent studies combine measurements, CFD, and optimization to examine how the location of the source affects the dispersion of CO₂, aerosols, and gases.

- Sensors in the breathing zone vs. sensors mounted on the wall/ceiling. Sensor placement strongly influences IAQ assessment but remains understudied. Breathing-zone measurements often show higher exposure to CO₂ and PM than wall or ceiling sensors [59,60]. Although nearby CO₂ sensors provide moderate agreement with personal exposure ($R^2 \approx 0.4$), PM measurements are highly dependent on air-flow, with wall-mounted or exhaust-located sensors achieving much better accuracy ($R^2 \approx 0.8\text{--}0.9$) [60,61].

Figure 2 hits a critical point: proxy reliability depends on pollutant behavior, so conventional placement habits are not always optimal. Sensor placement should follow the location of the occupant or be guided by smarter positions.

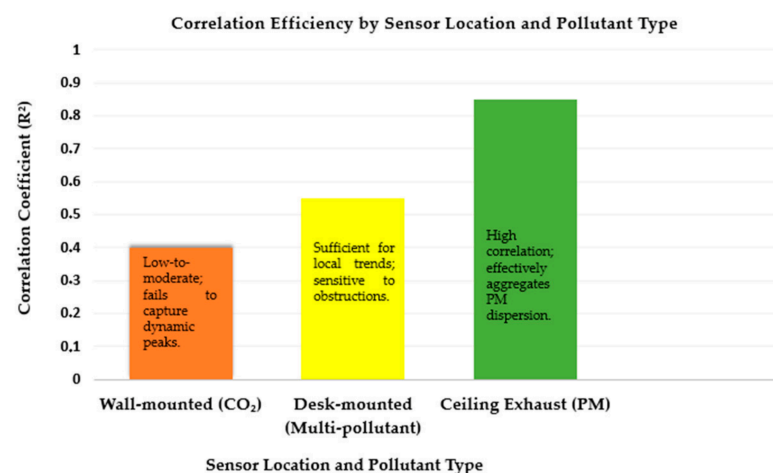


Figure 2. Comparison of correlation efficiency (R^2) and analytical performance in various locations of sensors and types of pollutants.

The spatial distribution within a room also affects the accuracy of monitoring. In well-mixed office spaces, the variability of CO₂ and TVOC is often low, allowing a single high-resolution return-air sensor to perform, as well as multiple low-cost sensors [60,62]. In more complex environments, such as classrooms, sensor placement and ventilation strategy can influence readings by more than 100 ppm CO₂ [63]. Because temperature and humidity show greater spatial variation than CO₂ [23], optimized placement is often required. As a result, CFD and optimization methods are increasingly being used to design sensor layouts that improve coverage and compliance with standards such as LEED [64].

Model-based analyses reveal the limitations of random sensor placement. CFD-adjoint studies show that about 25% of potential locations provide CFD-adjoint information, while most perform far worse than optimal positions [65]. Sensor effectiveness depends on both placement and sensitivity, as improved detection limits can expand monitoring coverage [65]. To optimize performance and cost, wireless sensor networks increasingly use statistical methods to identify the most representative sensor locations [66]. These findings highlight the essential role of CFD in designing effective IAQ monitoring systems within the TIAF.

Figure 3 highlights the weakness of conventional sensor placement: most locations provide lower monitoring coverage than optimal sites [65]. This demonstrates the need for CFD-based analysis to identify poorly monitored zones and determine sensor effectiveness before deployment [65,66].

Understanding IAQ requires tracking spatial and temporal variations, not only mean concentration. Studies show strong pollutant gradients within buildings, with PM_{2.5} levels varying significantly by source location and distance [67,68]. In multi-story, educational,

and open-plan buildings, pollutant distribution is further influenced by room function, height, and occupancy, making dense sensor networks and spatial modeling necessary for accurate assessment [69,70].

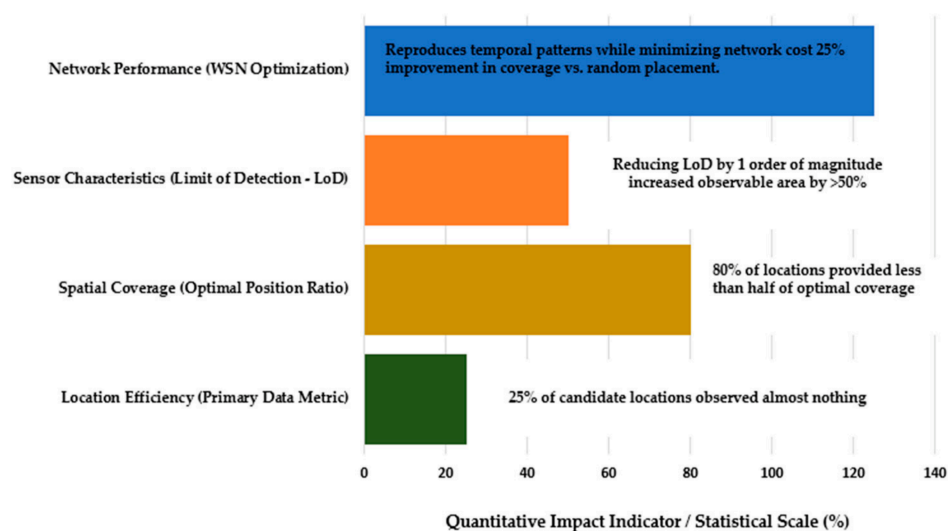


Figure 3. Quantitative metrics for explicit sensor placement optimization.

Table 3 shows that indoor environments are spatially heterogeneous. Variations related to floor level and room function often make single-point measurements unreliable, highlighting the need for sensor placement strategies that reflect building layout and occupancy patterns rather than generic interpolation methods.

Table 3. Empirical findings on spatial heterogeneity in indoor environments.

Monitoring Context	Key Quantitative/Technical Finding	Citations
Residential (PM _{2.5})	Strong intra-apartment gradients and time lags; source strength/distance explains 79% of variation.	[67]
Microenvironments	Sensor placement, occupancy, and activity log are crucial for source interpretation.	[68]
Educational Buildings	The accumulation of heat and pollutants is strongly dependent on the use of the room, elevation and floor level.	[69]
Large Offices	Grouping locations with similar characteristics improves estimation at unsensed points (better than IDW/Kriging).	[70]

Breathing-zone measurements provide the most accurate estimate of occupant exposure, but practical constraints often require fixed sensors. Locations near occupants, such as desks, adjacent walls, or ceiling vents, can estimate CO₂ and PM levels when occupancy patterns are considered. In well-ventilated spaces, return-duct CO₂ sensors may adequately represent average conditions. However, pollutant sources, airflow patterns, building geometry, and vertical stratification can make randomly placed sensors unrepresentative of both local exposure and room-wide conditions. Integrating CFD, multipoint monitoring, and appropriate detection limits improves accuracy in complex environments.

Because sensor representativeness depends on three-dimensional airflow patterns, monitoring alone is insufficient. These findings support an integrated TIAF approach in which CFD informs sensor placement, data quality is continuously validated, and monitoring results are interpreted alongside occupant exposure assessments.

3.2. Direction 2: Numerical Simulations via Ansys Fluent

Recent reviews identify Ansys Fluent as the leading commercial CFD platform for indoor airflow, ventilation, and contaminant transport, combining robust modeling capabilities with practical implementation advantages [71,72]. Comparative studies show that Ansys Fluent, OpenFOAM, and STAR-CCM+ achieve similar accuracy, while differences in computational efficiency influence project costs and engineering effort [71]. Extensive validation against laboratory and field measurements has established Ansys Fluent as a reliable tool to predict IAQ-related metrics such as air change rates, air age, and airflow patterns [72]. Applications in complex environments, including indoor swimming pools, further demonstrate their value in evaluating ventilation strategies through a rapid comparison of multiple design options validated against experimental data [72].

