Optimizing Indoor Air Quality with Multi-Zone Modeling: Comparative Calibration Using Ensemble Kalman Filter & Genetic Algorithm

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ABSTRACT

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Eslam Fathelbab

Indoor air quality (IAQ) modeling is essential for evaluating and optimizing modern buildings' ventilation systems, pollutant dispersion, and occupant health. Accurate IAQ predictions rely on calibrated models that effectively represent real-world conditions. This study focuses on calibrating the CONTAM multi-zone airflow model using two advanced methodologies: the Ensemble Kalman Filter (ENKF) and the Genetic Algorithm (GA). To improve the model's predictive accuracy, calibration efforts targeted key parameters, including initial CO_2 concentrations, generation rates, and occupancy counts. These methods were validated using CO_2 tracer gas experiments conducted across multiple test scenarios, including room-to-floor and floor-to-floor dispersion dynamics. Results demonstrate that ENKF calibration achieved RMSE reductions of approximately 25% in complex multi-zone airflow scenarios, with CVRMSE consistently below the ASHRAE-recommended threshold of 15%. The GA method performed similarly in accuracy but required higher computational resources, making it more suitable for static or offline calibration processes. The calibrated models were subsequently applied in a case study to analyze CO_2 quanta dispersion in an experimental building with controlled ventilation strategies. This study investigated the effects of varying fresh air percentages (10% to 100%) and stairwell pressurization on contaminant transport. Results from the calibrated models revealed critical insights, such as the effectiveness of high fresh air intake in mitigating pollutant concentrations and the impact of pressurization strategies on inter-zone airflow. These findings highlight the practical value of calibration in refining IAQ predictions and informing operational strategies. This research underscores the importance of hybrid calibration techniques for improving the reliability of multi-zone IAQ models and their application in dynamic building environments. By integrating calibrated models into operational planning, stakeholders can optimize ventilation performance, reduce energy consumption, and enhance occupant safety in diverse building types.

Keywords: Indoor Air Quality (IAQ), CONTAM, Ensemble Kalman Filter, Genetic Algorithm, Calibration, Multi-Zone Airflow, CO_2 Dispersion, Building Performance Optimization.

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Chapter 1

1. Introduction

1.1 Problem Statement

Indoor air quality (IAQ) plays a pivotal role in ensuring building occupants' health, productivity, and overall well-being. The quality of indoor environments directly impacts human comfort and performance, making it an essential consideration in building design and operation. Globally, buildings contribute to around 30% of total energy consumption, with heating, ventilation, and air conditioning (HVAC) systems accounting for a substantial share of this usage (International Energy Agency, 2021). Efficient HVAC systems are crucial for regulating IAQ, as they manage the levels of indoor pollutants, maintain thermal comfort, and support energy-efficient building operations. However, balancing healthy IAQ and energy efficiency is a complex challenge.

High-performance buildings, characterized by airtight envelopes and sophisticated mechanical systems, have been designed to reduce energy losses and improve sustainability. While these features enhance energy efficiency, they can inadvertently increase the risk of pollutant buildup due to reduced natural ventilation. This scenario necessitates using advanced ventilation strategies and predictive models to optimize IAQ and mitigate risks. However, accurate prediction of IAQ in such buildings remains challenging due to the dynamic nature of contaminants, occupant activities, and the operational variability of ventilation systems (Dols et al., 2016).

Multizone modeling tools, such as CONTAM, have emerged as vital platforms for simulating airflow, contaminant dispersion, and ventilation performance in complex building environments

(Wang et al., 2010). These tools allow researchers and practitioners to evaluate various design scenarios and operational strategies, supporting informed decision-making. However, the accuracy of these models depends on their calibration against reliable field data. Tracer gas techniques, including the use of carbon dioxide (CO_2) and sulfur hexafluoride (SF_6), are widely employed to measure ventilation rates and airflow patterns, providing the data required for model validation (Sherman, 1990; Cui et al., 2015). Despite their utility, calibration processes are often complicated by uncertainties arising from unpredictable occupant behavior, variations in contaminant sources, and the inherent complexity of building systems.

Advanced calibration methods such as the Ensemble Kalman Filter (ENKF) and Genetic Algorithms (GA) have been developed to address these uncertainties. The ENKF is a powerful tool that uses iterative data assimilation to dynamically improve model predictions, making it particularly effective for systems with time-dependent variables (Higdon et al., 2013). On the other hand, GA applies principles of natural selection to optimize calibration by identifying parameter sets that minimize errors between model outputs and observational data (Pandey et al., 2020). While both methods have shown promise in related applications, their comparative effectiveness in calibrating multizone IAQ models is an area that requires further exploration. This research integrates ENKF and GA calibration methods with multizone modeling tools in CONTAM to improve the accuracy and reliability of IAQ predictions. By utilizing field data from tracer gas experiments, the study evaluates the performance of these calibration techniques and their potential to enhance the modeling of IAQ across diverse building configurations. The findings aim to contribute to the advancement of energy-efficient, sustainable, and healthy building environments.

1.2 Research Objectives

To address the multifaceted challenges outlined in Section 1.1, this research establishes two primary objectives:

1. Calibration of Multizone IAQ Models: This study employs ENKF and GA to calibrate multizone IAQ models developed in CONTAM, using field measurements from tracer gas experiments in high-rise buildings. The calibration process systematically varies critical parameters, such as ventilation rates, contaminant generation, and occupant behavior to identify the most accurate model configurations. By comparing the performance of ENKF and GA, the study provides insights into the strengths and limitations of each method, offering a framework for selecting appropriate calibration techniques for specific scenarios.
2. Simulation and Analysis of Ventilation Strategies: The calibrated models are applied to simulate various ventilation strategies, including adjustments to airflow distribution, changes in mechanical ventilation rates, and pressurization scenarios. These simulations aim to evaluate the impacts of different strategies on IAQ, energy consumption, and contaminant transport in diverse building environments. The analysis highlights how advanced calibration techniques can enhance HVAC system performance, guiding optimizing energy efficiency while ensuring occupant comfort and health.

By integrating advanced calibration methods with IAQ modeling, this research contributes to developing robust, data-driven approaches for addressing the dual challenges of energy efficiency and indoor air quality. The study's findings have significant implications for designing and operating buildings in regions with high cooling demands, offering valuable insights for improving urban sustainability.

Chapter 2

2. Literature Review

2.1 Overview

Indoor air quality (IAQ) is a critical determinant of health, comfort, and productivity in modern building environments. With increasing urbanization and stringent energy efficiency requirements, the design and optimization of ventilation systems have become pivotal in mitigating indoor air pollutants, ensuring occupant well-being, and maintaining environmental sustainability. Multi-zone airflow modeling has emerged as a powerful tool to analyze and predict the transport of contaminants, evaluate ventilation effectiveness, and design pressurization strategies in complex building layouts. However, the accuracy and reliability of these models are often constrained by uncertainties in input parameters, necessitating robust calibration techniques.

Calibration bridges the gap between simulation outputs and real-world measurements, enhancing the predictive power of multi-zone models. Advanced approaches, such as the Ensemble Kalman Filter (ENKF) and Genetic Algorithms (GA), have shown promise in refining these models by dynamically updating parameters based on sensor data and optimizing solutions across multi-objective landscapes. While ENKF excels in the real-time assimilation of measurement data, GAs offer robust optimization capabilities for exploring large and complex parameter spaces. Combining these methodologies offers a unique opportunity to address the limitations of traditional calibration methods and advance the state of IAQ modeling.

This thesis explores the comparative performance of ENKF and GA in optimizing multi-zone airflow models for IAQ, focusing on ventilation and pressurization strategies. By integrating these techniques into practical applications, this work aims to provide actionable insights into achieving energy-efficient, health-conscious, and adaptive ventilation solutions. The findings contribute to the growing field of IAQ management by bridging theoretical advancements with practical applications, ultimately supporting healthier and more sustainable indoor environments.

2.2 IAQ Analysis Using Multi-Zone Models

Multi-zone modeling using CONTAM is critical for analyzing IAQ, airflow dynamics, and contaminant transport in various building environments. This review incorporates 26 key studies detailing advancements, applications, and challenges associated with multi-zone modeling and CONTAM.

2.2.1 CONTAM in Multi-Zone Modeling

Dols et al. (2016) demonstrated the integration of CONTAM with TRNSYS to evaluate building energy and IAQ trade-offs. This co-simulation approach proved effective in optimizing energy efficiency while maintaining acceptable IAQ. Wang et al. (2010) introduced CFD capabilities into CONTAM, enhancing the accuracy of airflow and contaminant transport simulations in irregularly shaped spaces. Yan et al. (2022) combined CONTAM with Wells-Riley models to simulate SARS-CoV-2 transmission in various building types. The study emphasized the importance of ventilation and filtration in mitigating airborne disease risks. Guo et al. (2021) applied CONTAM to validate pressure zone control strategies in isolation wards, effectively limiting pathogen transmission risks. Wu et al. (2016) employed tracer gas techniques within CONTAM to examine cross-infection risks in residential units adjacent to healthcare facilities. Chao and Wan (2004) utilized constant concentration dosing in CONTAM simulations, effectively measuring ventilation performance in complex environments.

2.2.2 Modeling Across Different Building Types

In residential applications, Lo and Novoselac (2012) explored cross-ventilation dynamics in multi-zone residential buildings, focusing on airflow through tiny openings. Their work provided insights into ventilation challenges under varied pressure conditions. Fine and Touchie (2021) used CONTAM to analyze inter-suite contaminant transfer in high-rise buildings, identifying air leakage and ventilation inefficiencies.

In commercial applications, Kabirikopaei and Lau (2020) assessed seasonal ventilation performance in classrooms, emphasizing the role of HVAC systems in achieving stable IAQ conditions. Na et al. (2023) evaluated HRVs and air purifiers in schools, highlighting their dual benefits of IAQ improvement and noise reduction using CONTAM simulations.

As for Healthcare facilities applications, Guo et al. (2021) demonstrated the utility of CONTAM in modeling airflow and pressure differentials in isolation wards, aiding infection control efforts. Wu et al. (2016) validated multi-zone modeling for identifying airborne pathogen risks in healthcare-adjacent residential flats.

2.2.3 Advancements in Modeling Techniques

CONTAM has also been incorporated with multiple energy analysis software packages to optimize combined Energy and IAQ. Qi et al. (2020) applied CONTAM to optimize hybrid ventilation systems in high-rise buildings. The study highlighted the potential for predictive control to balance energy efficiency with IAQ improvements. Alonso et al. (2022) used CONTAM and EnergyPlus co-simulations to develop demand-controlled ventilation strategies, achieving significant energy savings while maintaining occupant comfort.

Bivolarova et al. (2017) compared the behavior of tracer gases and aerosols in indoor spaces, emphasizing the role of ventilation rates and airflows in particle dispersion. Reda et al. (2023) proposed a modified decay method incorporating a uniformity index to better account for non-uniform air mixing in large spaces.

Berquist et al. (2023) evaluated BAS-grade sensors for real-time IAQ assessments in CONTAM simulations, showcasing their accuracy and utility in dynamic monitoring. Hou et al. (2023) introduced Bayesian inference models combined with CO_2 sensors for evaluating school ventilation conditions, offering a data-driven approach to IAQ management.

2.2.4 Challenges and Future Directions

After carefully considering what has been mentioned above, it is clear that accurate calibration of CONTAM models remains a challenge, particularly in non-standard building designs or under variable occupancy and usage conditions. Integrating IoT devices and AI-driven analytics offers a promising direction for enhancing CONTAM's predictive and adaptive capabilities. Tsang et al. (2023) reviewed the role of multi-zone modeling in evaluating airborne transmission risks in hospitals, emphasizing the importance of dynamic ventilation strategies for infection control. Table 1 provides a comparison between selected studies.

Table 1. Comparison between different IAQ analysis studies

Study	Building Type	Focus	Model Used	Key Findings
Dols et al. (2016).	Office	Energy-IAQ optimization	CONTAM + TRNSYS	Balanced energy efficiency and IAQ.
Wang et al. (2010).	Mixed-use	CFD integration in CONTAM	CONTAM + CFD	Enhanced airflow modeling in complex geometries.
Yan et al. (2022).	Mixed	Pathogen dispersion	CONTAM + Wells-Riley	Quantified infection risks and mitigation strategies.
Guo et al. (2021).	Healthcare	Pressure control in isolation wards	CONTAM	Validated airflow management for infection control.
Pease et al. (2021).	Office/Retail	HVAC modifications for SARS-CoV-2	CONTAM	Highlighted effective filtration strategies.
Qi et al. (2020).	High-rise buildings	Hybrid ventilation	CONTAM	Improved IAQ and energy use with predictive controls.
Kabirikopaei and Lau	Classrooms	Seasonal HVAC impact on IAQ	CONTAM	Identified significant seasonal variations in IAQ.
Lo and Novoselac (2012)	Residential	Cross-ventilation performance	CONTAM	Modeled airflow interactions in multi-zone systems.

Alonso et al. (2022).	Office	Demand-controlled ventilation	CONTAM + EnergyPlus	Simultaneous IAQ improvement and energy savings.
Wu et al. (2016).	Residential	Cross-infection risks	CONTAM	Assessed airborne contaminant transmission.

2.3 Tracer Gas Analysis

2.3.1 Overview

Tracer gas analysis is vital for evaluating indoor air quality (IAQ), providing insights into ventilation performance, contaminant transport, and airflow dynamics. By tracking the movement of gases like CO_2, SF_6, and perfluorocarbons (PFCs), researchers can quantify air change rates, identify pollutant sources, and assess ventilation strategies. This review explores the evolution of tracer gas techniques, their methodological advancements, and applications across diverse environments, integrating insights from recent and classical studies.

The use of tracer gas for IAQ analysis began with studies like Lidwell and Lovelock (1946) and evolved with the establishment of standardized methodologies. These methodologies, like ASTM E741 (2017) and ISO 12569 (2017), provide guidelines for using tracer gas to determine building air exchange rates. Sherman (1990) and Persily (2015) emphasized the critical role of tracer gas in understanding single-zone and multi-zone ventilation dynamics. Nazaroff (2021) reviewed residential air-change rates, highlighting the variability across different housing types and the role of natural ventilation. These foundational studies set the stage for contemporary applications in IAQ analysis.

2.3.2 Methodological Advancements in Tracer Gas Analysis

Tracer gas techniques are categorized into decay, constant concentration, and pulse injection. Cui et al. (2015) developed a CO_2 tracer gas decay method to estimate air change rates, emphasizing its applicability in naturally ventilated spaces. Chao and Wan (2004) used the constant concentration method to measure ventilation rates in dynamic, multi-zone setups. Paralovo et al.

(2020) introduced a passive tracer gas test, enabling air change rate measurements without active gas injection.

Modern studies have expanded tracer gas applications with advanced methodologies**.** Reda et al. (2023) and Hou et al. (2023) refined decay methods by integrating Bayesian inference and uniformity indices, addressing non-uniform air mixing challenges. Tsang et al. (2023) introduced IoT-enabled wireless sensor grids for real-time tracer gas monitoring, enabling spatial and temporal evaluations of pollutant dispersion. Shinohara et al. (2010) adapted the PFC method to measure effective multizone air exchange rates, offering a novel approach to validating IAQ models.

In South Korea, mandatory standards for ventilation systems, such as an air change rate (ACH) of 0.5, were introduced to ensure satisfactory IAQ in residential buildings. However, research indicates that this prescriptive metric, based solely on volumetric airflows, does not account for actual airflow patterns and air distribution within spaces (Son & Yang, 2020; Yang et al., 2021). These studies suggest that existing evaluation methods may fail to eliminate pollutants adequately, further underscoring the importance of advanced tracer gas methodologies in validating ventilation performance.

Concerns over the environmental impact of SF_6 as a tracer gas have prompted a shift toward more sustainable alternatives. Edouard et al. (2016) compared CO_2 and SF_6 tracer gas methods, demonstrating that CO_2 offers a viable, environmentally friendly solution for air change rate measurements. Seol et al. (2023) explored occupant-generated CO_2 as a low-cost alternative, particularly for natural ventilation studies.

Despite these advancements, challenges remain in achieving widespread adoption of mechanical ventilation systems. Surveys by Son and Yang (2020) revealed that 35.5% of South Korean apartment residents did not use their mechanical ventilation systems, even though these systems were legally mandated. Similarly, Yang et al. (2021) found that many residents preferred natural ventilation or misunderstood the role of air purifiers. These findings highlight the need for enhanced awareness and user-friendly systems to maximize the benefits of ventilation technologies.

2.3.3 Comprehensive Comparison of Tracer Gas Studies

Due to the wide range of studies conducted, the table below will try to summarize.