3.2.1. Governing Equations and the CFD Framework

CFD has become a primary tool for analyzing indoor ventilation, thermal stratification, and pollutant transport. By solving conservation equations with turbulence, species transport, and particle-tracking models, it predicts airflow, temperature, and contaminant distributions at spatial resolutions unattainable through sensor networks. Although monitoring provides detailed temporal data, CFD provides comprehensive spatial information and depends on accurate boundary conditions derived from measurements. This section reviews the mathematical basis for pollutant transport in Ansys Fluent, turbulence-model selection, gaseous and particle dispersion, and boundary-condition strategies that determine model reliability and physical validity [72–77].

- **Navier–Stokes Framework for Indoor Airflows.** Most indoor CFD studies use Reynolds average Navier–Stokes (RANS) models to represent turbulent air flow [72,74]. In Ansys Fluent, airflow is predicted by solving mass and momentum conservation equations, while turbulence is commonly modeled using Standard, RNG, or Realizable k – ε formulations with wall functions for near-wall regions [73–76]. These approaches generate velocity and pressure fields that govern the transport of heat and pollutants in buildings ranging from offices and classrooms to green buildings [72,74,75,78–81]. By solving the Navier–Stokes equations with appropriate turbulence models, Fluent produces detailed three-dimensional distributions of airflow and pollutant concentrations driven by ventilation and thermal effects [76,79].
- **The Conservation of Mass Principle (Continuity Equation).** Ensures air mass entering the zone is conserved over time—a fundamental requirement for stable simulation [76].

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (1)$$

- **The Momentum Conservation Equation (Navier–Stokes).** Computes volumetric flow and pressure distributions from viscous effects, pressure differentials, and turbulent fluctuations [73,76].

$$\rho \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) = -\nabla p + \mu \nabla^2 u + f \quad (2)$$

- **Turbulent Viscosity Equation.** Under RANS, the eddy viscosity (μ_t) relates k and ε to the velocity distribution, estimating turbulent dispersion without solving every vortex [74,75].

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (3)$$

where

ρ : Air density (kg/m³);
 t : Time (s);
 ∇ : Del (gradient) operator;
 u : Velocity vector (m/s);
 μ : Absolute (Dynamic) Viscosity (kg/m·s);
 f : External body forces (e.g., gravity) (N/m³);
 μ_t : Turbulent viscosity (kg/m·s);
 C_μ : Experimental coefficient (standardly valued at 0.09 within the default k – ε framework);
 k : Turbulent kinetic energy (m²/s²);
 ε : Turbulent dissipation rate (m²/s³).

- Species Transport for Pollutants and Humidity. Beyond airflow and energy, Ansys Fluent 2025 R1 (and tools such as Airpak) typically computes chemical transport for IAQ, integrating one or more variables for CO₂, water vapor, radon, particulate matter (as a passive scalar), or other pollutants [75,76,79–82].
- The Governing Transport Equation. The convection–diffusion transport equation, solved for the mass fraction of each species with terms for emissions, decay, and reactions, where applicable [74,75,77,80].

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) = -\nabla \cdot J_i + S_i \quad (4)$$

where:

ρ : Density of the mixture (kg/m³);
 Y_i : Loca mass proportion of the chemical constituent;
 u : Flow velocity vector (m/s);
 J_i : Diffusion flux of the species (kg/m²·s);
 S_i : Source or sink term (representing emission, decay, or reactions) (kg/m³·s).

Table 4 confirms that IAQ monitoring is geometry dependent. Species-specific equations (UDF-defined inhalation sources or mass-fraction moisture transfer) let the framework account for local source/receiver boundaries often oversimplified in standard experiments [82–84].

Table 4. Specific IAQ applications of the species transport framework.

Application/Building Type	Pollutant/Scalar Studied	Citation
Classrooms	CO ₂ and aerosols.	[79]
Swimming Pools	Humidity (water vapor transport).	[74]
Green Buildings	Integrated pollutant species equations.	[77]
Transport Cabins	Water vapor diffusion.	[78]
Inhalation Studies	Inhalation of PM _{2.5} using passive scalars and UDF sources.	[82]

- Justification for Selecting Ansys Fluent for Indoor Simulations. Table 5 shows the preference for Ansys Fluent stems from its integrated ecosystem: advanced meshing plus robust turbulence and species libraries enable stable simulation of complex multi-zone environments with higher computational efficiency than other commercial CFD software (eg. Ansys 16.2) [71,80,83].

Table 5. Technical merits and rationale for selecting Ansys Fluent in IAQ research.

Selection Criterion	Technical Advantage and Impact	Citation
Market Leadership	The most widely used indoor CFD code recognized for exceptional heat transfer and pollutant dispersion modeling.	[71,72]
Industrial Robustness	Ideal for complex industrial simulations (e.g., poultry, enclosed environments) with a comprehensive physics library.	[73]
Pre-processing Efficiency	The Built-in Airpak technology provides automatic meshing, local refinement, and mesh-quality cheques.	[80]
Performance Benchmark	Demonstrated similar accuracy to STAR-CCM+ with slightly better performance in detailed indoor cases.	[83]
Versatile Geometry	Validated choice of complex rooms, swimming pools, cabins and multi-zone building geometries.	[71,80,82,83]

3.2.2. Turbulence Modeling: RANS vs. LES Effectiveness

Most comparative studies focus on large indoor spaces or urban-scale applications, but the underlying airflow mechanisms are like those in indoor ventilation. Across models, accuracy in predicting turbulence and mixing is balanced against computational cost.

Table 6 reflects the current preference for RANS models in building engineering, although this choice remains pragmatic. Blocken et al. [84] argued that advances in computing have reduced the cost gap between LES and RANS, while LES provides a better representation of separation, recirculation, and transient dispersion. This issue may be even more relevant indoors, where airflow is strongly influenced by buoyancy, human heat plumes, furniture, occupant posture, and near-wall concentration gradients. Consequently, RANS remains suitable for routine design, but its uncertainty in exposure assessment may be greater than acknowledged. More systematic LES–RANS comparisons are needed to quantify these limitations in indoor environments [84].

Table 6. Overall performance trends and benchmarking of turbulence models.

Turbulence Model	Accuracy and Capabilities	Limitations and Computational Requirements	Citation
LES	Provides the highest accuracy for mean velocities and pollutant fields; captures jet flapping and intermittent mixing.	High computational cost (80–100 times higher than RANS); requires resolving unsteady structures.	[85–91]
Standard $k-\epsilon$	Effective for large simple isothermal spaces; accuracy within the factor 0.5 to 2 of the experimental data.	Underpredicts wake turbulence; sensitive to the turbulent Schmidt number.	[88,90,92,93]
RNG $k-\epsilon$	Outperforms Standard $k-\epsilon$ in cross-ventilation cases and flow rate predictions.	Accuracy is lower than LES; struggles with detailed transient behavior in building-induced turbulence.	[84,89,94]
$k-\omega$ SST	Frequently the best RANS model for separated flows; 78% of predictions are within factor 2 of breathing-zone data.	Meets the quality criteria of the VDI (FAC2 $\approx$ 0.6–0.67) for the dispersion of pollutants around isolated buildings.	[86,91,93,94]

Table 7 summarizes the model-selection criteria by objective. For standard building-scale IAQ studies, RANS (particularly $k-\omega$ SST) offers a reliable and cost-effective prediction of mean concentrations of breathing zones. In accidents or situations that are critical to safety dominated by transient dynamics, the higher fidelity of LES is required [84,86,89].

Table 7. Strategic selection matrix for indoor pollutant dispersion models.

Study Scale/Nature	Recommended CFD Model	Key Rationale and Capabilities	Citation
Engineering-scale IAQ	RANS (RNG $k-\epsilon$ or especially $k-\omega$ SST)	Offers the best balance, much cheaper than LES. Reproduces mean flow and time-averaged pollutant fields.	[89,91,92]
Research/Safety-Critical	LES (or well-designed hybrid RANS-LES)	Preferably despite the cost for problems that need accurate near-source peaks, transient plumes, or detailed turbulence.	[84,89–91]

Among practical options, $k-\omega$ SST and RNG $k-\epsilon$ RANS models consistently deliver the best compromise, with $k-\omega$ SST generally emerging as the most reliable single choice for complex separated flows and heavy-gas or passive tracer dispersion, and standard $k-\epsilon$ remaining acceptable only for relatively simple, isothermal, well-mixed indoor spaces.