Table 2. Comparison between previous tracer gas studies

Study	Building Type	Tracer Gas	Measurement Method	Key Findings
Sherman (1990)	Single-zone	SF_6, CO_2	Decay, constant concentration	Established foundational tracer gas methodologies.
Persily (1988, 2016)	General	SF_6, CO_2	Various	Reviewed ventilation rate measurement techniques.
Reardon et al. (2002).	Atrium office building	SF_6, CO_2	Decay	Examined ventilation and air infiltration in atrium spaces.
Men et al. (2020).	General	SF_6	Decay	Assessed infiltration rates in varying conditions.
Kabirikopaei and Lau (2020)	Classrooms	CO_2	Seasonal analysis	Highlighted HVAC systems' role in ventilation variability.
Berquist et al. (2023)	Various	CO_2	BAS-grade sensor analysis	Evaluated BAS sensors for accuracy in infiltration measurements.
Ishigaki et al. (2022)	Geriatric care facility	CO_2	Decay	Investigated airborne transmission mitigation strategies.
Jiang et al. (2023).	High-rise building	SF_6, CO_2	Decay	Provided evidence of aerosol transmission of SARS-CoV-2.
Wu et al. (2016).	Residential	SF_6	Step-up/down	Evaluated cross-infection risks in adjacent flats.
Sung et al. (2018).	Hospital	SF_6, CO_2	Decay, CFD integration	Modeled airflow in MERS transmission scenarios.
Cui et al. (2015).	Office	CO_2	Decay	Reliable method for air change rate calculation.
Liu et al. (2022).	Office	CO_2, Aerosol	Mixing vs. displacement	Assessed exposure in mixed/displacement ventilation.
Batterman (2017)	Classrooms	CO_2	Decay	Extended CO_2-based methods for school ventilation rates.
Laussmann and Helm (2011)	Residential	SF_6, CO_2	Decay	Analyzed the significance of air change for IAQ.
Hou et al. (2023).	Schools	CO_2	Bayesian inference	Bayesian models for ventilation assessment.
Reda et al. (2023).	Worship places	CO_2	Modified decay	Proposed uniformity index for non-uniform air spaces.

Danlin et al. (2021).	Schools	CO_2	Bayesian calibration	Linked CO_2 conditions to COVID-19 risk in classrooms.
Lo and Novoselac (2012)	Test building	SF_6, CO_2	Cross-ventilation assessment	Measured small opening effects in multi-zone buildings.
Ai et al. (2020).	Various	SF_6, CO_2	Simulation and experiments	Validated tracer gases as surrogates for airborne droplets.
Bivolarova et al. (2017)	Indoor spaces	SF_6, Aerosols	Comparative analysis	Tracer gas and particle behavior were compared under different ventilation rates.
Zhang et al. (2009).	Airliner cabin	SF_6	Experimental & CFD	Investigated contaminant transport in confined spaces.
Tsang et al. (2023).	Hospitals	SF_6, CO_2	Systematic review	Analyzed airborne transmission studies in healthcare.
Zhao et al. (2022).	Enclosed spaces	SF_6, CO_2	Overview of methods	Reviewed airborne COVID-19 transmission in buildings.
Reda et al. (2023).	Non-uniform air spaces	CO_2	Modified decay	Addressed challenges of non-uniform air mixing.

The above table clearly shows that SF6 has been widely used as a tracer gas for most studies. However, due to its environmental impact, multiple complications are associated with its usage.

2.4 Sensitivity Analysis

Sensitivity analysis (SA) is fundamental in identifying and quantifying the influence of model parameters on the output, ensuring that resources are focused on the most influential variables during calibration. This is particularly important in building models, where large numbers of parameters (e.g., infiltration rates, CO_2 generation rates, HVAC settings) exist and can interact non-linearly.

2.4.1 Sensitivity Analysis Types

1. Local Sensitivity Analysis (LSA):

LSA evaluates how changes in one input parameter affect model output while keeping all other parameters constant. While this approach is computationally inexpensive and intuitive, it may fail to capture the interactions between parameters, particularly in highly complex and non-linear models. This limitation can lead to an incomplete understanding of the model's behavior under various conditions.

2. Global Sensitivity Analysis (GSA):

GSA provides a more comprehensive assessment by considering the entire parameter space and all parameter interactions. The Sobol variance decomposition method is particularly useful in GSA, as it quantifies the contributions of both individual parameters and their interactions to the total output variance. This method is highly suited for non-linear and multi-dimensional models like multi-zone building models, where the relationship between inputs and outputs is not straightforward.

Monte Carlo Simulations are often used alongside Sobol's method to evaluate the range of possible outcomes by sampling from distributions of uncertain input parameters. This approach is especially beneficial when dealing with parameter uncertainties in complex models.

2.4.2 Key Parameters Analyzed in Sensitivity Studies

Sensitivity analysis is critical for identifying and prioritizing the parameters significantly influencing building model outputs. Systematic evaluation of the effects of various inputs allows researchers to focus on the variables that have the most significant impact on energy performance, indoor air quality (IAQ), and occupant comfort. This process streamlines calibration efforts and provides insights into the underlying dynamics of building systems, enabling more efficient and accurate modeling.

The following section highlights key parameters frequently examined in sensitivity studies, emphasizing their role in shaping simulation accuracy and calibration outcomes.

1. Infiltration Rates: These rates determine the exchange of indoor and outdoor air, influencing energy consumption and IAQ.
2. CO_2 Generation Rates: Occupant density and activity levels determine the CO_2 generated indoors, impacting energy modeling and ventilation system performance.
3. HVAC Operational Parameters: The efficiency of HVAC systems, including airflow rates, temperature setpoints, and system controls, directly affects energy efficiency and comfort levels.
4. Building Envelope Characteristics: Parameters such as wall insulation, window type, and airtightness influence energy demand and indoor air quality by affecting heating, cooling, and ventilation loads.

Sensitivity analysis and calibration techniques have been widely applied across various building types to improve the accuracy of simulations and optimize performance. These applications demonstrate the practical value of identifying key parameters and refining models for specific use cases, such as educational facilities, healthcare environments, and residential buildings. The following section highlights notable case studies that illustrate the effectiveness of these methods in addressing real-world challenges.

Studies like Batterman (2017) have demonstrated the importance of natural ventilation in classrooms, where airflow and CO_2 removal rates significantly impact indoor air quality and occupant comfort. Sensitivity analysis indicated that natural ventilation rates and internal heat generation are key determinants for IAQ in classroom environments.

In infection control studies, Guo et al. (2021) utilized GSA to assess how ventilation strategies in hospital isolation rooms affect airborne pathogen control. The analysis emphasized the critical role of airflow distribution and pressure control in minimizing the spread of pathogens.

Cheng et al. (2021) conducted groundbreaking work using CFD simulations for multi-zone indoor airflow analysis. Their research revealed that MVAC (Mechanical Ventilation and Air Conditioning) layouts and room settings significantly impact thermal comfort and air quality parameters, emphasizing the need for detailed sensitivity analysis in building design phases.

Recent research by Haleem et al. (2020) has shown that uncertainty in HVAC systems with advanced control sequences significantly impacts energy use and indoor environmental quality. Their Monte Carlo uncertainty analysis revealed complex interactions between control parameters and IAQ outcomes, particularly in CO_2 concentration management.

Sensitivity analysis in indoor air quality research has evolved significantly, providing crucial insights for building design and operation. The field continues to advance with new technologies and methodologies, though several challenges remain. Future research should focus on developing more comprehensive approaches to handle the increasing complexity of modern building systems while maintaining computational efficiency.

It is vital to develop standardized methodologies that can account for the dynamic nature of indoor environments while providing actionable insights for building designers and operators. As we face new challenges related to climate change and public health, the role of sensitivity analysis in understanding and optimizing indoor air quality will become increasingly critical.

2.5 Ensemble Kalman Filter for Model Calibration

The Ensemble Kalman Filter (EnKF) is a widely used data assimilation technique that combines model predictions with observational data to improve model accuracy. Initially developed for meteorological and geophysical applications, its adaptability has made it an essential tool in various domains, including building energy modeling, thermal system calibration, and airflow simulations. For CONTAM, a multizone modeling tool, EnKF's iterative updating capabilities enable efficient calibration of input parameters, accounting for uncertainties in boundary conditions, sensor data, and model structure. This section explores the theoretical underpinnings, advancements, and applications of EnKF, mainly focusing on its role in improving the reliability of CONTAM models.

2.5.1 Advancements in EnKF Methodology

Higdon et al. (2013) introduced a novel approach to computer model calibration using EnKF. The method's strength lies in its ability to handle high-dimensional problems and incorporate observational uncertainties into the calibration process, making it particularly relevant for CONTAM, where models often involve extensive parameter spaces; Bach and Gill (2022) advanced the multi-model EnKF framework, improving data assimilation for systems involving multiple interacting sub-models, a feature highly applicable to complex CONTAM simulations in multizone buildings.

Beer et al. (2024) proposed the Ensemble Kalman Inversion method, which improves parameter convergence rates in complex systems like geothermal reservoirs. This method's reduced computational demand offers potential advantages for CONTAM calibration. Martincevic et al. introduced a constrained Kalman filter for identifying semi-physical building thermal models, which integrate constraints reflecting physical system limits. This approach can be directly translated into CONTAM to ensure parameter realism.

2.5.2 Applications Performance Calibration

EnKF has been instrumental in building energy modeling and HVAC system calibration. Lin et al. (2020) demonstrated EnKF's capability to dynamically forecast cooling loads in hybrid ventilation systems, emphasizing its potential to optimize HVAC operations under variable occupancy conditions. This dynamic calibration aligns with CONTAM's need for real-time adjustments to reflect changes in indoor airflow. Rui et al. (2018) leveraged a Gature Model-based EnKF to calibrate machine parameters in energy systems. This probabilistic extension of EnKF enhances its ability to capture nonlinear interactions within building systems, a common challenge in CONTAM modeling.

Tanaka et al. (2021) applied Assisted Enate thermal states in complex environments, showcasing the method's ability to integrate sparse data and improve model fidelity. This approach can address CONTAM's sensitivity to input data quality, particularly in multizone airflow analyses. Similarly, Lou et al. (2018) explored EnKF's capabilities in calibrating HVAC systems under uncertainty, a challenge analogous to CONTAM's sensitivity to infiltration and occupant behavior inputs.

2.5.3 Hybrid and Reduced-Order Methods

Hybrid methods are a practical solution for integrating EnKF into computationally intensive workflows. Silva et al. (2024) introduced an adaptive hierarchical EnKF approach, combining reduced-order models with EnKF to balance accuracy and computational efficiency. This methodology is particularly relevant for CONTAM models requiring extensive sensitivity analyses across multizone setups. Bach and Gill (2022) also demonstrated a multi-model approach, enabling the calibration of interconnected subsystems, a feature applicable to CONTAM when modeling interlinked zones or mixed ventilation strategies.

While EnKF offers significant advancement regarding CONTAM calibration, several challenges remain. These include:

1. Handling Sparse Data**:** CONTAM's reliance on high-quality input data makes it vulnerable to errors in sensor placements or observational inconsistencies. Methods such as those proposed by Beer et al. (2024) and Hou et al. (2023), which refine EnKF for sparse datasets, offer promising solutions.
2. Nonlinear Dynamics**:** CONTAM's multizone models often involve nonlinear airflow and contaminants. As Rui et al. (2018) demonstrated, integrating Gaussian mixture models could help better capture these complexities.
3. Computational Efficiency**:** Given the high-dimensional nature of CONTAM simulations, reduced-order hybrids, such as those by Silva et al. (2024) and Martincevic et al. (2020), are essential for real-time applications.

Future research should focus on further integrating EnKF with machine learning techniques to enhance calibration efficiency. Developing user-friendly EnKF frameworks tailored to CONTAM could encourage its broader adoption among practitioners.

2.6 Genetic Algorithm for Model Calibration

Accurately calibrating indoor air quality (IAQ) and energy models is crucial for designing efficient and sustainable buildings. Genetic Algorithms (GAs), a robust optimization technique inspired by natural selection, have emerged as a reliable tool for model calibration due to their ability to solve complex, nonlinear problems. By iteratively searching the solution space, GAs optimizes model parameters, balancing computational efficiency and accuracy. This review explores the use of GAs in calibrating IAQ and energy models, focusing on key advancements, applications, and integration with other computational techniques.

2.6.1 Application of GAs in IAQ Model Calibration

Mengjie et al. (2021) utilized GAs to optimize ventilation systems in a single-family house in Sweden. Their study integrated GAs with demand-based control strategies, significantly improving IAQ while reducing energy consumption. This highlighted GAs' suitability for real-time ventilation management in residential settings.

Albert et al. (2014) employed GAs to calibrate air quality models around an electric power plant. By aligning pollutant concentration predictions with real-world measurements, they demonstrated the efficacy of GAs in reducing calibration errors and enhancing model accuracy.

Zhe et al. (2013) explored the integration of GAs with artificial neural networks (ANNs) to assess IAQ. Optimizing the ANN architecture with GAs improved the prediction accuracy of pollutant levels in indoor environments.

Shirish et al. (2020) extended the GA-ANN framework to simulate air quality estimations in dynamic environments. Their findings showcased GAs' robustness in managing nonlinear relationships between ventilation parameters and IAQ outcomes.

Shirish et al. (2020) extended the GA-ANN framework by simulating air quality estimations in complex environments. Their findings highlighted GAs' robustness in handling highly nonlinear relationships between ventilation parameters and IAQ outcomes.

2.6.2 Optimization of Energy Models Using GAs

Subhi et al. (2020) optimized energy consumption and thermal comfort in intelligent building management systems using GAs. Their multi-objective optimization approach balanced energy efficiency with occupant comfort, demonstrating GAs' ability to tackle competing objectives effectively.

Tony and Nassif (2015) applied GAs to optimize HVAC systems, achieving substantial energy savings while maintaining IAQ standards—this underlined GAs' adaptability in dynamically adjusting HVAC settings to environmental changes.

Kele (2020) employed GAs in energy-saving parameterized building designs. By optimizing materials and configurations during the early design stage, GAs facilitated reductions in building energy loads.

Marius et al. (2019) focused on industrial ventilation systems using gas to evaluate energy efficiency and ventilation effectiveness. Their framework highlighted how GAs could meet industrial IAQ requirements while minimizing energy costs.

2.6.3 Integration with Advanced Techniques

Florent et al. (2012) proposed a GA-based optimization of ANN architectures for predicting indoor discomfort and energy consumption. The hybrid method achieved higher prediction accuracy by tailoring the ANN to specific building datasets than standalone models.

Ali and Aydin (2014) introduced GAs as an intelligent optimization technique for parameter estimation in complex models. Their study demonstrated GAs' versatility in calibrating both IAQ and energy parameters in multi-zone simulations.

Thirumal et al. (2014) applied multi-objective GAs to optimize indoor air quality in air-conditioned cars. The study underscored GAs' applicability in confined spaces, where air distribution dynamics are constrained.

While GAs have demonstrated remarkable potential, their application in IAQ and energy model calibration faces challenges:

1. Computational Demand: GAs' iterative nature can make them computationally intensive, particularly for complex, multi-zone models. Hybrid approaches, such as GA-ANN integrations, have shown promise in mitigating this issue.
2. Parameter Sensitivity: GAs require careful tuning of key parameters, such as mutation rates and population sizes, to ensure effective convergence. Studies by Mengjie et al. (2021) and Subhi et al. (2020) emphasized the importance of adaptive parameterization in improving GA performance.
3. Real-Time Integration: Integrating GAs with real-time monitoring systems could significantly enhance their applicability in IAQ and energy management, enabling dynamic calibration and prediction in response to changing conditions.

Genetic Algorithms offer a robust framework for calibrating IAQ and energy models, solving complex optimization problems that traditional techniques often struggle to address. Their ability to integrate with machine learning and other advanced methods positions GAs as a key tool in achieving sustainable building design and operation. Future research should prioritize hybrid models, adaptive GA frameworks, and real-time integrations to unlock their full potential.

2.7 Discussion

The comprehensive review of the existing literature highlights significant advancements in the application of advanced computational techniques, such as Genetic Algorithms (GAs) and the Ensemble Kalman Filter (ENKF), for the calibration of indoor air quality (IAQ) and energy models. These methodologies have been pivotal in addressing the inherent complexities of multi-zone airflow modeling, tracer gas analysis, and the optimization of ventilation systems. Despite these advancements, critical gaps persist, particularly in the practical implementation and real-time calibration of models tailored for dynamic environments like those examined in this thesis.

The integration of GAs and ENKF has demonstrated significant potential to improve model calibration accuracy and adaptability. However, previous studies often lack a unified framework that effectively combines these methods with real-world measurement data, especially in IAQ models built using platforms like CONTAM. Furthermore, while literature underscores the value of sensitivity analyses and optimization techniques, there is a limited focus on systematically comparing different calibration methodologies and their impact on building performance metrics such as energy efficiency, ventilation effectiveness, and occupant comfort.

This thesis addresses these gaps by introducing an innovative calibration framework that leverages GAs and ENKF to enhance the accuracy and reliability of CONTAM-based IAQ models. By conducting extensive sensitivity analyses and incorporating real-world measurement data, the work aims to overcome limitations identified in the literature, such as computational inefficiency, parameter uncertainty, and inadequate consideration of dynamic environmental conditions. Additionally, the comparative analysis between GAs and ENKF provides a deeper understanding of their strengths and limitations, offering valuable insights for future applications in building performance modeling.

In conclusion, while the reviewed literature underscores the potential of advanced optimization and calibration techniques, the work presented in this thesis represents a critical step toward developing robust, real-time, and data-driven calibration methodologies for IAQ models. By bridging theoretical advancements and practical implementation, this research lays a foundation for enhancing the performance and sustainability of indoor environments, meeting the growing demand for healthier, more energy-efficient buildings.

Chapter 3

3. Methodology

The methodology for this study is a comprehensive approach that involves field measurements, simulation modeling, calibration, and analysis. The goal is to simulate CO2 dispersion within a multi-zone institutional building, validate the model against real-world data, refine it using different calibration techniques, and analyze the effect of different HVAC and pressurization strategies on particle spread.

3.1 Field Measurement Overview

3.1.1 Objective of Filed Measurement

The primary objective of the field experiments is to measure the dispersion of CO2 as a tracer gas in a multi-zone institutional building and to validate the multi-zone airflow model developed for indoor air quality (IAQ) analysis. CO2 is used due to its correlation with ventilation effectiveness, providing critical data on how air moves between rooms and floors.

The field measurements are specifically designed to assess the performance of the building's ventilation system under various operating conditions. The focus is identifying areas of insufficient ventilation, which is crucial for improving IAQ management. The data collected during these experiments will later be used to calibrate the multi-zone airflow model, ensuring that it reflects real-world conditions and can predict the spread of airborne contaminants in different zones.

The experiments are not just about data collection but also about understanding airflow patterns, contaminant transport, and the effectiveness of the building's HVAC system in managing indoor air quality. This is achieved by conducting single-zone and multi-zone CO_2 tracer gas tests, which provide an overview of the building's air dynamics.

In real-world applications, buildings like hospitals, offices, schools, and high-rise structures are often divided into multiple zones that operate independently yet are connected through shared HVAC systems. Variations in door openings, air pressure differences, temperature gradients, and occupancy in these zones can all significantly impact how air—and, by extension, contaminants—moves throughout the building. This variability underscores the practical relevance of our research, making it essential to analyze the system rather than focusing on individual zones in isolation.

By conducting multi-zone CO_2 tracer gas tests, we can observe:

- Inter-zone airflows: How air travels between adjacent rooms and floors, mainly through corridors, stairwells, and other shared spaces.
- Pressure-driven airflow patterns: The influence of pressure differences between zones can either enhance or hinder adequate ventilation.
- Contaminant spread and removal: How effectively are contaminants (simulated by CO_2) dispersed and removed in each zone, considering the operation of the HVAC system under various conditions?
- Cross-zone ventilation interactions: The impact of one zone's ventilation (e.g., a room with an open door) on neighboring zones, highlighting potential areas of insufficient air exchange.

This multi-zone approach provides a realistic view of the entire building's ventilation performance. Testing in multiple zones simultaneously allows for a deeper analysis of potential dead zones (areas with poor airflow), recirculation patterns, or pressure differentials that could lead to ineffective ventilation. Ultimately, these insights are crucial for optimizing HVAC system performance, ensuring consistent air quality across the entire building, and improving occupant health and safety by reducing exposure to airborne contaminants.

3.1.2 Building Overview

The field measurements were conducted in a 16-story institutional high-rise building at the Longueuil Campus, Université de Sherbrooke, in Montreal, Canada. The building houses various spaces, including classrooms, laboratories, and reception areas, each with distinct ventilation requirements.

The building has a centralized air conditioning system managed by a Building Automation System (BAS). The BAS plays a critical role in controlling key aspects of the HVAC system, including fresh air intake, air distribution, and zone-specific ventilation rates. This system allows for real-time adjustments of the HVAC parameters based on occupancy and environmental conditions, ensuring that ventilation needs are met efficiently across the building's diverse spaces.

The classrooms utilize a mixed-ventilation system that includes supply air ceiling diffusers, linear slot diffusers, and return air ceiling grilles, ensuring effective air distribution within the space. These elements facilitate uniform air mixing, improve indoor air quality (IAQ), and help maintain comfortable and safe environmental conditions for occupants.

3.2 Experimental Design and Setup

3.2.1 CO2 Tracer Gas Testing Overview

To evaluate the performance of the building's ventilation system and its ability to manage indoor air quality (IAQ), CO2 tracer gas testing was employed. CO2 was selected as the tracer gas due to its well-established use as a surrogate for human exhalation and occupant-generated contaminants. Studies have shown that elevated indoor CO2 concentrations are closely associated with inadequate ventilation and can be a reliable proxy for air exchange effectiveness and contaminant buildup in indoor environments (ASHRAE, 2016).

CO2 was injected into selected zones of the building at controlled rates, with concentrations monitored over time to assess both the dispersion of air and the removal rate of CO2. This approach enabled a detailed examination of airflow patterns within individual zones and across multiple floors, providing critical data for subsequent calibration of the multi-zone airflow model.

3.2.2 Measurement Phases

The experimental design involved two distinct phases of CO2 tracer gas testing to capture airflow behaviors in different contexts:

1. **Phase1: Room-to-Floor Testing**

   CO2 was injected into Room 5670 on the 5th floor in the first phase. The aim was to monitor how the gas dispersed from the room into adjacent spaces on the same floor under various HVAC conditions. Measurements were taken at locations within the room and surrounding areas to observe local dispersion patterns. This phase helped to identify how contaminants spread from a single room to other zones, providing insights into localized ventilation performance.

2. **Phase 2: Floor-to-Floor Testing**

   The second phase involved injecting CO_2 into the 5th-floor corridor and tracking its spread to adjacent floors (4th and 6th floors). This phase assessed vertical airflows between floors, simulating how airborne contaminants move through shared spaces such as stairwells and corridors. This is particularly important in large multi-zone buildings where inter-zone airflows are critical for IAQ control (Rayegan et al., 2023).

3.2.3 CO2 Injection and Measurement Setup

CO_2 was injected into the test zones using an Alicat Mass Flow Controller, which regulated the injection rate with high precision. The gas was introduced 1.5 meters from the floor, simulating human breathing height by ASHRAE/ANSI Standard 55. The injection points were carefully selected to mimic real-world scenarios where contaminants might originate from human occupants.

Silicon rubber tubes connected the CO_2 cylinders to the mass controller to ensure uniformity and accuracy while tripods held the injection points at the designated height. Table 3 provides the technical specifications of the Alicat Mass Flow Controller used in the experiment.

Table 3. Mass Flow Meter Technical Characteristics

Range	0-500 LPM
Response Time	≤ 10 M.S
Accuracy	± 0.8% of reading ± 0.2% of full scale

CO_2 concentrations were measured using a Universal Gas Analyzer (UGA 100). The UGA 100 was connected to a manifold system with multiple outlets, allowing air samples to be drawn simultaneously from different rooms. This ensured efficient data collection, especially from rooms on different floors or distant locations. A vacuum pump assisted in drawing air samples into the analyzer, particularly from rooms far from the central measurement setup. Table 4 provides the details of the UGA 100 Device.

Table 4. UGA 100 Technical Details

Range	100 amu (atomic mass unit)
Response Time	< 200 M.S
Accuracy	± 5% of reading

3.2.4 Testing Protocols and Environmental Conditions

Before the start of each test, background CO_2 levels were measured to ensure baseline concentrations were accounted for. The environmental conditions of each room (temperature, humidity, HVAC settings) were monitored through the Building Automation System (BAS). The BAS provided real-time data on ventilation rates, temperature, and airflow settings, ensuring the experiments were conducted under controlled and repeatable conditions.

The tests were designed to simulate occupancy-driven ventilation scenarios (high CO_2 generation) and non-occupancy periods (low or no CO_2 generation). This approach allowed for the evaluation of the ventilation system's performance across different usage patterns and operating conditions.

Following the injection, CO_2 concentrations were continuously monitored until they returned to baseline levels, providing decay curves that were later used to evaluate the effectiveness of ventilation in removing contaminants from the air.

3.2.5 Experimental Assumptions and Limitations

For all tests, it was assumed that each zone represented a well-mixed air volume, meaning that CO_2 concentrations were uniform throughout the zone during each measurement period. Although this assumption simplifies the analysis, localized variations in airflow may still need to be fully captured. Future work could incorporate Computational Fluid Dynamics (CFD) to analyze more granular airflows at specific points (Dols & Polidoro, 2015).

3.3 Simulation Model Setup

3.3.1 Overview of the CONTAM Model

The simulation model used in this research was developed using the CONTAM 3.2 software, a widely recognized multi-zone airflow and contaminant transport modeling tool developed by the National Institute of Standards and Technology (NIST). CONTAM is designed to simulate indoor air quality (IAQ) and ventilation performance in large buildings by predicting how air and contaminants move through different zones (Dols & Polidoro, 2015).

The simulation model is designed with a crucial goal in mind: to accurately replicate real-world airflow and contaminant dispersion in a complex multi-zone building. This model represents the 16-story institutional high-rise at the Longueuil Campus of the Université de Sherbrooke, complete with a centralized HVAC system and various room types. Its primary function is to simulate CO2 concentrations under varying ventilation conditions, using CO2 as a tracer gas to mimic occupant-generated contaminants.

3.3.2 Modeling Assumptions and Parameters

The CONTAM model operates based on several key assumptions, simplifying large buildings' airflow and contaminant transport dynamics. These assumptions are commonly used in multi-zone modeling to balance computational efficiency with accuracy:

1. Well-Mixed Zones: Each room or zone in the building is assumed to be "well-mixed," meaning that air properties—such as temperature, pressure, and CO2 concentration—are

considered uniform throughout the zone. Localized effects such as stratification or turbulence are not explicitly modeled (Dols & Polidoro, 2015).

2. Mass Balance Equations: CONTAM uses mass balance equations to simulate contaminant concentrations within each zone. These equations account for:
    - Air exchange between zones via doors, windows, and ventilation ducts.
    - Contaminant sources, such as CO2 generation from occupants.
    - Infiltration and exfiltration through building envelopes.
3. Boundary Conditions: The boundary conditions for the simulation are determined by external weather data, including outdoor temperature, wind speed, and CO2 concentrations. These values are critical for determining infiltration and exfiltration rates across the building envelope (ASHRAE, 2019).
4. Ventilation System Dynamics: The model incorporates the building's ventilation system, controlled by the Building Automation System (BAS). The HVAC system is modeled to reflect its operation during field measurements, including supply and return airflow rates and pressure differences between zones.

3.3.3 Mass Balance Model for CO2 Concentration

The mass balance equation governs the simulation of contaminant concentrations in each room. It is based on the principle that the change in contaminant concentration within a room is determined by the balance between the incoming and outgoing airflows, internal sources of contamination, and the volume of the room. The general form of the mass balance equation is as follows:

$$\frac{dC(t)}{dt} = \frac{Q_{in} . C_{in} - Q_{out} . C(t) + S(t)}{V} \qquad (2.1)$$

Where:

- $C(t)$ is the contaminant concentration in the room at time t.
- Q_{in} is the flow rate of air into the room.
- C_{in} is the concentration of the contaminant in the inflow air.
- Q_{out} is the outflow rate of air from the room.
- $S(t)$ is the source term representing the rate of contaminant generation within the room.
- V is the volume of the room.

3.3.4 Discretization of the Mass Balance Equation

The continuous form of the mass balance equation is discretized for a numerical solution to simulate the evolution of CO2 concentrations over time in the CONTAM model. The discretized explicit form of the equation, used for iterative simulations at each time step, is given by:

$$C_{k+1} = C_k + \Delta t \frac{dC(t)}{dt} \qquad (2.2)$$

Where:

- C_{k+1} is the contaminant concentration at the next time step,

- C_k is the contaminant concentration at the current time step,

- Δt is the time step used for the numerical solution,

- $\frac{dC(t)}{dt}$It is the change in contaminant concentration over time, which is computed using the mass balance equation.

This discretized equation allows CONTAM to simulate contaminant concentrations iteratively, updating the concentration at each time step based on the current airflows, source terms, and ventilation rates. Depending on the required accuracy, numerical methods such as the Euler or Runge-Kutta method can solve this equation (Press et al., 2007).

3.3.5 Input Data for the Simulation

The CONTAM model relies on input data to simulate airflow and contaminant transport within the building. The key inputs for the simulation model include:

- Building Geometry: The physical layout of the building, including room volumes, door and window sizes, and inter-zone airflow paths, was recreated in CONTAM. CAD drawings accurately represented each floor's dimensions; this geometry was essential for defining the boundaries between zones (Figure 1).

- Ventilation Rates: The HVAC system parameters were imported from the BAS, which controls fresh air intake, exchange rates, and temperature set points. Where direct airflow measurements were unavailable, the BAS data was used to estimate each zone's supply and return flow rates.

- Occupancy Data: Occupancy levels were modeled to reflect the CO2 generation rate from human occupants. The CO2 generation rate was set based on standards, ranging between

0.002 and 0.01 l/s per person, depending on room type and occupancy density (ASHRAE, 2019).

- Infiltration and Exfiltration Rates: The infiltration rates were estimated based on typical values for buildings of this size and construction type regarding the Quebec Building Code for envelope performance (Quebec Code, 2015). Internal infiltration rates, such as air leakage between floors and zones, were similarly estimated.
- CO2 Source Term: CO2 was introduced into the model to simulate occupant-generated contamination. CO2 injection rates were based on real-world field data collected during the CO2 tracer gas tests. This input data allowed for an accurate representation of how contaminants would spread through the building during different operational scenarios.

Figure 1. Layout of the 5th Floor

3.3.6 Simulation Process

Once the input data was incorporated into the CONTAM model, the simulation was run for multiple scenarios, reflecting different ventilation and HVAC settings used during the field measurements. The following steps were taken during the simulation:

1. Baseline Simulation: A baseline simulation was conducted using standard HVAC settings (ventilation rates, temperature set points) as recorded by the BAS during non-occupancy periods. This provided a reference point for CO2 levels under normal operating conditions.

2. Contaminant Transport Simulation: CO2 injection was simulated in key zones (e.g., classrooms and corridors) to replicate the field measurements conducted during the tracer gas tests. The model tracked how CO2 dispersed through the building's ventilation system and between different floors.

3. Model Calibration: The simulation results from CONTAM were compared with the field measurement data. This comparison is essential for calibrating the model, ensuring that the simulation results align with real-world observations (Chapter 5 will discuss the calibration process in detail).

3.3.7 Model Output

The model produced time-dependent predictions of CO2 concentrations in each zone, allowing for an analysis of air exchange rates and contaminant dispersion throughout the building. These outputs were then used to evaluate the ventilation system's performance and identify areas with suboptimal airflow patterns.

The simulation results formed the basis for subsequent parametric analysis and calibration, in which specific parameters were systematically adjusted better to align the model's predictions with real-world data.

3.4 Parametric Simulation and Sampling

3.4.1 Parametric Simulation

Manual calibration of multi-zone airflow models is complex due to the numerous interacting parameters. To overcome this challenge, a parametric simulation approach was adopted to automatically explore the potential range of critical simulation parameters. The goal was to identify parameter sets that produce results closely aligned with experimental data.

Eight key parameters, including infiltration rates, CO2 generation rates, and occupancy levels, were selected for the parametric analysis based on their influence on model predictions.

A uniform distribution was assumed for each parameter to facilitate an unbiased parameter space exploration. This approach ensured an equal likelihood of all values within each range being selected during simulations.

The parametric analysis was implemented using CONTAM's Parametric Analysis Utilities (ContamFactorial 1.0). This utility generated multiple simulation project files with varying parameter values. A Python script was developed to run the simulations, extract results, and convert the data into a spreadsheet format for streamlined analysis.

3.4.2 Sampling

Given the vast number of possible parameter combinations, a full factorial simulation would have required millions of runs, making it computationally unfeasible. To address this, a sampling technique based on the Sobol method was applied. The Sobol method is a variance-based sensitivity analysis technique that effectively captures linear and non-linear correlations between inputs and outputs.

Using the Sobol method, the total number of simulations was reduced to 1,152 cases. This reduction allowed for efficient parameter space exploration while maintaining simulation accuracy.

3.5 Sensitivity Analysis

Sensitivity analysis was conducted to identify the most influential parameters affecting the accuracy of the multi-zone airflow model. This step simplifies the calibration process by focusing on parameters significantly impacting the model's predictions. The sensitivity analysis helped determine which uncertain parameters should be retained for calibration and which could be excluded without compromising model accuracy.

3.5.1 Objective of Sensitivity Analysis

The primary objective of the sensitivity analysis was to quantify the relative importance of key parameters influencing the model's predictions. This analysis was essential in prioritizing the calibration of those parameters that had the most significant impact on the simulated CO2 concentrations.

3.5.2 Sensitivity Analysis Methodology

A variance-based sensitivity analysis technique, specifically the Sobol Method, was employed to evaluate the effect of input parameters on model outputs. The Sobol method is particularly suited for multi-zone airflow models with non-linear parameter interactions, as it decomposes the total variance in model outputs into contributions from individual input parameters and their interactions.

Steps for Sensitivity Analysis:

1. Parameter Identification: Key uncertain parameters related to infiltration rates, internal CO2 generation rates, occupancy, and ventilation settings were selected based on their potential impact on the model's predictions. These parameters were identified through initial domain knowledge and a literature review.