3.2.3. Pollutant Transport: Gas-Phase vs. Particle Dynamics

In Fluent-based IAQ studies, gas-phase pollutants are usually modeled with the Species Transport (or passive scalar) equation, while particulate matter (PM) is often modelled with the Discrete Phase Model (DPM) or Eulerian particle analogues. The choice of model affects how sources (breathing, materials) and wall interactions are implemented.

- Gas-Phase Pollutants: Species/Passive Scalar Models. The transport of indoor pollutants is simulated by considering gaseous pollutants and fine particles as constant or non-constant quantities. Table 8 summarizes the technical details of this application.

Table 8. Modeling strategies for gas-phase pollutants and particulates.

Modeling Approach	Technical Implementation and Methodology	Citation
Continuous Scalar	Gas pollutants or PM are solved using a convection–diffusion transport equation with emission terms.	[95–97]
Passive Scalar	PM _{2.5} modeled around thermal manikins; inhalation is represented by a constant sink at the breathing boundary.	[82]
Scalar Source Types	Includes various steady or pulse sources: diffusive, momentum, and body-surface types.	[82]
Tracer Gas Proxy	Use of species such as SF ₆ or N ₂ O as proxy for PM to optimize computational cost in urban/indoor studies.	[95,96,98]

Table 8 illustrates the flexibility of scalar representations: using tracer gases such as sulfur hexafluoride (SF₆) as particulate substitutes reduces computational load while maintaining precision in predicting inhalation risk and diffusion profiles.

- Numerical Strategies for the transport of PMs. Accurately resolving suspended-particle dynamics, especially for respiratory and worker-safety studies, requires a robust framework. The Eulerian-versus-Lagrangian choice depends on the detail needed at the particle–wall interface and available resources, as Table 9 summarizes.

Table 9. Modeling approaches for particulate matter in indoor environments.

Model Category	Methodology and Physical Interactions	Performance and Best Use Cases	Citation
Eulerian–Lagrangian (DPM)	Air flow solved as a continuous phase; particles tracked individually under drag, gravity, Brownian forces, and Saffman lift.	Excels for particle–wall interactions; accurate for complex geometries and near-source dispersion.	[99–103]
Species Transport (Eulerian)	Particles are treated as a continuous species phase.	Computationally cheaper but limited to concentration fields; adequate for simple flows.	[97,102,103]
Eulerian–Eulerian	Two-phase modeling with mechanistic interphase interaction.	Offers airflow accuracy like Lagrangian but provides a more detailed mechanistic interaction.	[104]

Table 9 justifies the use of DPM for an accurate assessment of individual-exposure: unlike simplified species-transport models, the Lagrangian approach captures Brownian motion and Saffman lift, essential for simulating deposition in complex geometries.

- Numerical Implementation of Human Breathing Dynamics. The accuracy of the simulation depends on realistically representing the human presence as both a source and a reservoir of pollutants. Modeling the breathing zone requires precise boundary conditions that capture the interaction between exhaled and ambient air flow, summarized in Table 10.

Table 10. Boundary conditions and modeling approaches for human respiration.

Breathing Mechanism	Numerical Implementation/Boundary Condition	Impact on IAQ Accuracy	Citation
Exhalation (Gas/Aerosol)	Mouth/nose boundaries with specified mass flow rates and species source terms.	Validated against in situ measurements for CO ₂ and aerosol dispersion.	[80]
Exhalation Jets	Time-dependent sinusoidal velocity profiles vs. steady velocity conditions.	Sinusoidal profiles provide realistic momentum for better jet penetration matching.	[98,105]
Inhalation (Deposition)	Injection of DPM into the nostrils combined with “trap” boundary conditions in the airway.	Enables precise prediction of deposition fractions within the respiratory tract.	[100]
General Exposure	Constant inhalation is modeled as a sink for scalar pollutants at the mouth.	Allows rapid intake of fraction computation without explicit particle tracking.	[82]

Table 10’s breathing boundary conditions link whole-room airflow to individual micro-scale exposure; time-varying sinusoidal models, rather than constant flow rates, capture the transient nature of pollutant diffusion.

- Modeling of Emission Sources and Surface Interactions. Beyond human-generated pollutants, IAQ is strongly shaped by localized sources and pollutant–surface interaction, modeled by approaches ranging from simple boundaries to UDFs for surface deposition, summarized in Table 11.

Table 11. Numerical configuration for emission sources and surface boundary conditions.

Source/Scenario Type	Numerical Implementation in Fluent	Technical Rationale and Application	Citation
Localized Emissions	UDF-based sources	Represents specific locations such as cooking zones, traffic lines, or sources near a manikin.	[82,95,106]
Urban/Traffic Proxy	Line-source boundaries	Used for tracer gas/PM proxies (e.g., SF ₆) at floor-level to mimic traffic emissions.	[95]
Wall Deposition	Drift-flux Eulerian models	Coupled via UDFs to implement semi-empirical models for size-dependent deposition on surfaces.	[107]
Kitchen IAQ	Scalar vapor source	Calibrated to measured fume concentrations to assess removal efficiency by range of hoods.	[108]

UDF-based source models (Table 11) provide an accurate representation of size-dependent pollutant transport and deposition, while line-source tracer gases efficiently simulate traffic-related infiltration without the computational cost of particle tracking.

In Fluent, scalar transport models are commonly used for gaseous pollutants and some fine particles, providing efficient estimates of room-scale concentrations and exposure. However, they cannot accurately capture particle–wall interactions. Lagrangian approaches such as the Discrete Phase Model (DPM) explicitly simulate particle motion, forces, and deposition, improving predictions of near-field exposure in complex geometries, albeit at higher computational cost.

By generating detailed three-dimensional distributions of airflow and contaminants, CFD reveals source-to-receptor pathways that cannot be captured through physical monitoring alone. Identify stagnation zones, ventilation short-circuits and spatial exposure inequalities, supporting ventilation designs that improve pollutant dilution and providing a robust basis for validation and exposure assessment.

3.3. Direction 3: The Integrated Approach (The Bridge)

3.3.1. Experimental Validation Protocols

Linking CFD simulations with physical measurements requires rigorous verification and validation, which are often not adequately addressed in the literature. Validation assesses agreement with measurements, while verification ensures that the governing equations are solved correctly. Distinguishing between these processes is essential for quantifying model uncertainty and determining the reliability of CFD predictions. The analysis of systematic discrepancies, commonly caused by simplified boundary conditions and limitations of the turbulence model, highlights current challenges in sensor–CFD integration. It also supports emerging approaches such as data assimilation and surrogate modeling, which use high-quality monitoring data to continuously improve simulation accuracy.

- Validation Framework and Statistical Reliability. A rigorous verification mechanism compared CFD results with the experimental measurements by aligning the sensor and probe coordinates and applying standardized statistical indices, as detailed in Table 12.

Table 12. Framework for CFD validation and statistical performance indicators.

Validation Phase	Methodology and Key Requirements	Statistical Indicators and Thresholds	Citation
Data Collection	Use of co-located sensors and CFD probes; measurement of velocity, temperature, and concentration.	Focus on sensor accuracy, range, and calibration to minimize gap errors.	[109–112]
Error Magnitude	RMSE (Root Mean Square Error)	Typical performance: 2.02 °C for temperature; 1.91–5.61 µg/m ³ for PM.	[113,114]
Normalized Error	MAPE/MRE (Mean Relative Error)	Acceptance criteria: 3–15% for temperature and velocity fields.	[110,111,114]
Trend Agreement	R ² (Coefficient of Determination)	Target performance: R ² > 0.90 to capture spatial/temporal variability.	[113,114]

Table 12 establishes a clear, replicable system for confirming the reliability of the model: exceeding these thresholds, particularly keeping relative discrepancies below 15%, demonstrates the simulation’s proficiency in tracking airflow and contaminant dispersion [110,113,114].

- Benchmarking Numerical Accuracy: Case Studies of High Concordance. Documented cases of strong CFD–sensor agreement across diverse indoor and urban settings provide a benchmark for acceptable error margins, summarized in Figure 4.

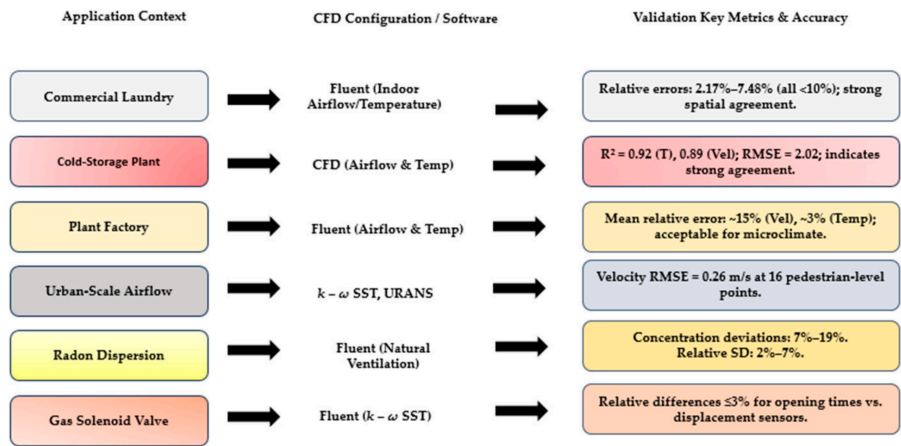


Figure 4. Summary of benchmarked CFD validation cases and performance metrics.

Figure 4 confirms the predictive accuracy of the selected models: relative errors in temperature and velocity consistently fall between 3% and 15% across scenarios (e.g., industrial laundry, factories), establishing a clear success threshold. High correlation coefficients ($R^2 > 0.90$) and low RMSE values reinforce the reliability of Ansys Fluent and the k – ω SST model for complex IAQ and pollutant-dispersion analysis [110,111,113,115–117].

- Methodological Recommendations and Quality Assurance in IAQ Modeling. To ensure robustness and avoid common errors, a set of best practices addressing validation integrity, sensor transparency, and sensitivity analysis was adopted, summarized in Table 13.

Table 13. Methodological challenges and recommended best practices for indoor CFD.

Potential Pitfall	Methodological Recommendation	Strategic Impact on Research Quality	Citation
Inconsistent Validation	Validate both physical parameters (Temp/Velocity) and pollutant species concentrations.	Strengthens IAQ claims by ensuring that both flow and chemistry are accurate.	[112]
Insufficient Sensor Data	Document complete sensor specifications, calibration status, and spatial alignment with CFD probes.	Improves reproducibility and limits uncertainty in experimental–numerical comparisons.	[112]
Sensitivity Uncertainty	Perform mandatory mesh- and model-sensitivity cheques before final validation.	Identifies the optimal configuration that yields the best agreement with the experimental data.	[111,112,115]
Single-Case Reliance	Validate across multiple operating conditions (e.g., varied fan speeds or configurations).	Tests the robustness of the model across different physical scenarios, not just a single point.	[113,116,118]

Table 13 provides a quality-assurance framework for CFD validation. Verifying pollutant dispersion against thermal fields, together with multi-condition validation and sensitivity analysis, reduces numerical uncertainty and strengthens conclusions on environmental safety and building performance [112,113,115]. Best practice requires multiple validation of metrics, clear acceptance criteria, and detailed reporting of sensor characteristics and boundary conditions to demonstrate robust CFD–measurement agreement.

3.3.2. Discrepancy Analysis: Why Do CFD and Reality Differ

Post-2020 studies show that CFD–reality differences often stem less from the analyst than from uncertain or oversimplified boundary conditions, unmodeled occupant behavior, and thermal effects that are difficult to accurately measure [119–123].

- Boundary Condition Uncertainty and Non-Isothermal Effects. CFD reliability for microclimate prediction depends strongly on boundary-condition accuracy; simplifying geometric detail and thermal loads often causes discrepancies, as Table 14 summarizes.

Table 14. Drivers of numerical discrepancies and boundary condition challenges.

Factor/Scenario	Impact on Simulation Accuracy	Key Findings and Recommendations	Citation
BC Simplification	Crucial accuracy and stability; uncertainties arise from the oversimplification of inlets, outlets, and heat sources.	The correct specification of sources is the main driver for model stability.	[72]
Natural Convection	The stand-alone CFD is limited by fixed BCs over extended periods.	Year-long accuracy requires dynamic coupling with Building Energy Simulation (BES).	[124]

Table 14. Cont.

Factor/Scenario	Impact on Simulation Accuracy	Key Findings and Recommendations	Citation
Inflow Jet Dynamics	Temperature and velocity errors near windows or openings.	Discrepancies are often related to uncertain thermal BCs and unsteady inflow jets.	[120]
Inlet Directionality	Significant deviations from experimental data if the direction is not imposed correctly.	The direction of the velocity is more critical than the BC temperature for details in ventilated rooms.	[122]
Thermal Stratification	Buoyancy-driven flows are sensitive to Reynolds numbers and near-wall behavior.	Challenges arise in natural-ventilation CFD due to solar gains and thermal mass effects.	[72,125]

Table 14 highlights the model sensitivity to thermal and directional inputs: non-isothermal natural ventilation requires precise matching of thermal conditions and near-wall behavior. Since velocity direction and unsteady airflow are the main sources of error, this research uses optimized boundary configurations to reduce variability and improve pollutant-diffusion reliability [120,122,125].

- Impact of Infiltration and Air Exchange Rates on IAQ Predictions. Air exchange through leaks and ventilation is crucial for indoor particulate levels and energy efficiency; oversimplifying leakage causes major thermal and pollution discrepancies, as Table 15 summarizes.

Table 15. Effects of infiltration and air exchange on indoor environment modeling.

Infiltration Driver	Numerical Modeling Challenge/Impact	Consequences of Model Simplification	Citation
Envelope Infiltration	Co-simulation of building energy and CFD requires dynamic outdoor/indoor temperature BCs.	Fixed BCs lead to “considerable differences” in energy and stratification predictions.	[124]
Wind and Buoyancy	Air-change rates (ACH) are highly dependent on wind pressure and thermal buoyancy.	Using static pressure coefficients instead of CFD-derived façade pressures propagate large uncertainties.	[126]
Occupant Behavior	The opening/closing of the windows/doors changes the effective levels of infiltration and outdoor particulate (OPL).	Mismatches between modeled and actual infiltration patterns cause major discrepancies in IAQ predictions.	[127]

Dynamic leakage rates (Table 15) reduce the transfer of uncertainty from external conditions to internal flow fields. Recognizing leakage as a product of wind, buoyancy, and occupant interaction (not a constant) improves the accuracy of PM prediction, which is crucial for assessing the environmental safety of certified facilities [124,126,127].

- Stochastic Occupant Behavior and Its Impact on Model Fidelity. IAQ prediction is related to the stochastic nature of the accuracy of occupant behavior; actions such as opening windows or changing position introduce variability that deviates from steady-state assumptions, as Table 16 summarizes.

Table 16. Influence of stochastic occupancy factors on IAQ and infection risk predictions.