2. Sampling Approach: A uniform distribution was assumed for each parameter, allowing for an unbiased parameter space exploration. The Sobol Sampling Method was applied to generate a comprehensive set of simulation parameter combinations. This method effectively captures both linear and non-linear interactions among parameters.
3. Simulation Runs: Using the CONTAM model, simulations were run for each combination of parameters generated by the Sobol sampling. The results provided a dataset of model outputs, which was used to calculate the sensitivity indices for each parameter.
4. Calculation of Sensitivity Indices: The Sensitivity Index (SI) for each parameter was computed using the Sobol method. The SI quantifies the proportion of variance in the model output attributable to each input parameter. Parameters with an SI greater than 0.05 significantly impacted model accuracy, while those with an SI below this threshold were deemed less influential.

3.5.3 Results of Sensitivity Analysis

The sensitivity analysis revealed that parameters related to initial indoor CO2 levels, indoor CO2 generation rates, and occupancy exhibited the highest sensitivity indices. These parameters were prioritized during the calibration process. Conversely, parameters with low sensitivity indices were excluded from further calibration to streamline the process and reduce computational costs.

The sensitivity analysis results guided the subsequent calibration efforts by focusing on the most influential parameters. This targeted approach helped improve the efficiency and accuracy of the model calibration using the Ensemble Kalman Filter (ENKF) and the Genetic Algorithm (GA).

3.6 Calibration

The multi-zone airflow model was calibrated to align the simulated CO2 dispersion results with observed field measurements. This section outlines the two primary calibration techniques employed: manual and automatic calibration using the Ensemble Kalman Filter (ENKF) and a Genetic Algorithm (GA).

3.6.1 Manual Calibration

Manual calibration served as the initial refinement step. Key parameters, such as infiltration and CO2 generation rates, were manually adjusted based on sensitivity analysis and expert judgment. The objective was to reasonably align simulation results and measured CO2 concentrations before employing more advanced automatic calibration techniques.

3.6.2 Ensemble Kalman Filter

The Ensemble Kalman Filter (ENKF) was employed to refine key model parameters using observational data iteratively. The ENKF is a data assimilation technique that extends the traditional Kalman Filter by utilizing an ensemble of model states, making it particularly effective for non-linear systems. The workflow for the ENKF calibration process is outlined as follows:

ENKF Workflow:

1. Initialization and Ensemble Generation: The ENKF generates an initial ensemble of model states. Each ensemble member represents a unique combination of key model parameters, such as infiltration rates, CO2 generation rates, and HVAC operational settings. The ensemble size is chosen based on computational considerations and the complexity of the

model. Parameter values for each ensemble member are drawn from probability distributions defined by the initial parameter ranges.

2. Forecast Step: During the forecast step, each ensemble member simulates CO2 concentrations across multiple building zones using the CONTAM model. The simulation results from each ensemble member are treated as predictions of the system's state.
3. Observation Integration: The observational data, consisting of measured CO2 concentrations at different locations and times, is integrated into the calibration process. The difference between the observed and forecasted CO2 concentrations is used to compute the Kalman Gain.
4. Update Step: The state of each ensemble member is updated using the Kalman Gain, which determines the extent to which the ensemble predictions are corrected based on observational data. The Kalman Gain is calculated by comparing the error covariance between the forecasted and observed states. This update step allows for real-time adjustment of model parameters, ensuring that the simulation results progressively converge toward the observed data.
5. Iterative Refinement: The ENKF process is repeated iteratively, with each forecast-update cycle producing increasingly accurate model predictions. The iteration continues until the model's performance meets predefined accuracy criteria, such as achieving a Coefficient of Variation of Root Mean Square Error (CVRMSE) below 15% and a Normalized Mean Bias Error (NMBE) below 5%.

The Ensemble Kalman Filter (ENKF) approach provides several advantages in multizone airflow modeling. One of its key strengths lies in its ability to refine parameters in real-time by continuously incorporating observational data as it becomes available. This dynamic feature enhances the model's predictive accuracy and responsiveness to changing conditions. Additionally, the ensemble-based nature of the ENKF makes it particularly effective for handling complex non-linear relationships, which are often present in multizone airflow models. This capability ensures that the method can accommodate intricate interactions between variables, resulting in more reliable simulations.

3.6.3 Genetic Algorithm (GA)

A Genetic Algorithm (GA) was used as an alternative automatic calibration method to systematically explore the parameter space. The GA approach leverages natural selection and evolution principles to identify the optimal set of parameters that minimize the fitness function, defined as the Root Mean Square Error (RMSE) between observed and simulated CO2 concentrations.

Genetic Algorithm Workflow: The GA was implemented using the following workflow:

1. Initialization and Parameter Setup: The algorithm starts by initializing a population of solutions, where each solution (or chromosome) represents a unique combination of perturbed parameters. The algorithm uses configuration data from a .csv file, including the number of perturbed parameters, measurement locations, crossover and mutation rates, and generations.
2. Simulation Execution for Each Generation: The GA perturbs parameters based on the current population and modifies the CONTAM input files accordingly for each generation. It then executes the CONTAM simulations. Simulation outputs are processed and matched with corresponding measurement locations and time tags.
3. Fitness Evaluation: The fitness of each solution is evaluated using the RMSE between simulated outputs and observed measurements. The GA reads the observations from the specified observation file, which includes measurement locations, time tags, and error ratios.
4. Selection and Genetic Operations: The algorithm selects the best-performing solutions as parents for the next generation. It applies crossover operations to combine selected parent solutions and mutation operations to introduce variability. Crossover is conducted using a

uniform crossover method, while mutation is applied to individual genes based on the predefined mutation rate.

5. Updating the Population and Repeating the Process: The new population of solutions is generated and repeated for a specified number of generations. After each generation, the GA saves the updated population and best-performing solutions to an output file.

The Genetic Algorithm (GA) approach provides distinct advantages over traditional manual calibration methods, particularly in multizone airflow modeling. One notable benefit is its ability to efficiently explore the parameter space by leveraging evolutionary operations such as crossover and mutation. This systematic exploration increases the likelihood of identifying optimal parameter combinations. Additionally, the GA is highly robust when dealing with non-linear relationships, enabling it to handle the complex interactions between parameters often encountered in multizone airflow models. This versatility makes it a powerful tool for addressing calibration challenges in such systems.

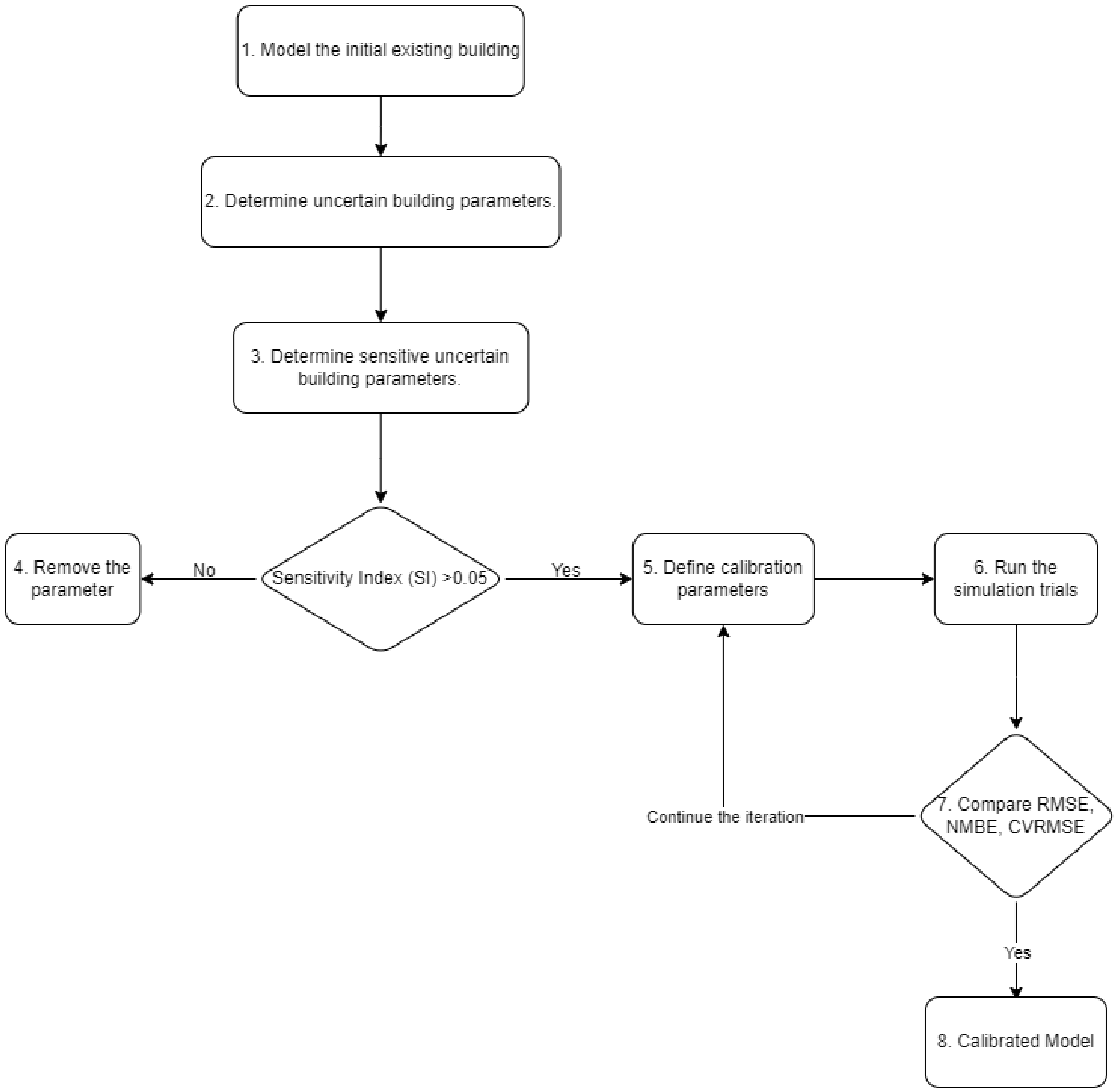


Figure 2. Calibration Methodology Diagram

Chapter 4

4. Experimental Measurements

4.1 Overview

This chapter presents the findings from CO_2 tracer gas tests conducted to evaluate the effectiveness of the ventilation system and the behavior of CO_2 dispersion in a multi-zone building. The experiments consisted of two types of tests: Room-to-Floor and Floor-to-Floor. These tests provided critical insights into the cross-zone and cross-floor movement of airborne contaminants, highlighting potential areas for improvement in air quality management.

4.2 Experimental Setup

4.2.1 CO_2 Injection and Measurement System

CO_2 was injected using a mass flow controller at carefully selected points on the fifth floor. Sensors were placed in key locations to capture variations in CO_2 concentrations within the injection zones and adjacent areas. These measurements were recorded using a Universal Gas Analyzer (UGA) system, which continuously monitored the CO_2 levels.

CO_2 was introduced into rooms or corridors to simulate localized sources of CO_2 emissions. The injection rate was controlled to replicate human breathing at a height of 1.5 meters. Sensor Placement: Sensors were installed near the injection points, in adjoining rooms, and in shared spaces such as stairwells and corridors to capture both horizontal and vertical dispersion of CO_2.

4.2.2 Types of Tests Conducted

Two types of tests were conducted to examine both horizontal and vertical contaminant movement within the building. The first type, referred to as room-to-floor tests, focused on monitoring CO_2 dispersion across rooms on the same floor. These tests aimed to analyze how CO_2 spreads horizontally through various spaces under different conditions, such as door positions and HVAC system configurations. The second type, floor-to-floor tests, investigated CO_2 movement between floors, emphasizing the role of shared spaces like stairwells in facilitating cross-floor contaminant transport. These tests provided insights into both localized and vertical airflow dynamics.

Figure 3 shows the exterior layout of the building. The floor plan in Figure 4 illustrates the locations of CO2 injection points and sensors on the fifth floor. CO2 was injected at the red-marked points, while sensors were installed in other rooms to capture CO2 concentrations in adjacent rooms and shared spaces. The legend also illustrates room functions.

Figure 3. Building Exterior

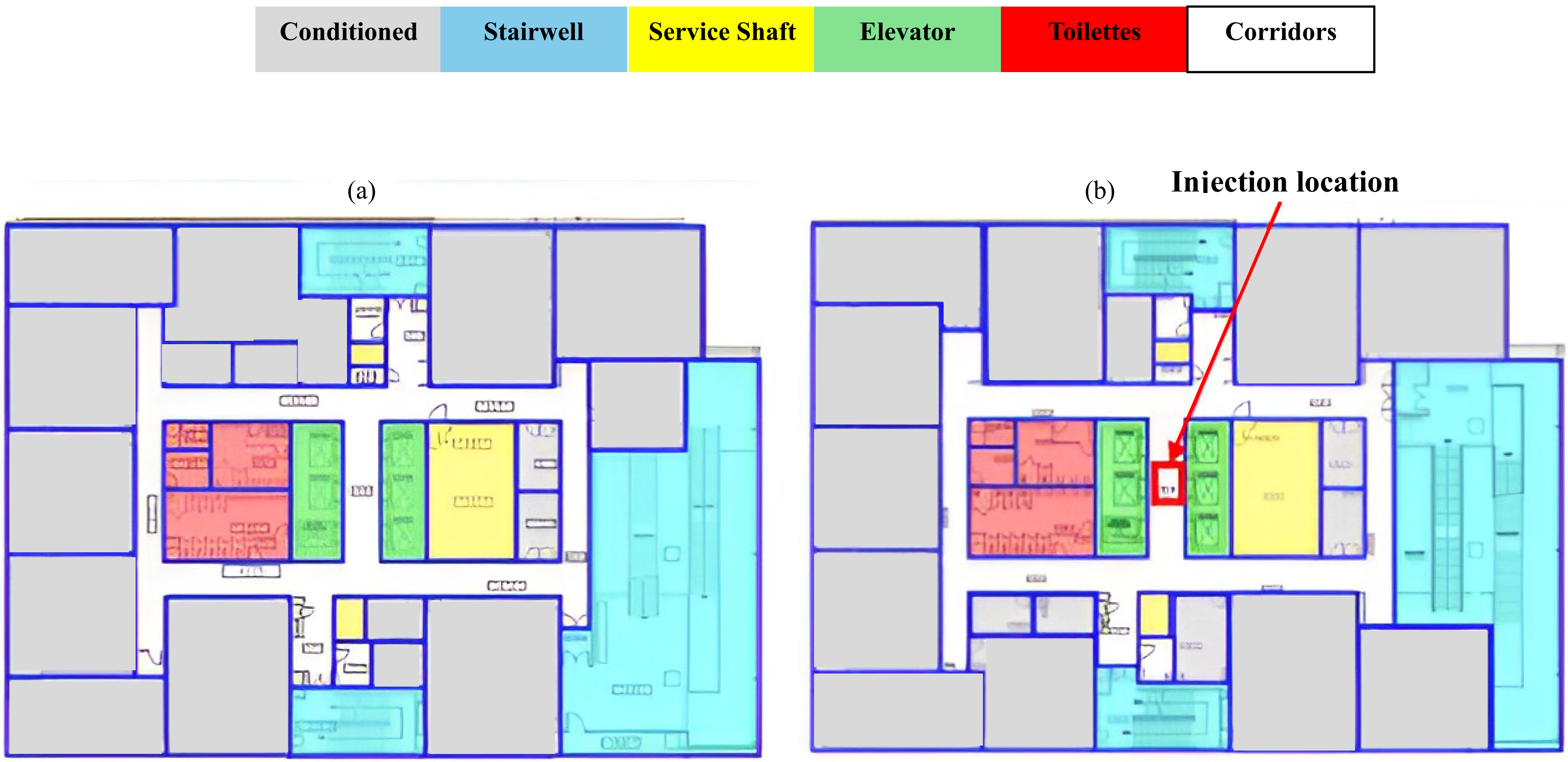


Figure 4. (a) 4th Floor layout, (b) 5th Floor layout

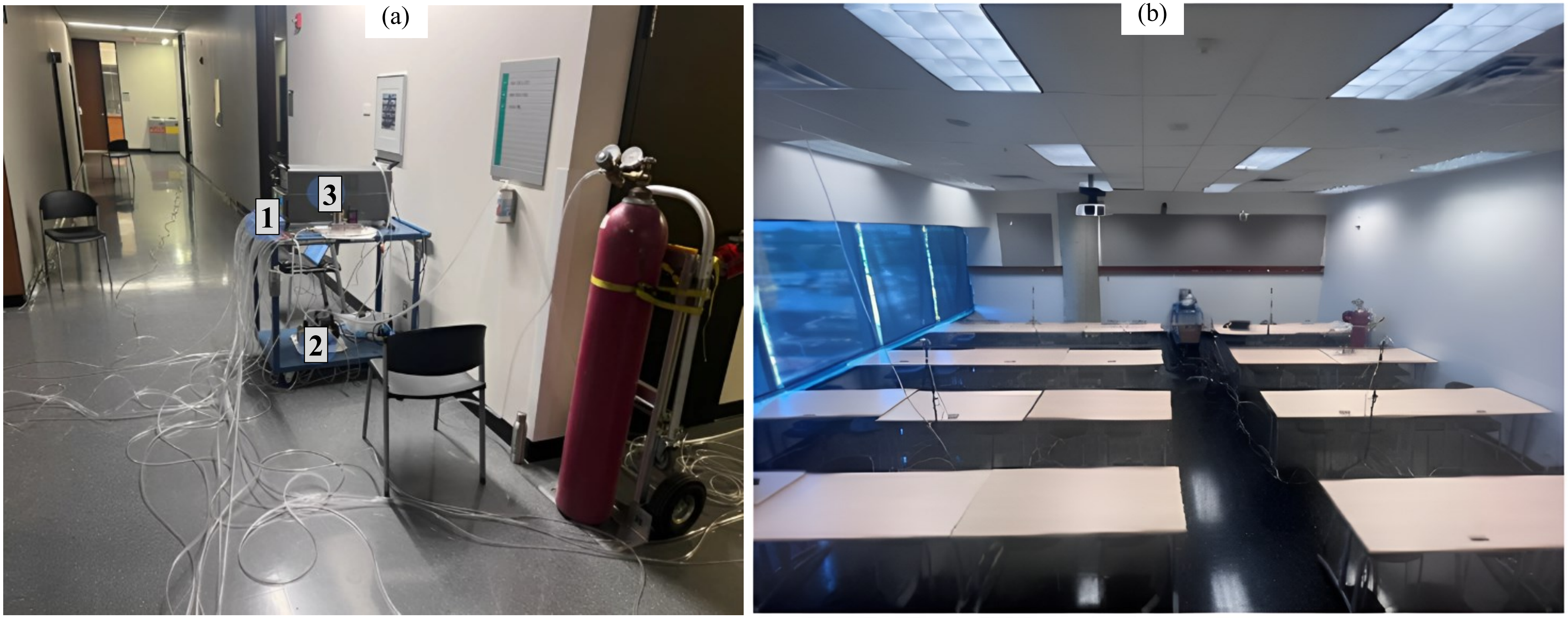


Figure 5. (a) UGA, CO2 cylinder, and sampling tubes in the corridor, (b) Tripods and sampling tubes in room 5670