Stochastic Factor	Mechanistic Influence on IAQ	Observed Numerical/Physical Impact	Citation
Occupancy Actions	Modification of infiltration rates (e.g., window opening).	Identified as the main determinant of indoor PM levels; steady models tend to mispredict concentrations.	[127]
Location and Distance	Alterations in local air patterns and separation distances.	Produced up to 220% variation in individual infection probabilities in classroom scenarios.	[128]
Human Posture	Variability in physical states (Seated, Standing, Mixed).	This leads to different CO ₂ stratification patterns and causes deviations from deterministic CFD cases.	[129]

Table 16 underscores the importance of incorporating randomness: up to 220% variation in infection risk shows that slight, often-overlooked changes in occupant position can produce quite different safety outcomes. A major challenge in CFD validation is the temporal mismatch between continuous sensor measurements and CFD outputs. Sensor data captures dynamic changes driven by occupancy, ventilation schedules, pollutant sources, and thermal cycles, whereas CFD often produces steady-state or scenario-specific results. Reliable comparison therefore requires clear definition of averaging periods, alignment between measurement intervals and CFD boundary conditions, and treatment of transient events. Existing validation frameworks provide limited guidance on this issue [72], and the TIAF addresses this gap through concurrent data collection and temporal alignment procedures.

- **Advanced Strategies for Mitigating Model–Data Discrepancies.** Advanced data integration and hybrid frameworks reduce boundary-condition uncertainty by using real-time sensor data to correct numerical fields and surrogate models to explore uncertainty, as Table 17 summarizes.

Table 17. Advanced frameworks for data assimilation and mitigation of uncertainty.

Strategy/Approach	Methodology and Technical Implementation	Impact on Model Accuracy	Citation
Data Assimilation (EnKF)	Use of Ensemble Kalman Filter (EnKF) frameworks to explicitly target BC uncertainty.	Significantly reduces simulation errors by using limited measurements to correct flow/temperature fields.	[121,123]
Sensor Optimization	Aligning the number of sensors with the number of uncertain BC variables.	Correlation between assimilation error and measurement noise; identifies optimal sensor placement.	[123]
ML Surrogates	Training machine learning models on CFD measurement datasets for fast predictions.	Offers fast emulation of complex flows in multiple configurations where full CFD is too expensive.	[130–134]
Sensitivity Analysis	Performing sensitivity cheques on inlet velocities, internal gains, and sources.	Identifies which uncertainties dominate the prediction error to focus on co-simulation efforts there.	[72,124]
Polynomial Chaos Expansion	Quantifying uncertainty in outdoor and thermal mass surface temperatures.	Clarifies which BCs must be characterized more accurately in experiments to reduce variance.	[120]

Table 17 marks a fundamental shift from static CFD verification to sensor-driven dynamic modeling. Surrogate ML models allow for a comprehensive exploration of space uncertainty, providing a solid basis for building-performance certification tools based on high-resolution environmental data [72,121,123,130].

3.4. Direction 4: Human Perception and Acceptance

3.4.1. Perceived Air Quality (PAQ) and Psychometric Tools

The ultimate measure of IAQ adequacy is occupant perception. A building may meet all regulatory limits, yet it can still be perceived as uncomfortable or unhealthy. Therefore, understanding air-quality perception and the gap between risk awareness and protective behavior is essential. Data alone rarely changes behavior; effective visualization can make environmental information more meaningful and actionable. Excluding this perceptual dimension leaves even advanced CFD analyses incomplete, as human experience cannot be fully captured by measurements or simulations. Integrating occupant assessment ensures that IAQ solutions are not only technically sound but also socially effective and acceptable.

- **Correlation Between Sensor Data and Perceived Air Quality (PAQ).** Human satisfaction is often shaped more by thermal sensation than by invisible pollutant concentrations, creating a gap between legal safety limits and occupant comfort, as Figure 5 summarizes.

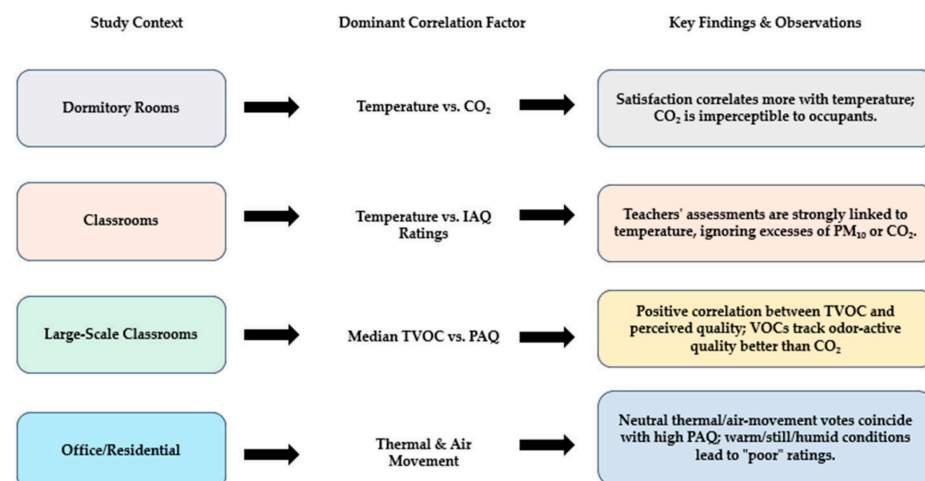


Figure 5. Relationships between measured environmental data and occupancy PAQ.

Figure 5 reveals a major perception gap: while the sensors reliably detect elevated CO₂ and PM₁₀, occupants, including trained professionals, often judge air quality through thermal comfort [135,136]. As a result, perceived air quality (PAQ) is a poor indicator of actual pollutant exposure. Building management systems focused only on comfort may, therefore, overlook harmful concentrations of CO₂ or TVOCs, making high-accuracy monitoring essential for managing invisible risks [137,138].

This limitation also challenges traditional comfort-based design. Occupants frequently use temperature and airflow as proxies for air quality, perceiving cool, moving air as fresh and warm, and stagnant air as polluted regardless of actual concentrations. Consequently, acceptable PMV/PPD values do not guarantee IAQ satisfaction, and standards such as ASHRAE 55 and ASHRAE 62.1 cannot fully predict occupant perception. These findings support the integrated assessment of thermal, chemical and perceptual factors to identify gaps between technical compliance and occupant experience.

- **Methodological Critique of Subjective IAQ Assessment Tools.** PAQ assessment remains dependent on subjective methods, with assessment of PAQ using structured questionnaires, often based on 7-point Likert scales, to evaluate perceived air quality [139]. Standardized frameworks such as the BUS and ASHRAE surveys allow comparison between buildings and have revealed performance gaps in offices and universities [22,140]. However, these approaches remain in post-occupancy indicators and are rarely linked to high-resolution CFD or sensor data. Although tools such as the Occupant Survey System (OSS) provide more detailed feedback [141], perceived IAQ is often assessed without direct correlation to local CO₂ or PM levels. Integrating standardized surveys with validated, high-resolution measurements is therefore essential to align occupant well-being with actual environmental safety.
- **Psychological and Physical Dissonance in Air Quality Perception.** Occupant perception reveals a key paradox: perceived air quality (PAQ) often differs from actual pollutant concentrations. Because occupants cannot directly detect pollutants such as CO₂, they commonly rely on temperature, airflow, and comfort as indicators of air quality [135,136,142]. Studies show that spaces can be considered acceptable despite elevated levels of pollutants, while feelings of “stuffiness” are more strongly associated with warm, humid and poorly ventilated conditions [137]. Perception is also influenced by odors and VOCs, which often affect satisfaction more than CO₂ concentrations [143]. In addition, psychological factors, such as information about ventilation quality or perceived environmental control, can increase satisfaction without physical changes to IAQ [144–146]. These findings highlight the limitations of subjective assessment and the need to complement it with high-resolution sensor measurements and CFD analysis, particularly in certification and other high-stakes applications [147].

Malodorous compounds can affect the perception of the occupant even at concentrations below the detection limits of the sensor, creating additional discrepancies between the measured and perceived air quality [143]. This effect is amplified when the occupants cannot control the ventilation. These findings support the treatment of PAQ as a distinct dimension of IAQ and emphasize the need for a concurrent assessment that combines perception, monitoring, and modeling.