1. Sampling tubes
2. Vacuum pump.
3. UGA 100.

4.3 Presentation of Results

4.3.1 Room-to-Floor Test Results

The room-to-floor tests revealed notable variations in CO2 concentrations across different rooms on the same floor. The highest concentrations were recorded in Room 5670, where the CO2 was directly injected. The rapid increase in CO2 concentration within Room 5670 was due to the proximity to the injection source. Consequently, the decay of CO2 in this room was also faster as the initial dispersion phase resulted in higher CO2 levels compared to other rooms.

The test results highlighted the significant influence of airflow dynamics, such as the positioning of doors and the effectiveness of the HVAC system, on the spread and removal of CO2. Figures X and Y below illustrate the concentration profiles in Room 5670 and four adjacent rooms located at the corners of the floor.

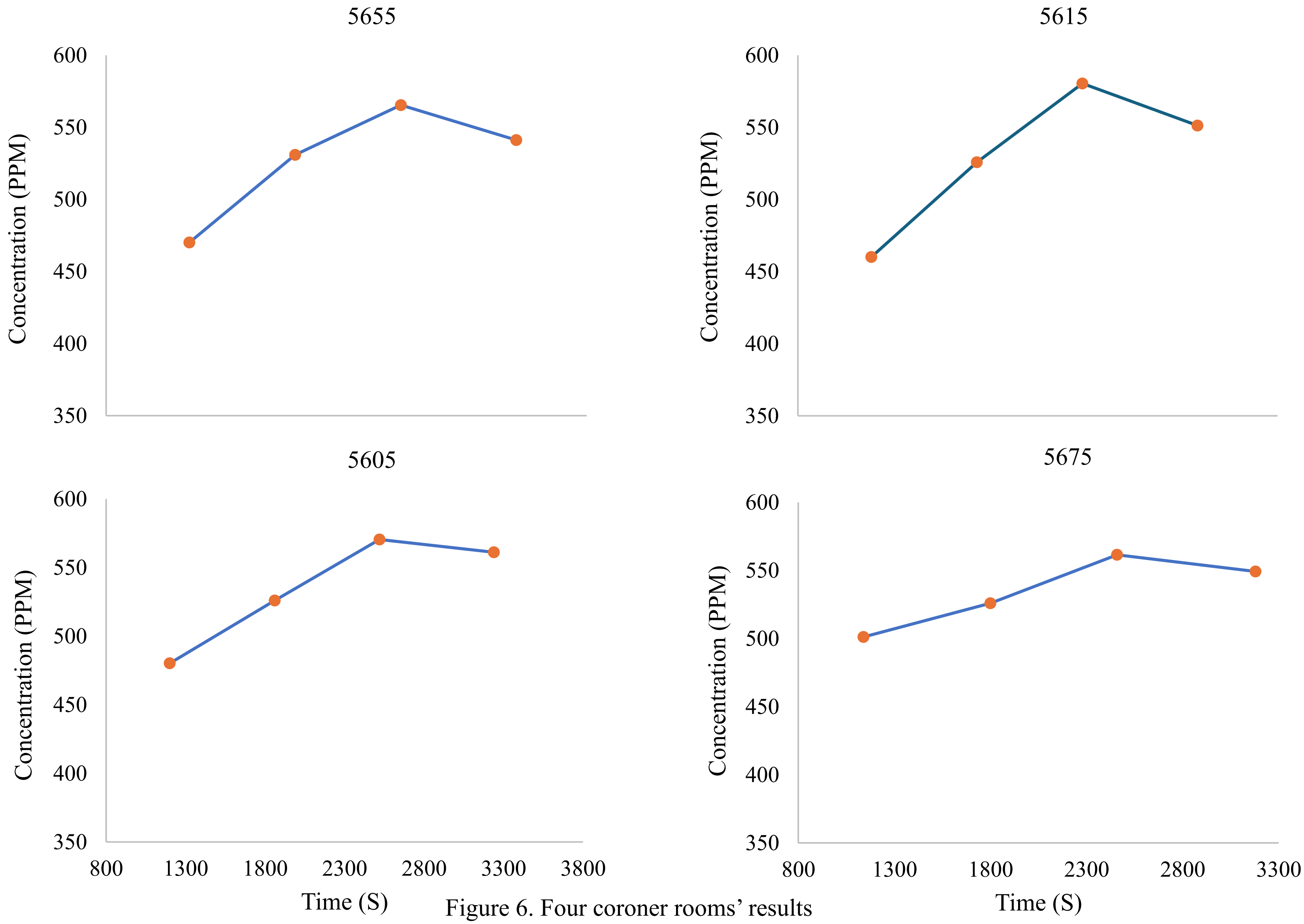


Figure 6. Four coroner rooms' results

In adjacent rooms, the rise in CO_2 concentration occurred more gradually. This delayed increase can be attributed to the dependency on CO_2 transport through multiple airflow pathways, including open doors, HVAC ducts, and return airflows. Specifically, CO_2 migrated from Room 5670 to neighboring rooms via both direct openings and the operation of the HVAC system, which recirculated air between rooms through the return air vents to the central Air Handling Unit (AHU). The AHU then redistributed the air back into different rooms, contributing to the delayed rise in CO_2 concentration outside of Room 5670.

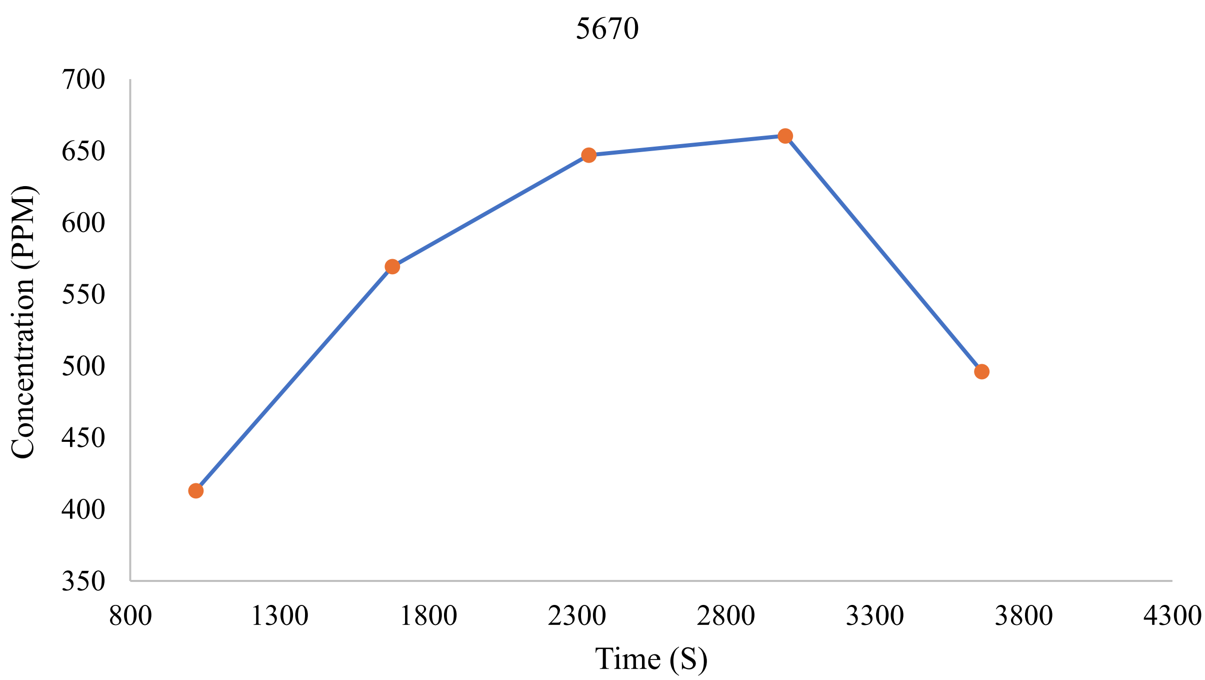


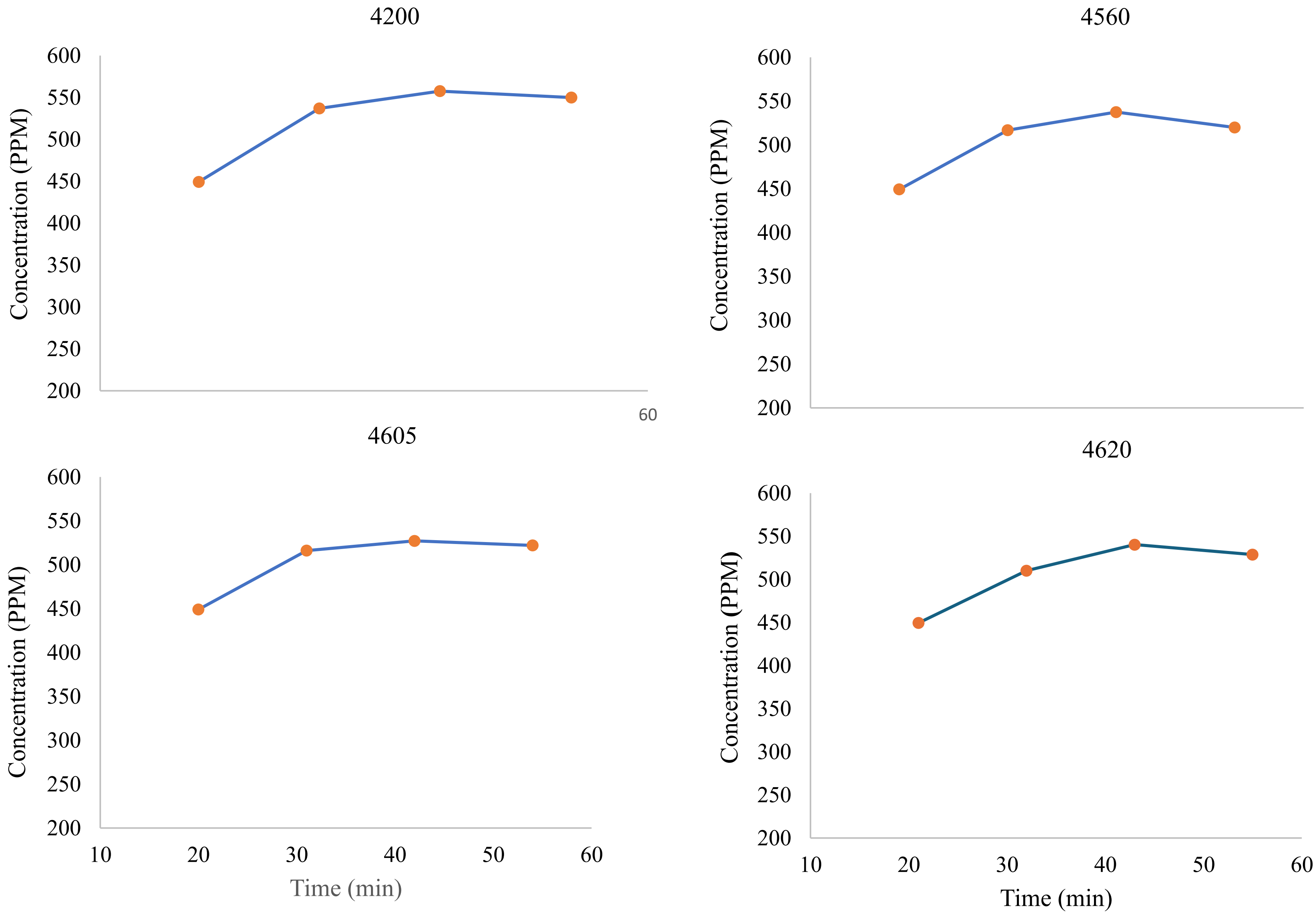
Figure 7. Results for room 5670, where the injection took place

4.3.2 Floor-to-Floor Test Results

The floor-to-floor tests demonstrated that CO2 spread vertically between floors predominantly through shared spaces such as stairwells and corridors. Elevated concentrations of CO2 were recorded in rooms directly connected to these spaces, indicating that the vertical transport of CO2 was significantly influenced by stairwell pressurization and the airflow dynamics within these areas.

The primary objective of these tests was to evaluate the extent and pathways of CO2 dispersion across multiple floors. Various infiltration pathways, including floor and wall penetrations, stairwells, and utility shafts, facilitated the spread of CO2 between floors. The return air system also contributed to redistributing CO2 between floors. A return air containing elevated CO2 concentrations was drawn back to the Air Handling Unit (AHU), and it was subsequently circulated through the supply ducts to different rooms, contributing to the vertical transport of CO2.

The test results highlighted the significant influence of airflow dynamics, such as door positioning and the effectiveness of the HVAC system, on the spread and removal of CO2. The figures below illustrate the concentration profiles in rooms on the 4th,5th, and 6th floors.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Concentration (PPM)
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4560
Concentration (PPM)
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300
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4605
Concentration (PPM)
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550
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450
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200
10
20
30
40
50
60
Time (min)
4620
Concentration (PPM)
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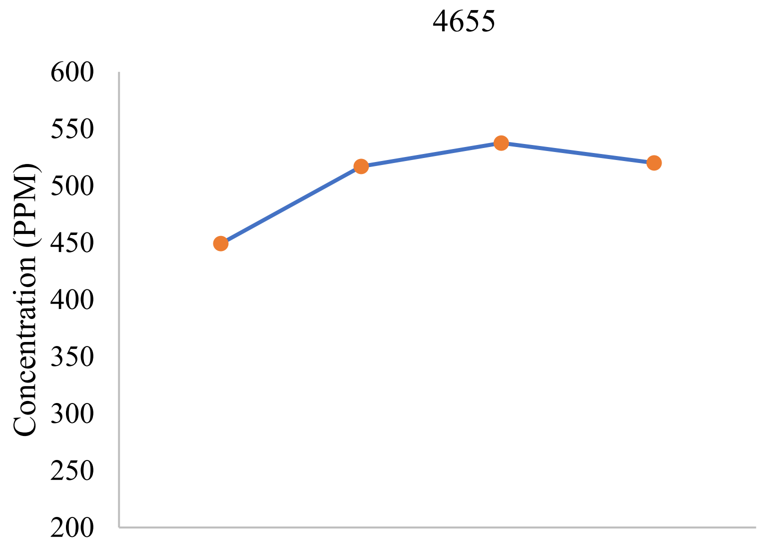
Time (min)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Concentration (PPM)
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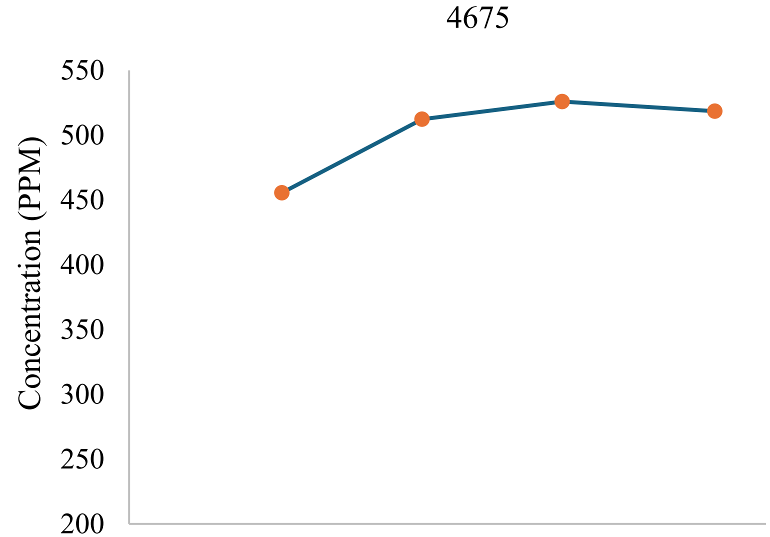
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Concentration (PPM)
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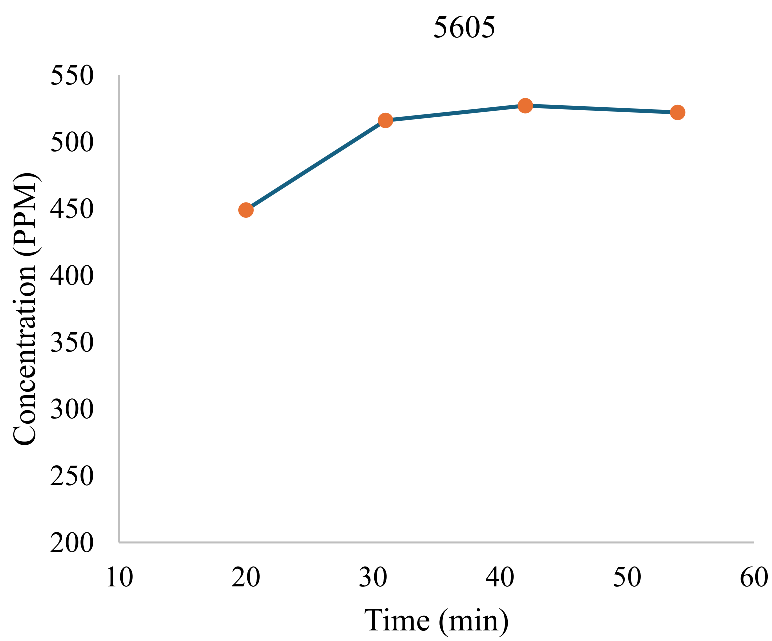
5605
Concentration (PPM)
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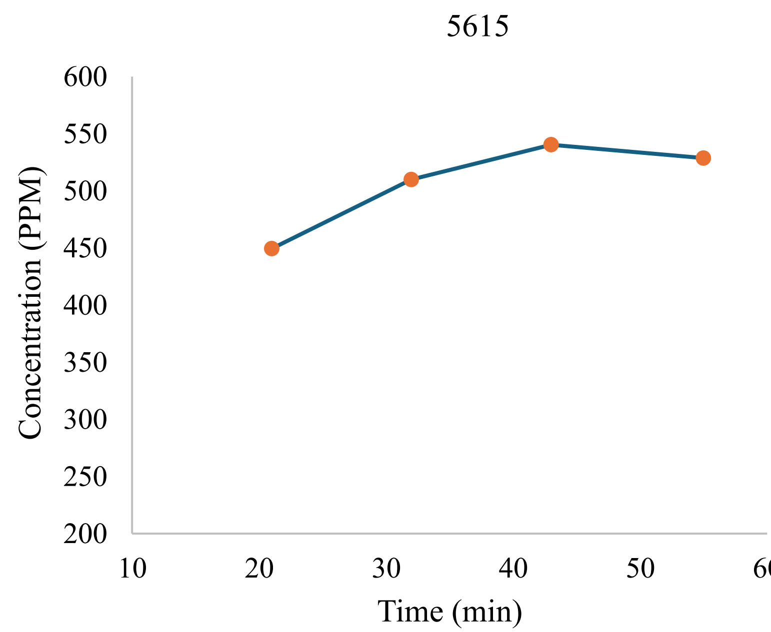
Time (min)


5615
Concentration (PPM)
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Time (min)

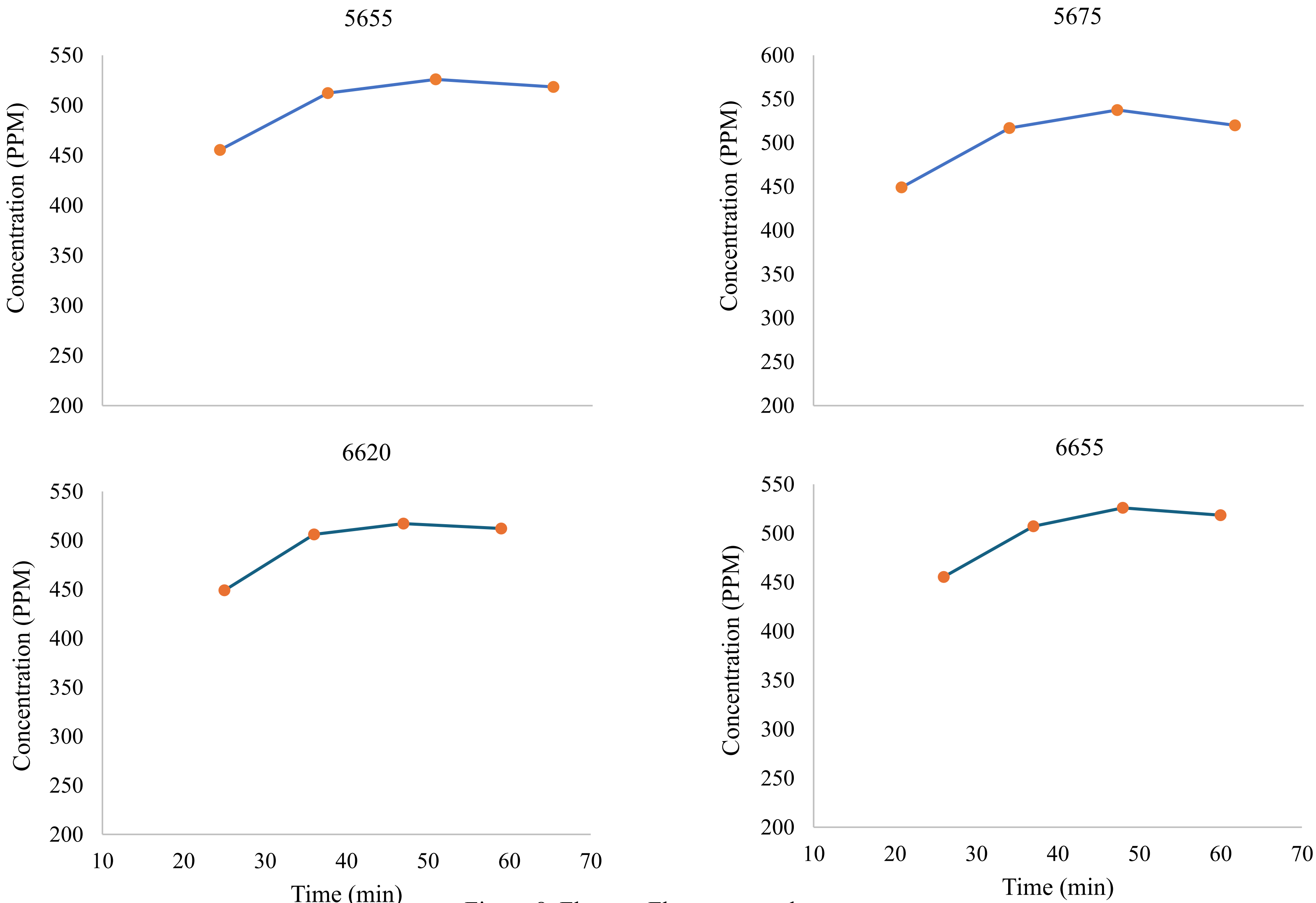


Figure 8. Floor-to-Floor test results

4.4 Analysis of the results

4.4.1 Room-to-Floor Test Analysis

Understanding airflow distribution and direction is crucial to explaining the complex relationship between CO_2 concentrations and the building's ventilation system. The 5th floor of the building, where the experiments were conducted, is positively pressurized, with a pressurization rate equal 10% of the total airflow. In contrast, restrooms are negatively pressurized, with air supply rates matching those used to pressurize other zones on the floor. This differential pressurization significantly affects CO_2 dispersion patterns across the floor.

The results, depicted in Figure 8, show that zones with negative pressure, such as the restrooms and the air handling unit (AHU) return location, exhibited significantly higher CO_2 concentrations when the ventilation system was enabled. Specifically, ΔCO_2 concentrations in these areas increased by 19%, 15%, and 33%, respectively. Similarly, the central corridor (Room 5200), which serves as a shared space, experienced a 10% higher exposure to ΔCO_2 concentrations than rooms with positive pressurization.

Interestingly, rooms closer to the CO_2 injection source exhibited lower exposure to CO_2, with reductions of 29% and 38%, respectively. This counterintuitive result is likely due to the more effective ventilation near the injection source, which rapidly removes CO_2 from the immediate area.

The four corner rooms presented inconsistent exposure values. For example, the nearest corners (Rooms 5675 and 5655) showed a significant increase in CO_2 concentrations by 34% and 32%, respectively, while the more distant corners (Rooms 5605 and 5615) experienced lower concentration increases of 37% and 1%. This suggests that the airflow dynamics in the building may not be distributed uniformly across the entire floor, with proximity to ventilation outlets and other architectural features playing a significant role.

4.4.2 Floor-to-Floor Test Analysis

In the inter-floor tracer tests, CO_2 was injected at the midpoint of the 5th floor, with six locations monitored on the 4th, 5th, and 6th floors. These locations included four corner zones (positive pressurization), a restroom (negative pressurization), and the central corridor. As with the room-to-floor tests, these experiments explored the impact of the ventilation system (on/off) with the doors closed.

On the lower (4th) floor, the CO_2 concentration was generally lower than on the 5th floor, with the lowest increase observed at one of the corner zones (Room 4620). However, the central corridor (Room 4200) exhibited the highest relative increase when the ventilation system was enabled. This suggests that shared spaces such as corridors, where airflow is directed, are key areas for vertical contaminant transport.

As expected, the highest concentration was observed on the 5th floor near the CO_2 injection point (Room 5200). Enabling the ventilation system resulted in a significant increase in CO_2 concentration in the corridor compared to when the ventilation system was disabled, highlighting the role of mechanical ventilation in recirculating air within the floor. In contrast, some corner zones (e.g., Room 5605) experienced lower CO_2 increases, suggesting that airflow distribution was uneven across the floor.

The same pattern was observed on the upper (6th) floor as on the 4th floor, with the corridor (Room 6200) showing the highest increase in CO_2 concentration when the ventilation system was enabled, while the southeast corner (Room 6675) experienced the smallest relative increase. This indicates that shared spaces like corridors accumulate more CO_2 due to vertical air movement, while corner rooms are less affected by cross-floor transport.

Key findings from these measurements can be summarized as follows:

The maximum CO_2 exposure on both the upper and lower floors occurred in the corridors when the ventilation system was enabled, and the doors were closed, representing approximately 15% of the peak concentration measured near the source on the 5th floor. In contrast, the minimal CO_2 exposure, around 4% of the peak concentration, was observed in one of the corner zones on the 6th floor under the same conditions. This highlights the significant role that ventilation systems and shared spaces play in the vertical transport of airborne contaminants in multi-zone buildings.

Chapter 5

5. Numerical Simulation and Calibration

5.1 CONTAM Model Setup and Implementation

The CONTAM model simulated the multi-zone airflow and CO_2 dispersion within the selected high-rise building. The model aimed to replicate the conditions observed in the field experiments, focusing on the interaction between the building's pressurization system, ventilation, and contaminant transport. This section provides an in-depth discussion of the critical features of the model setup, including boundary conditions, input parameters, and the specific modifications made to represent the building's ventilation system accurately.

5.1.1 Building Layout and Zoning

The CONTAM model was developed to represent the layouts of the 4th, 5th, and 6th floors, which were the primary focus of the experimental tests. Each floor was divided into zones based on their physical characteristics and functional purposes. Four corner rooms on each floor were modeled as individual zones with positive pressurization to reflect their controlled airflow conditions. Restrooms were assigned negative pressurization to replicate their actual ventilation setup. Corridors and stairwells, functioning as shared spaces, were modeled with neutral or slightly positive pressurization to align with the airflow dynamics observed during field measurements.

The geometry of the building was input into CONTAM using architectural floor plans, and the airflow paths between zones were defined by doorways, HVAC ductwork, and infiltration points (e.g., gaps around doors and windows).

5.1.2 Airflow and Pressurization Parameters

Pressurization levels played a crucial role in the simulation, determining the direction and airflow volume between different zones. To accurately replicate real-world conditions, the model included several key pressurization parameters. Positive pressure was applied to all zones except restrooms, set at a 10% rate. This ensured a more excellent supply of air compared to the return, effectively preventing the inflow of contaminants from adjacent areas. In contrast, restrooms were modeled with negative pressurization, reflecting their actual ventilation systems where exhaust airflow exceeded the supply. This pressure differential encouraged CO_2 inflow from nearby spaces, such as the central corridor. Meanwhile, corridors and stairwells were modeled with neutral or slightly positive pressurization, as these spaces were identified during experimental tests as critical pathways for contaminant transport both within and between floors.5.1.3 Ventilation System Configuration

The ventilation system, including the supply and return air paths, was meticulously modeled in CONTAM to replicate the experimental setup. The model featured an Air Handling Unit (AHU) that supplied conditioned air to the various zones on each floor. The flow rate of the supplied air was proportional to each zone's size and ventilation needs, ensuring adequate airflow to maintain intended pressurization levels. Excess air from the zones was routed back to the AHU via return air ducts.

The return air and recirculation processes were critical in redistributing CO_2 throughout the building. The model simulated CO_2-laden air being returned from individual zones to the AHU, mixed with fresh air before being recirculated to other areas. This recirculation mechanism significantly influenced CO_2 concentrations, particularly in zones far from the source, contributing to the buildup and transport of contaminants across floors.

5.1.3 Infiltration and Leakage

The model also accounted for infiltration pathways, such as door gaps, window cracks, and wall penetrations, which contributed to uncontrolled air exchange between zones and the external environment. These pathways were integrated into the simulation to capture their impact on airflow and contaminant movement. Infiltration rates were initially estimated based on standard building leakage rates and subsequently adjusted during calibration to align with observed CO_2 dispersion patterns.

Wall and floor infiltration was modeled using standard construction tolerances, with the rates varied to replicate the conditions observed in the field experiments. Additionally, stairwells and shafts connecting multiple floors were assigned higher infiltration rates to reflect their role in facilitating vertical airflow. These areas were identified during tracer gas experiments as critical conduits for cross-floor CO_2 transport, making their accurate representation essential to the model's ability to simulate contaminant dispersion realistically.

5.1.4 CO_2 Injection and Monitoring

CO_2 was injected into the model at the same points and rates as in the field tests to replicate the experimental conditions. CO_2 was injected into Room 5670 on the 5th floor for the room-to-floor tests. For the inter-floor tests, CO_2 was injected at the midpoint of the 5th floor to simulate cross-floor dispersion. The CO_2 concentrations were monitored at different locations on each floor, matching the sensor placement used in the experimental tests.

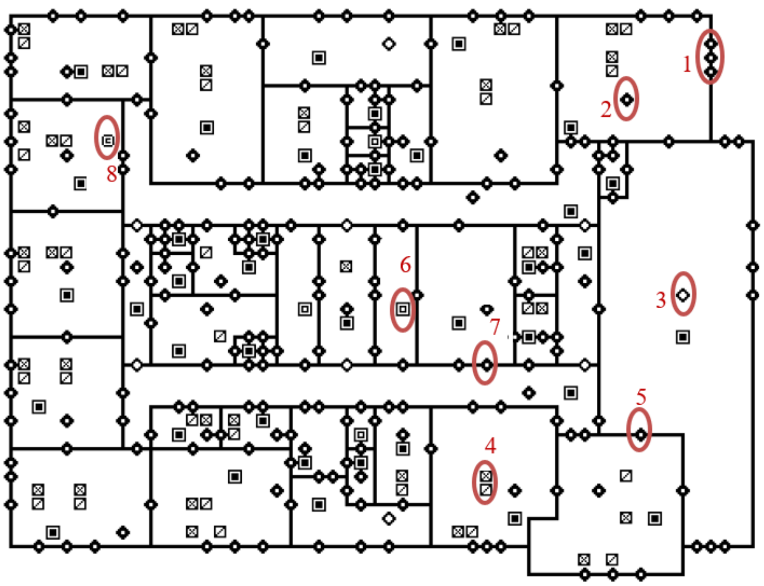
CONTAM simulated the transport of CO_2 through both mechanical ventilation (via supply and return ducts) and infiltration pathways. The model accounted for the time-varying nature of CO_2 concentration as air circulated between zones and floors.