3.4.2. The Knowledge–Action Gap and Behavioral Barriers

Improving IAQ involves not only technical solutions but also social and behavioral factors. COM-B studies show that actions related to IAQ are often shaped more by cultural norms, socioeconomic conditions, and privacy concerns than by sensor data alone [148,149]. There is a persistent knowledge–action gap, even though well-informed occupants may not adopt preventive measures due to habits, practical constraints, or limited control over their environment [150–152]. Although automated HVAC systems can improve energy efficiency and satisfaction, concerns about privacy and data security often hinder acceptance [153,154]. Users prefer transparent participatory control strategies to fully autonomous operation [155]. Therefore, effective IAQ interventions should combine high-resolution data with user-centered support that addresses social constraints and occupants’ need for environmental control [156–158].

3.4.3. Visualization as a Catalyst for Change

Public response to IAQ information depends strongly on personalization and visualization. Higher risk awareness is associated with greater willingness to adopt protective behaviors [159]. Air-quality alerts have been linked to measurable reductions in PM-related health impacts [160], while personalized exposure maps from wearable sensors signifi-

cantly increase avoidance of high-risk activities [161–163]. Because conventional indicators often fail to motivate lasting behavioral change, advanced visual tools such as ML-based exposure maps and health-impact visualizations are increasingly used to make risks more tangible [164,165].

CFD has also evolved from a ventilation-design tool to a communication platform. Integrated with virtual reality, CFD visualizations help non-specialists understand airflow patterns and design decisions [166–171]. However, evidence that such visualizations increase public support for stricter ventilation regulations remains limited. This challenge is reinforced by the “clean but humid” paradox, where occupant satisfaction is influenced more by thermal comfort and air movement than by invisible pollutants such as CO₂ [164,165,167,168]. As a result, multidisciplinary CFD models are increasingly being developed to support both IAQ assessment and safety planning [127].

3.5. Tripartite Contradictions in Current IAQ Evidence

A building may meet all regulatory IAQ thresholds yet still be perceived as inadequate, highlighting a persistent challenge in IAQ research. Although CO₂ remains the primary indicator of ventilation performance in ASHRAE 62.1 [35] and EN 16798-1 [36], it often correlates poorly with PM_{2.5} and VOC concentrations. As a result, buildings compliant with older CO₂-based standards frequently fail the stricter WHO particulate limits introduced in 2021 [3]. Monitoring uncertainties further complicate assessment: low-cost PM sensors can underestimate concentrations by up to 50%, and ML calibration models that perform well in laboratories often lose accuracy in real buildings [47,48,52]. Sensor placement adds another source of error, as wall-mounted CO₂ sensors show only moderate agreement with breathing-zone exposure, while many conventional locations provide limited pollutant coverage [65,113,114].

CFD does not eliminate these uncertainties because its boundary conditions depend on measurement data. Moreover, continuous sensor records and time-averaged CFD results often represent different physical states, meaning apparent discrepancies may reflect real environmental variability rather than modeling errors [75,113].

Occupant perception introduces an additional dimension that cannot be captured by measurements or simulations alone. People typically judge air quality through thermal sensation and airflow rather than pollutant concentrations [135–137]. Consequently, a chemically compliant space may be perceived as stuffy, while a thermally comfortable one may be considered fresh regardless of actual pollutant levels [141,151]. Psychological factors further influence responses, as perceived ventilation quality or environmental control can improve satisfaction without changing physical conditions [144–146].

These contradictions point to a deeper epistemological problem. Physical monitoring, CFD simulation, and occupant perception are validated using discipline-specific criteria. As a result, they provide three valid but disconnected perspectives on the same phenomenon. None is sufficient on their own. This fragmentation is reinforced by existing regulations. ASHRAE 62.1 relies on prescriptive ventilation rates, whereas EN 16798-1 uses performance categories [35,36,155]. Because these frameworks are not directly interoperable, assessments are often confined to a single regulatory perspective, limiting cross-validation. The problem is therefore not a lack of knowledge within any individual domain. Rather, it is the absence of a framework capable of integrating sensor measurements, CFD assumptions, and occupant feedback into a common evaluation process. This gap remains unresolved by current compliance-based and discipline-specific assessment approaches.

3.6. The Operational Architecture of the Tripartite Indoor Air Quality Assessment Framework (TIAF)

The previous sections examined physical monitoring, CFD simulation, and occupant perception separately. However, IAQ is a single interconnected system. The proposed Tripartite IAQ Assessment Framework (TIAF) integrates these three domains through a closed-loop process that links sensor data, CFD predictions, and occupant feedback.

In TIAF, continuous data from IoT sensor networks are used as dynamic CFD boundary conditions, replacing static assumptions with measured conditions. Although low-cost sensors remain affected by calibration and placement limitations [54,56,62,170,172], they provide the dense datasets needed for realistic simulations. Data-assimilation methods such as the Ensemble Kalman Filter (EnKF) continuously update CFD results using incoming measurements, improving predictions of airflow and temperature fields [123,125]. This approach keeps simulations aligned with real operating conditions and reduces the gap between idealized CFD and actual building performance [122,125]. The $k-\omega$ SST model is particularly suitable because of its proven accuracy for indoor airflow and near-field dispersion [88,93].

TIAF also connects CFD outputs with occupant experience. High spatial accuracy does not guarantee perceived comfort; spaces that meet IAQ criteria may still be reported as stuffy or drafty [141,144]. To address this, CFD-derived airflow and pollutant patterns are compared directly with post-occupancy evaluation (POE) results collected from the same locations [17]. This enables identification of areas where compliance and occupant satisfaction diverge are measured. Where detailed perception of transient airflow is important, LES may provide better representation than time-averaged RANS models [101,104,125]. Combining CFD and survey data further helps distinguish thermal discomfort from IAQ-related dissatisfaction [140,144].

Occupant feedback is then used to improve monitoring. Reports of discomfort in areas where sensors indicate acceptable conditions may reveal inadequate sensor placement rather than true compliance [62,63,66]. Studies show that such mismatches occur systematically, particularly in classrooms and offices [33,168]. By treating repeated dissatisfaction as evidence of insufficient spatial coverage, TIAF uses occupant feedback to guide sensor-network refinement, creating a feedback mechanism absent from most current monitoring strategies.

The tripartite data fusion approach extends IAQ assessment beyond building-level diagnostics to support cross-jurisdictional governance. A major challenge is the difference between regulatory frameworks: ASHRAE 62.1/62.2 uses prescriptive ventilation-rate requirements [35], whereas EN 16798-1 applies performance categories based on occupant sensitivity [36]. Because these approaches are not directly interoperable, compliance assessments often remain framework-specific, creating inconsistencies across regions [150].

TIAF addresses this limitation by generating a framework-independent evidence base. CFD-derived concentration and ventilation fields, continuously updated with sensor data and validated through occupant feedback, can be evaluated against both ASHRAE [35] and EN 16798-1 criteria [36] without separate monitoring campaigns. This is particularly important for vulnerable populations, whose protection varies across national regulations [31,150,173]. By providing a continuously verified dataset that supports multiple regulatory frameworks, TIAF promotes more transparent IAQ assessment, sustainable building certification, and harmonized environmental governance across authorities.

In practice, TIAF is implemented through five sequential steps: (1) deployment and calibration of a distributed IoT sensor network; (2) creation and validation of a CFD model using measured building geometry and ventilation characteristics; (3) real-time assimilation of sensor data into the CFD environment through EnKF updating; (4) collection

of POE/PAQ responses from occupants in the same spatial zones represented within the CFD model; and (5) identification of discrepancies between measured, simulated, and perceived conditions to guide sensor repositioning, ventilation optimization, or operational interventions. This workflow transforms TIAF from a conceptual framework into a practical decision-support tool for IAQ management.

Validation is performed by comparing CFD predictions with co-located sensor measurements using established performance indicators such as RMSE, MAE, and correlation coefficients. Agreement between measured and simulated airflow, temperature, and pollutant concentrations is assessed before operational deployment. The framework is particularly suitable for offices, schools, healthcare facilities, and other occupied buildings where continuous monitoring data and periodic occupant-feedback surveys can be collected. In such environments, TIAF supports sensor-network optimization, ventilation management, and evidence-based building certification.

4. Discussion

4.1. Comparative Framework for IAQ Assessment: Sensors, CFD, and Occupant Surveys

IAQ assessment requires integrating physical monitoring, numerical modeling, and occupant perception. As shown in Table 18, no single method can fully characterize indoor environments; combining all three is essential to capture spatial variability, temporal changes, and occupant experience.

Table 18. Comparative analysis of primary IAQ assessment methodologies.

Methodology	Core Strengths	Fatal Flaws in Isolation	Citations
Physical Sensors (IoT/LCS)	High temporal resolution; real-time control; practical for source identification (cooking, cleaning); scalable/low-cost.	Measurement uncertainty/drift; poor spatial representativeness (point data); no direct link to human perception or health.	[61,67,174–177]
CFD Modeling (Numerical)	High spatial resolution; “What-if” scenario analysis; optimization of sensor placement and BMS design.	Strong dependence on uncertain boundary conditions; requires extensive validation data; computationally expensive/slow.	[168,177–179]
Occupancy Surveys (POE)	Captures subjective comfort and usability; contextualizes multi-domain experience (thermal, acoustic, visual).	Weak correlation with objective levels of pollutants (carbon dioxide, fine particles); significant bias due to perceived expectations/controls; no source identified.	[180–182]

Table 18 highlights the key limitations of the current IAQ assessment. Sensors provide continuous measurements but cannot capture pollutant distributions in space, whereas CFD offers detailed spatial mapping [168,178,179]. However, even highly accurate simulations may not predict occupant satisfaction, since perception is often driven by thermal comfort and airflow rather than pollutant concentrations [180,182]. In addition, low-cost sensors are prone to drift and interference without reference-grade calibration [174,176,177]. Therefore, reliable IAQ assessment requires methodological triangulation: combining sensor measurements, CFD simulations, and occupant feedback. This integrated approach helps align technical performance with occupant well-being and environmental safety.

4.2. Identified Gaps and the Road to Digital Twins

Current IAQ monitoring remains fragmented, limiting its value for real-time decision-making. Existing protocols provide little guidance on sampling density or data quality, while widespread use of poorly calibrated low-cost sensors reduces reliability [7,183,184]. Laboratory-focused approaches often fail under real-world conditions, and poor integration between building automation systems and IoT-AI platforms restrict data interoperability and automated control [7,185,186]. Consequently, many studies rely on short monitoring periods and limited metrics, producing weak links between IAQ conditions and long-term health outcomes [187]. Most systems also emphasize monitoring rather than predictive control and automated HVAC responses, while the lack of standardized AI benchmarking limits reproducibility and validation [7,185].

Digital twins offer a pathway toward dynamic IAQ management by integrating BIM, IoT data, AI, and CFD into real-time operational frameworks [188–190]. These systems can autonomously optimize HVAC performance using CO₂ and TVOC measurements [191], support predictive maintenance through sensor analytics and Bayesian models [185], and extend to urban-scale applications by linking CFD with meteorological data [192]. Emerging approaches also combine IAQ, energy performance, and physiological responses to enable personalized comfort prediction and health-oriented building control [186,193]. Open data standards, interoperable platforms, and long-term validation are essential for scaling these systems beyond pilot projects and supporting sustainable, occupant-centered building management [186,188,190,193–195]. Privacy protection and user engagement remain critical requirements for successful implementation [183,188].

4.3. Critical Synthesis and Framework Evaluation

Physical monitoring, CFD, and occupant assessment each captures a distinct aspect of IAQ. IoT sensor networks provide continuous measurements of pollutants and thermal conditions [1,2,8,85], CFD delivers detailed spatial distributions of airflow and contaminants [71,72], and occupant surveys capture perceived comfort and dissatisfaction that neither measurements nor simulations can fully explain [135,137,140]. Together, they form the basis of the Tripartite IAQ Assessment Framework (TIAF).

Excluding any pillar creates a specific limitation. Sensor-only approaches cannot resolve spatial variability and may miss localized exposure hotspots [60,61,65,66]. CFD without measurement data relies on simplified boundary conditions that can reduce prediction accuracy [120,122,123], while inconsistent validation and turbulence-model selection introduce additional uncertainty [96–100,187]. Without occupant feedback, discrepancies between technical compliance and perceived comfort remain undetected [134,135,142,143].

An effective integrated assessment therefore requires calibrated sensor networks [49,53,55], CFD models validated against experimental or field data [72,94,178], data-assimilation methods that continuously update simulations using measurements [119,121,123], and survey tools capable of distinguishing thermal discomfort from IAQ-related dissatisfaction [135,142,143]. Sensor data, CFD results, and occupant responses must also be compared within the same spatial zones rather than through building-wide averages [17].

Despite progress, important gaps remain. Sensor calibration and placement are often treated independently [52,53,60,61], CFD-IEQ validation lacks widely accepted standards [178], and differences between measured conditions and occupant perceptions are usually reported rather than used to improve assessment [134,141,142].

TIAF addresses these limitations through a bidirectional feedback process. Sensor data continuously updates CFD simulations through EnKF-based assimilation [121,123], while CFD results are linked to the same zones assessed through POE and PAQ

surveys [17,135,142,143]. Most importantly, persistent discrepancies between measurements and occupant feedback are used to identify inadequate sensor coverage and guide sensor-network refinement [54,64,134,141]. Because the framework is independent of a single metric, results can be evaluated against both ASHRAE 62.1/62.2 [35] and EN 16798-1 [36], supporting more consistent IAQ assessment across regulatory contexts [21,31,150,152].

The methodology follows three phases—preparation, experimentation, and data analysis—adapted from Dai et al. [193]. The preparatory phase identifies key IEQ and physiological parameters. The experimental phase combines continuous environmental monitoring with wearable sensing, while the final phase applies statistical analysis, correlation testing, and predictive modeling to interpret the integrated dataset [193].

4.4. Inherent Limitations of TIAF and Uncertainty Propagation Analysis

While TIAF addresses the fragmentation of IAQ assessment, it introduces its own methodological and operational constraints. These include the cost and complexity of multi-source data fusion, temporal synchronization challenges, limited transferability between building types, and barriers to large-scale implementation.

Beyond the limitations of its individual components, TIAF faces challenges inherent to integration. Combining IoT monitoring, EnKF-based CFD, and recurring POE/PAQ surveys increase costs, infrastructure requirements, and software dependencies compared with single-domain approaches [72,119,135]. Temporal synchronization is also difficult because sensors, simulations, and surveys operate on different timescales, introducing uncertainty during data integration [119,135,142,143]. In addition, the framework requires revalidation when applied to different building types, occupancy patterns, or ventilation conditions, while privacy and infrastructure constraints may limit large-scale adoption [87,89,94,150,151].

Grounded in the conceptual workflow developed by Dai et al. [193], the investigation implements an integrated procedural sequence designed to transition from preliminary parameters to advanced modeling. This cohesive structural design is visually mapped in Figure 6.

Uncertainty can also propagate across the framework. Sensor drift and cross-sensitivity may bias EnKF updates, affecting CFD boundary conditions and subsequent airflow predictions [53,119,121]. These errors can be amplified by turbulence-model limitations, particularly near walls and in buoyancy-driven flows, leading to inaccuracies in occupant-exposure estimates [87,89,91,92]. Further uncertainty arises when CFD results are linked to survey zones, potentially affecting comfort-compliance assessments [17,135]. As a result, incorrect attribution of perception-measurement discrepancies may trigger unnecessary sensor-network adjustments [58,64,134,141].

Each stage therefore requires specific mitigation measures. Sensor uncertainties can be reduced through periodic reference calibration and ML-based drift correction [49,53,119,122]. EnKF performance can be improved using tuning and multi-sensor redundancy [60,118,121]. CFD uncertainty should be managed through validation and selective LES benchmarking [84,87,91,178]. Consistent georeferenced zoning can reduce mapping errors between CFD, sensors, and surveys [17,135], while adaptive survey scheduling helps minimize temporal mismatches between occupant feedback and near-real-time environmental data [135,137,140,142,143].