5.1.5 Boundary Conditions and External Factors

The external environment, including outdoor air temperature, wind speed, and pressure conditions, was incorporated into the model as boundary conditions. These factors influenced the infiltration rates and the ventilation system's performance, particularly in areas near external walls and openings.

Outdoor Air Supply: The fresh air supply from the AHU was based on real-time outdoor conditions. The system was designed to introduce outdoor air at rates specified by ASHRAE standards. The model also accounted for fluctuations in outdoor CO_2 levels, which were monitored during the experiments to ensure accurate calibration of the indoor concentrations.

Figure 9 shows the CONTAM model layout for the fifth layout.



1- External Wall Leakage
2- Floor Leakage
3- Stair Leakage
4- AHU Supply & Return
5- Internal Wall Leakage
6- Elevator Shaft Leakage
7- Door Leakage
8- CO2 Injection Source

Figure 9. CONTAM Model Layout

5.2 Model Validation and Manual Calibration

5.2.1 Initial Model Validation

The CONTAM model was initially validated to assess its predictive accuracy before applying automatic calibration techniques. This process involved comparing the baseline simulation results with the experimental CO_2 measurements collected during the room-to-floor and floor-to-floor tests.

The baseline validation results indicated that while the model captured general CO_2 dispersion trends, there were discrepancies in certain zones, particularly in areas with complex airflow patterns or high variability in pressurization levels. These discrepancies underscored the need for further calibration to refine key parameters and improve the model's accuracy.

5.2.2 Manual Calibration Approach

A manual calibration process was performed to refine the initial simulation results and align them more closely with the observed data. This iterative approach focused on adjusting key model parameters to improve the predictive accuracy of the CONTAM model.

Infiltration rates for walls and floors were modified to represent better the observed air exchange and CO_2 transfer between zones. These adjustments ensured that the model accurately captured the uncontrolled airflow pathways contributing to contaminant dispersion. Additionally, the initial indoor CO_2 levels in various rooms were calibrated to reflect the observed buildup of CO_2 until the maximum concentration was reached. The calibration also accounted for the associated decay rates and the time required for CO_2 levels to return to baseline, further enhancing the model's ability to replicate real-world conditions.

Figure 10 shows the different trials for manually adjusting the parameters for one room. The trials involved changing the infiltration and outdoor CO2 values.

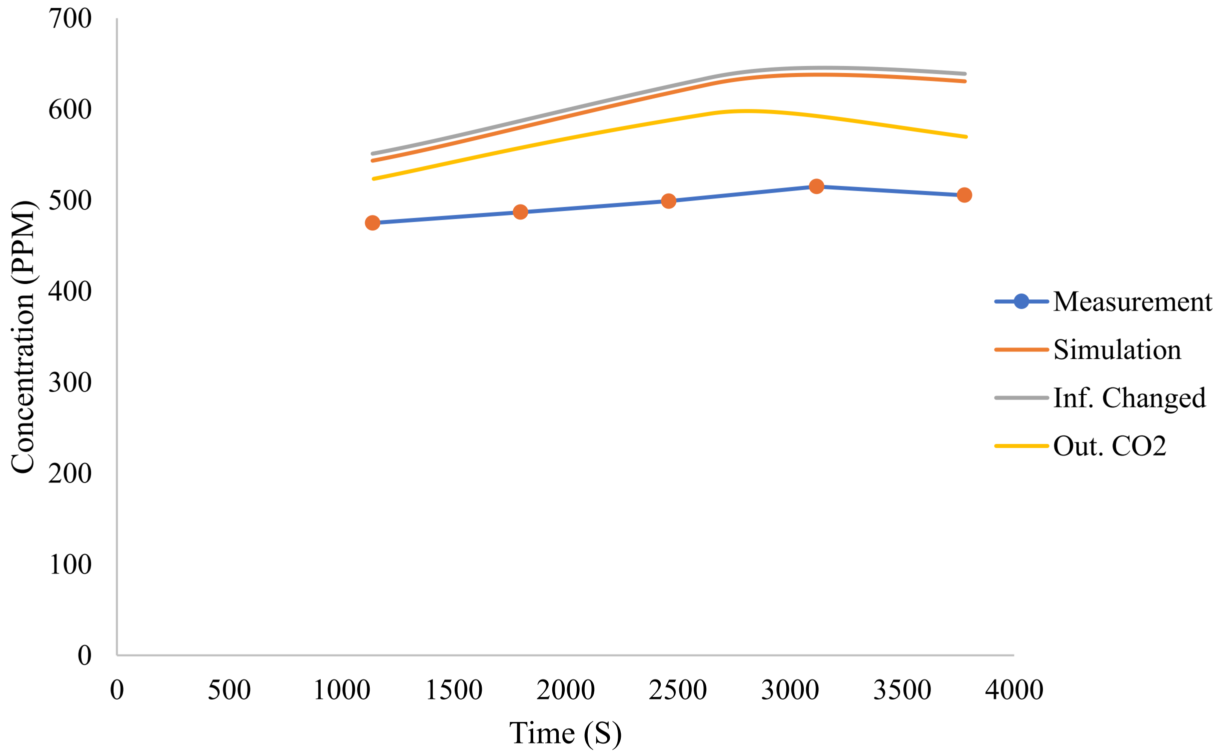


Figure 10. Manual Calibration Trials

5.3 Parametric Simulation and Sensitivity Analysis

5.3.1 Objectives of the Parametric Simulation

The parametric simulation was conducted to systematically explore the impact of critical parameters on CO_2 dispersion within the building model. This step was crucial for understanding how variations in each parameter affected the model's accuracy and identifying parameters with the most significant influence on CO_2 concentrations. These insights informed subsequent calibration efforts, allowing for a targeted model refining approach.

5.3.2 Selection of Key Parameters

Eight parameters were selected for the parametric simulation, which were informed by initial model validation and domain knowledge. These parameters were chosen due to their significant impact on indoor airflow and contaminant transport and their variability in real-world conditions.

Infiltration rates through walls, floors, and doors were included to represent the extent of air leakage between zones and floors. CO_2 generation rates were modeled to account for emissions from occupants and other sources within the building. Both outdoor and indoor CO_2 levels were considered to reflect the influence of external conditions on indoor air quality. Additionally, occupancy levels were included to simulate changes in CO_2 concentrations based on varying numbers of occupants.

Each parameter was systematically varied within a predefined range derived from field observations and standard building ventilation practices. This approach ensured that the simulation captured realistic variations and provided insights into the parameters' individual and combined effects on airflow and contaminant dynamics.

5.3.3 Simulation Setup

The parametric simulations were executed using a factorial design approach, enabling the exploration of multiple parameter combinations. CONTAM's Parametric Analysis Utilities (ContamFactorial 1.0) was employed to automate the process, generating separate simulation files for each parameter set. A Python script was developed to execute these simulations, extract CO_2 concentration data, and compile the results for sensitivity analysis.

The range for each parameter was set based on uniform distributions, allowing for equal probability across the selected range. Table 5 provides an overview of each parameter and its corresponding range.

Table 5. Ranges for Parameters used in the parametric simulation

Parameter	Uniform distribution range	Unit
External Wall Infiltration	0.25 +/- 20%	l/s.m^2
Internal Wall Infiltration	0.25 +/- 20%	l/s.m^2
Floor Infiltration	0.25 +/- 20%	l/s.m^2
Door Infiltration	4 – 27	cm^2
Outdoor CO2	396 – 416	ppm
Initial Indoor CO2	400 – 700	ppm
Indoor CO2 Generation Rate	0.002 – 0.01	l/s per person
Occupancy Count	0 – 40	-

5.3.4 Sensitivity Analysis Method

The sensitivity analysis employed the Sobol Method, a variance-based approach well-suited for non-linear models. This method decomposes the output variance into contributions from individual input parameters and their interactions, enabling a detailed understanding of parameter influence. The Sobol Method was selected for its ability to capture complex interactions between parameters, a critical requirement for accurately analyzing multizone airflow models.

Two key sensitivity indices were calculated to assess the parameters. The first-order sensitivity index (Si) quantified each parameter's direct effect on the model output, independent of interactions with other parameters. Meanwhile, the total-effect sensitivity index (STi) accounted for both the individual effects and the interactions, offering a more comprehensive evaluation of each parameter’s overall influence.

$$S_i = \frac{Var\ (E[Y|X_i])}{Var\ (Y)} \tag{5.1}$$

This measures the proportion of output variance Var (Y), which is explained by the variance of the conditional expectation of the output given the parameter X_i. It quantifies the direct contribution of X_i to the total variance.

$$S_{Ti} = 1 - \frac{Var\ (E[Y|X_{\sim i}])}{Var\ (Y)} \tag{5.2}$$

Where $X_{\sim i}$ represents all parameters except X_i. This index captures the direct effect of X_i and its interactions with other parameters provide a more comprehensive measure of its influence.

The sensitivity indices were computed based on variations in CO_2 concentrations at specific monitoring locations. Parameters with high sensitivity indices were identified as having the most significant impact on model accuracy and were prioritized in subsequent calibration steps to enhance the model's predictive performance.

5.3.5 Results of the Sensitivity Analysis

The sensitivity analysis identified the occupancy count, CO_2 generation rate, and initial indoor CO_2 concentration as the most influential parameters affecting the model's predictions. The initial indoor CO_2 concentration exhibited the highest total-effect sensitivity index, demonstrating its significant role in determining CO_2 levels. Starting concentrations strongly influenced how quickly CO_2 levels stabilized or reached equilibrium within each room.

Occupancy count ranked as the second most influential parameter, reflecting its substantial impact on CO_2 levels due to the emissions generated by additional occupants. Similarly, the CO_2 generation rate showed a high sensitivity index, as variations in per-person CO_2 production directly affected the concentration in each zone.

By contrast, parameters such as infiltration rates had notably lower sensitivity indices. This indicates that, under the modeled conditions, variations in infiltration had a relatively minor impact on CO_2 dispersion. This outcome can likely be attributed to the high efficiency of the mechanical ventilation system, which effectively regulated airflow and minimized the influence of uncontrolled air leakage across zones.

Table 6 shows the SI values for every parameter. Figure 11 shows the distribution of the indices.

Table 6. Sensitivity Index Value for Every Parameter

Parameter	Sensitivity Index (SI)
External Wall Infiltration	0.002
Internal Wall Infiltration	0.001
Floor Infiltration	0.001
Door Infiltration	0.005
Outdoor CO2	0.01
Initial Indoor CO2	0.461
Indoor CO2 Generation Rate	0.21
Occupancy Count	0.31

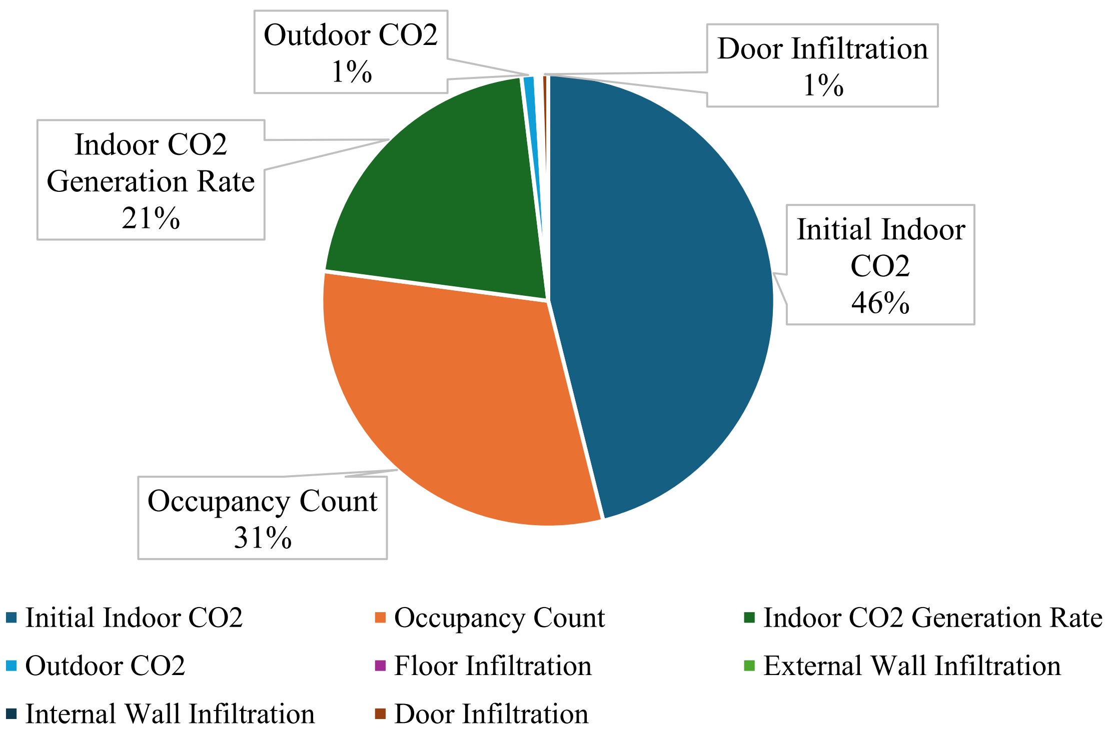


Figure 11.The percentage of contribution of every parameter

5.3.6 Implications for Model Calibration

The sensitivity analysis results provided a clear pathway for the calibration process. Calibration efforts were focused on these variables, with occupancy count, CO_2 generation rate, and initial indoor CO_2 concentration identified as the most impactful parameters. By prioritizing adjustments to these factors, the model could be optimized effectively without unnecessarily recalibrating less influential parameters, streamlining the calibration process and enhancing model accuracy.

5.4 Calibration Using ENKF and GA

Effective calibration of the CONTAM model was achieved through a combination of the Ensemble Kalman Filter (ENKF) and the Genetic Algorithm (GA). These complementary methods were applied to iteratively refine critical parameters, including occupancy count, CO_2 generation rate, and initial indoor CO_2 concentration, to improve the model's ability to simulate CO_2 dispersion accurately.

5.4.1 Ensemble Kalman Filter (ENKF) Calibration

The Ensemble Kalman Filter (ENKF) was employed to iteratively refine model parameters by integrating observational data. This approach followed a dynamic forecast-update cycle, making it highly effective for resolving real-time discrepancies between the model's predictions and experimental measurements.

The ENKF calibration process began with an initialization step, where an ensemble of 20 model realizations was generated. Each realization featured slightly varied values for the target parameters to introduce diversity and account for uncertainties. During the forecast step, each ensemble member was used to simulate CO_2 concentrations within the CONTAM model, producing a range of predicted outputs.

In the observation integration step, the simulated CO_2 concentrations were compared to the field measurements, and the differences between the two were quantified. These discrepancies informed the update step, where the Kalman Gain was calculated to adjust the parameter values of each ensemble member. This iterative adjustment processes reduced errors between the simulated and observed results, progressively improving the model's accuracy.

A. Room-To-Floor Test

The Room-to-Floor tests were conducted on the 5th floor to evaluate the horizontal dispersion of CO_2 across different zones. These zones were chosen to capture a range of ventilation and pressurization conditions, reflecting the building's airflow dynamics. The primary objective of these tests was to assess the effectiveness of the HVAC system and inter-zone airflow in managing CO_2 concentrations within a single floor. The ENKF was applied to calibrate the model parameters based on these measurements, focusing on reducing discrepancies between observed and simulated CO_2 levels.

Figure 12 compares simulated and observed CO_2 concentrations for monitored zones on the 5th floor (corner rooms) after ENKF calibration.

The figures show that the Root Mean Square Error (RMSE) decreased by approximately 25%, particularly in zones with complex airflow patterns. The method demonstrates its efficiency in refining parameters such as initial indoor CO_2 levels. ENKF proved effective for rapid adjustments, making it well-suited for cases requiring near-real-time calibration.

Comparisons between the RMSE, CVRMSE, and NMBE will be provided after the GA section to compare the results of the two algorithms.