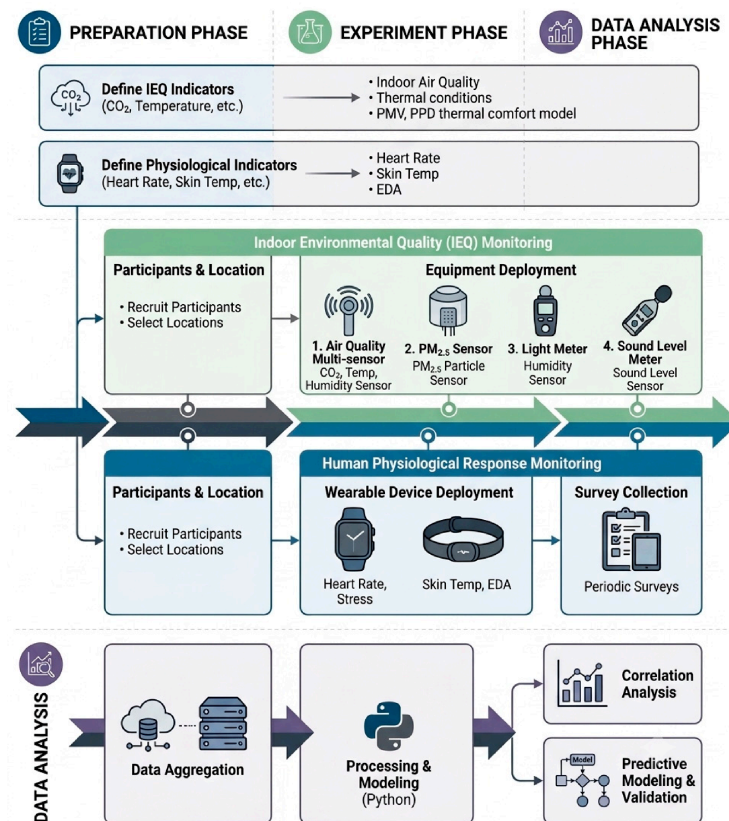


Figure 6. Three-phase experimental design and analytical workflow.

5. Conclusions

Isolating the three pillars of indoor air quality assessment physical sensing, numerical simulation, and subjective experience fragments our understanding of the built environment and obscures the true complexity of human exposure. This systematic review confirms that no single methodology possesses the epistemological depth to characterize IAQ with total reliability. Relying solely on IoT-integrated sensor networks provide high temporal granularity but ignore the mechanistic reality of three-dimensional airflow. These sensors often suffer from metrological drift and poor spatial representativeness, failing to capture the systematic discrepancy between wall-mounted readings and the actual breathing zone. Such measurement gaps necessitate the intervention of Computational Fluid Dynamics (CFD).

Deploying the $k-\omega$ SST formulation within the RANS framework transforms these discrete, retrospective sensor points into high-resolution deterministic maps of velocity and contaminant concentration. This numerical depth allows engineers to visualize source-receptor pathways that sensors simply cannot “see.” Achieving this level of predictive accuracy requires high-quality boundary conditions, forcing a technical marriage between physical monitoring and simulation. Implementing Ensemble Kalman Filter-based data assimilation frameworks reduces the inherent uncertainty of CFD, ensuring that the numerical environment reflects physical reality rather than idealized mathematics.

This technical precision remains hollow if it ignores the profound sensory paradoxes of the human occupant. Evidence consistently shows that people do not perceive chemical concentrations directly; they construct judgments of “freshness” from thermal cues, odor intensity, and a sense of personal control. These cognitive biases produce the “stuffy-but-clean” paradox, where thermally comfortable spaces with hazardous CO₂ levels are rated as satisfactory. Such behavioral inconsistencies make traditional Likert-scale surveys

scientifically insufficient when used in isolation. Addressing this fragmentation requires the adoption of the Tripartite IAQ Assessment Framework (TIAF).

Establishing TIAF forces a methodological triangulation that reconciles what the environment contains with what the occupant experiences. Physical measurements calibrate the CFD boundary conditions, while CFD outputs guide the intelligent placement of sensors within complex flow fields. Mapping these results against concurrent subjective data allows for the design of ventilation strategies that meet both regulatory thresholds and social acceptance. This integrated architecture becomes urgent in a post-COVID-19 landscape where the 2021 WHO Guidelines have rendered most contemporary buildings technically non-compliant. Bridging this compliance gap demands that we abandon disciplinary silos in favor of co-designed monitoring platforms. Future research must now focus on utilizing immersive VR representations of these CFD airflow fields to translate technical evidence into meaningful public action. Building environments must move beyond being measured as healthy; they must be trusted, sustained, and verified through this unified scientific lens.

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Abbreviations

IAQ	Indoor Air Quality
IEQ	Indoor Environmental Quality
PAQ	Perceived Air Quality
POE	Post-Occupancy Evaluation
PM	Particulate Matter
CO ₂	Carbon Dioxide
VOC/TVOC	Volatile Organic Compounds/Total VOCs
HCHO	Formaldehyde
NO ₂	Nitrogen Dioxide
MEK	Methyl Ethyl Ketone
SF ₆	Sulfur Hexafluoride
IoT	Internet of Things
LCS	Low-Cost Sensors
NDIR	Non-Dispersive Infrared
ML	Machine Learning
kNN	An instance-based learning algorithm utilizing k-Nearest Neighbors for classification or regression.

RF	A multi-decision tree ensemble technique known as Random Forest for robust predictive modeling.
CNN	A deep learning architecture specialized in processing structured arrays of data, specifically Convolutional Neural Networks.
LSTM	Long Short-Term Memory; a specialized recurrent architecture effective at preserving information over extended temporal sequences.
GRU	Gated Recurrent Unit; a streamlined recurrent model optimized for managing gradient flow in sequential processing.
RANS	Reynolds-Averaged Navier–Stokes: A computational framework used to approximate turbulent flow behavior through time-averaging.
LES	Large Eddy Simulation: a high-fidelity numerical technique that resolves large-scale turbulent structures while modeling smaller eddies.
DES	Detached Eddy Simulation; Hybrid turbulence model
URANS	Unsteady Reynolds-Averaged Navier–Stokes; Time-dependent RANS approach
DPM	Discrete Phase Model; Particle tracking model in CFD
UDF	User-Defined Function; Custom functions in CFD simulations
BIM	Building Information Modelling; Digital representation of building data
BES	Building Energy Simulation; Simulation of building energy performance
$k-\epsilon$	k-epsilon Model; a dual-equation closure scheme focusing on the dynamics of turbulent kinetic energy and its dissipation rate.
RNG $k-\epsilon$	Renormalization Group $k-\epsilon$; a statistical refinement of the standard k-epsilon model for better handling of strained flows.
$k-\omega$ SST	Shear Stress Transport Model; a robust hybrid formulation that enhances turbulence prediction near solid boundaries.
RMSE	Root Mean Square Error; a standard statistical measure used to quantify the magnitude of prediction residuals.
MAPE	Mean Absolute Percentage Error; an accuracy metric that expresses forecasting errors as a relative percentage.
MRE	Mean Relative Error: A performance indicator assessing the average deviation of predictions from observed values.
R^2	Coefficient of Determination; a statistical index representing the variance proportion captured by the regression model.
FAC2	Fraction of predictions within a factor of 2 of observations
HVAC	Heating, Ventilation, and Air Conditioning
DCV	Demand-Controlled Ventilation
ACH	Air Changes per Hour
AFCV	Air Flow Control Valve
EMA	Ecological Momentary Assessment
ESM	Experience Sampling Method
OSS	Occupancy Survey System
TIAF	Tripartite IAQ Assessment Framework
COM-B	Capability, Opportunity, Motivation-Behavior (behavioral model)
BUS	Building Use Studies (methodology)
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers; the global authority for establishing building environment and energy standards.
WSN	Wireless Sensor Network
IDW	Inverse Distance Weighting
VR	Virtual Reality
UDF	User-Defined Function
WHO	World Health Organization
AQG	Air Quality Guidelines

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