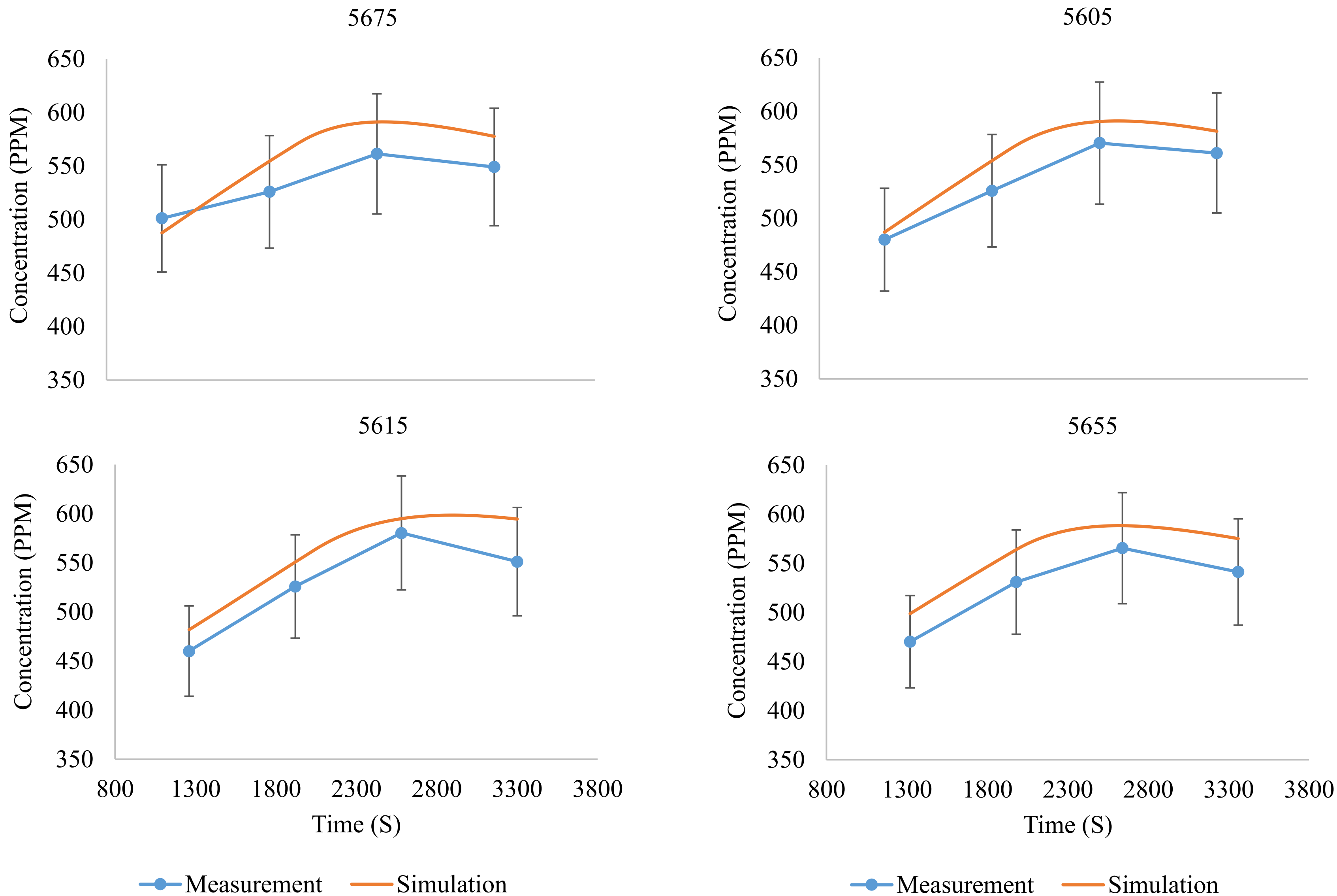


Figure 12. ENKF Results for Room-to-Floor test

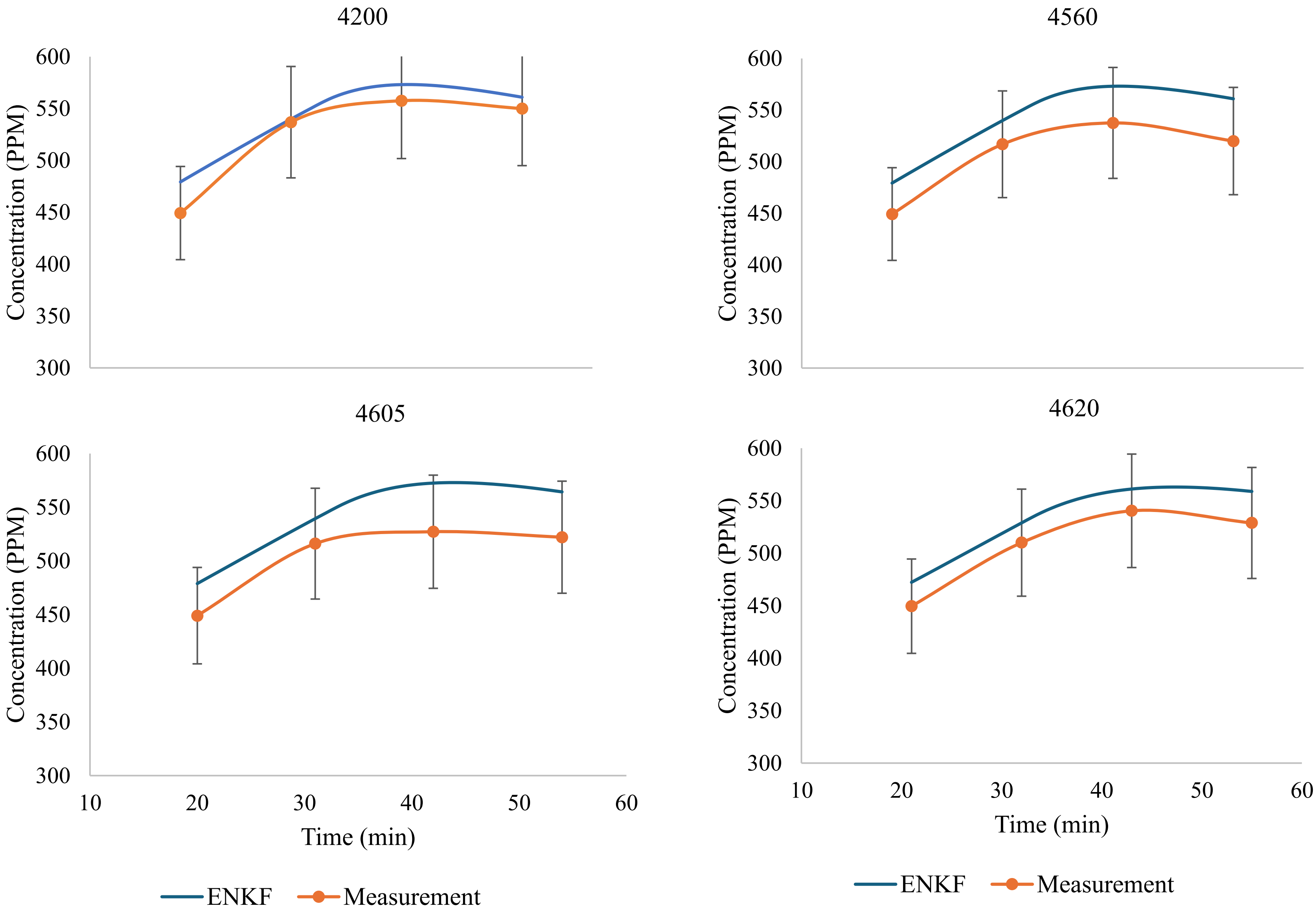
B. Floor-to-Floor Tests

The Floor-to-Floor tests were designed to examine the vertical transport of CO_2 between the 4th, 5th, and 6th floors, focusing on shared spaces like stairwells and corridors, as well as corner rooms and restrooms. These tests highlighted the role of cross-floor airflow and pressurization differences in contaminant transport. The calibration process uses the ENKF-targeted parameter adjustments to improve the model's ability to capture these vertical interactions and align simulated results with observed data.

Figure 13 compares simulated and observed CO_2 concentrations for monitored zones on the 5th floor (corner rooms) after ENKF calibration.

The figures show that the Root Mean Square Error (RMSE) decreased by approximately 25%, particularly in zones with complex airflow patterns. The method demonstrates its efficiency in refining parameters such as initial indoor CO_2 levels. ENKF proved effective for rapid adjustments, making it well-suited for cases requiring near-real-time calibration.

Comparisons between the RMSE, CVRMSE, and NMBE will be provided after the GA section to compare the results of the two algorithms.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Concentration (PPM)
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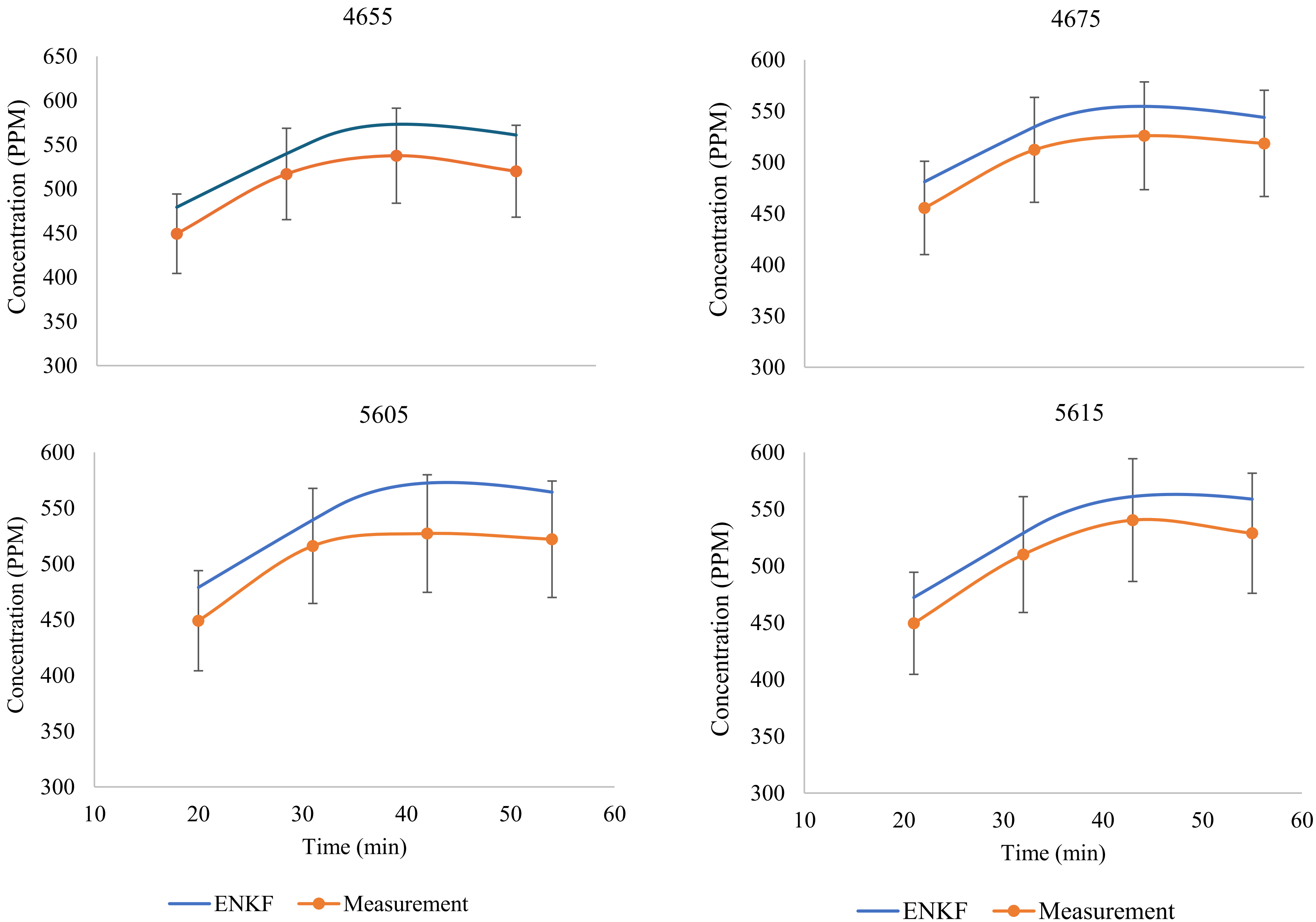
Time (min)
ENKF
Measurement


4655
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Concentration (PPM)
Time (min)
ENKF
Measurement

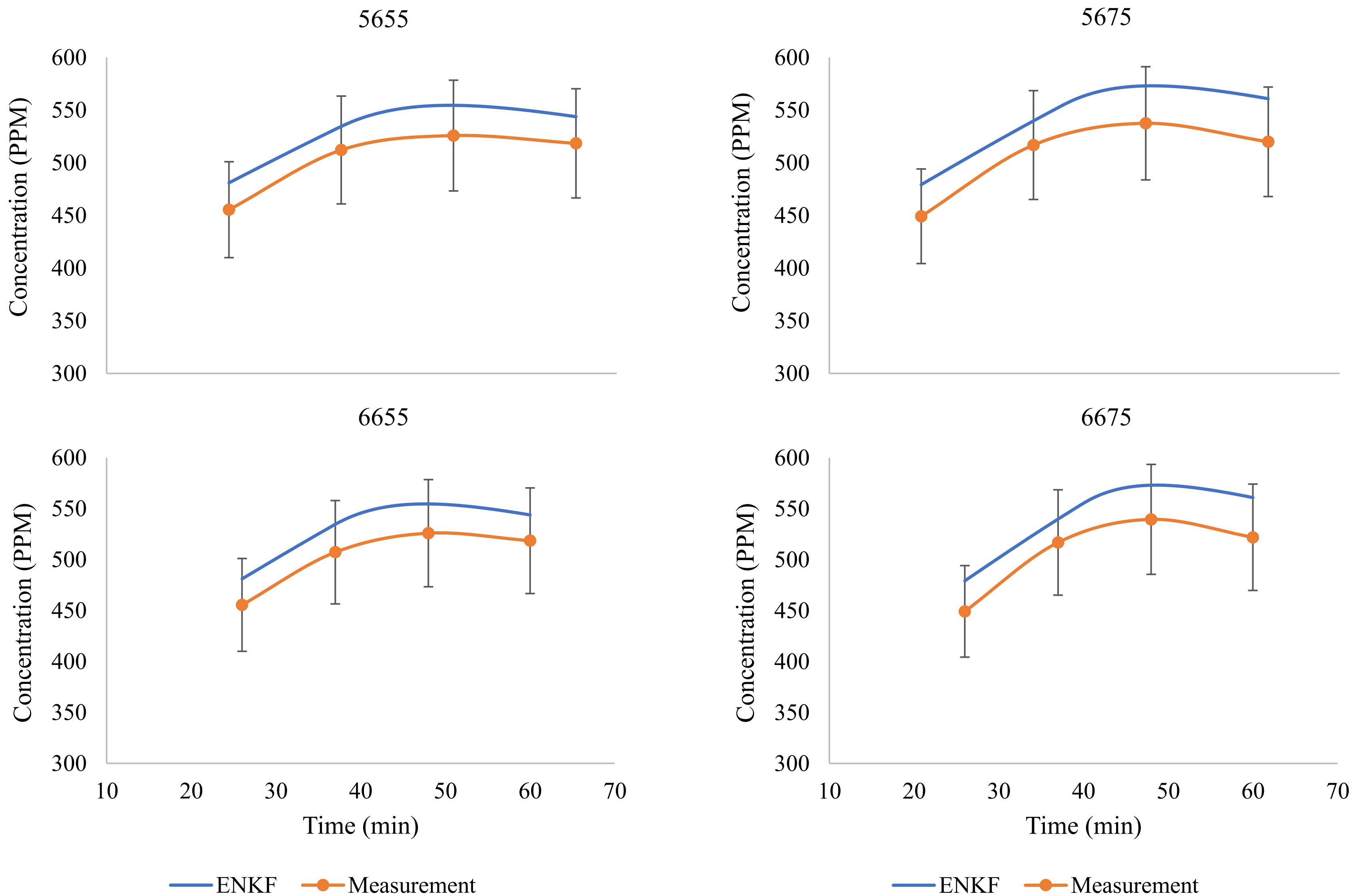


Figure 13. ENKF Results for Floor-to-Floor tests

5.4.2 Genetic Algorithm (GA) Calibration

The Genetic Algorithm (GA) was employed alongside the ENKF to explore a broader range of parameter combinations and address non-linear interactions that the ENKF might find challenging. Unlike ENKF, which relies on data assimilation, the GA leverages evolutionary principles to optimize model parameters through iterative improvement.

The GA calibration process began with the initialization of a population consisting of 50 chromosomes, each representing a unique parameter set. The fitness of each chromosome was then evaluated by calculating the root mean square error (RMSE) between simulated and observed CO_2 concentrations, providing a quantitative measure of accuracy.

Genetic operations were subsequently applied to refine the population. During the selection phase, the top-performing chromosomes were chosen as parents based on their fitness scores. These parent chromosomes were combined in the crossover step, where their parameters were recombined to produce offspring. To prevent the algorithm from converging on local optima, a mutation step was introduced, incorporating random changes to some of the parameters.

This iterative process of evaluation, selection, crossover, and mutation was repeated over 20 generations, gradually improving the population's overall fitness and converging on parameter sets that minimized errors between the model predictions and the observational data.

A. Room-to-Floor test

The Room-to-Floor tests provided a comprehensive dataset for evaluating the horizontal movement of CO_2 across zones with varying pressurization and ventilation conditions. The GA was applied to optimize parameters such as occupancy count, CO_2 generation rate, and initial CO_2 concentrations to align the simulated and observed data better. The iterative nature of the GA allowed for a thorough exploration of parameter interactions, particularly in zones with complex airflow patterns.

Figure 14 compares simulated and observed CO_2 concentrations for monitored zones on the 5th floor (corner rooms) after GA calibration.

The figures show that the Root Mean Square Error (RMSE) decreased by approximately 25%, particularly in zones with complex airflow patterns. The method demonstrates its efficiency in refining parameters such as initial indoor CO_2 levels. GA proved effective for rapid adjustments, making it well-suited for cases requiring near-real-time calibration.

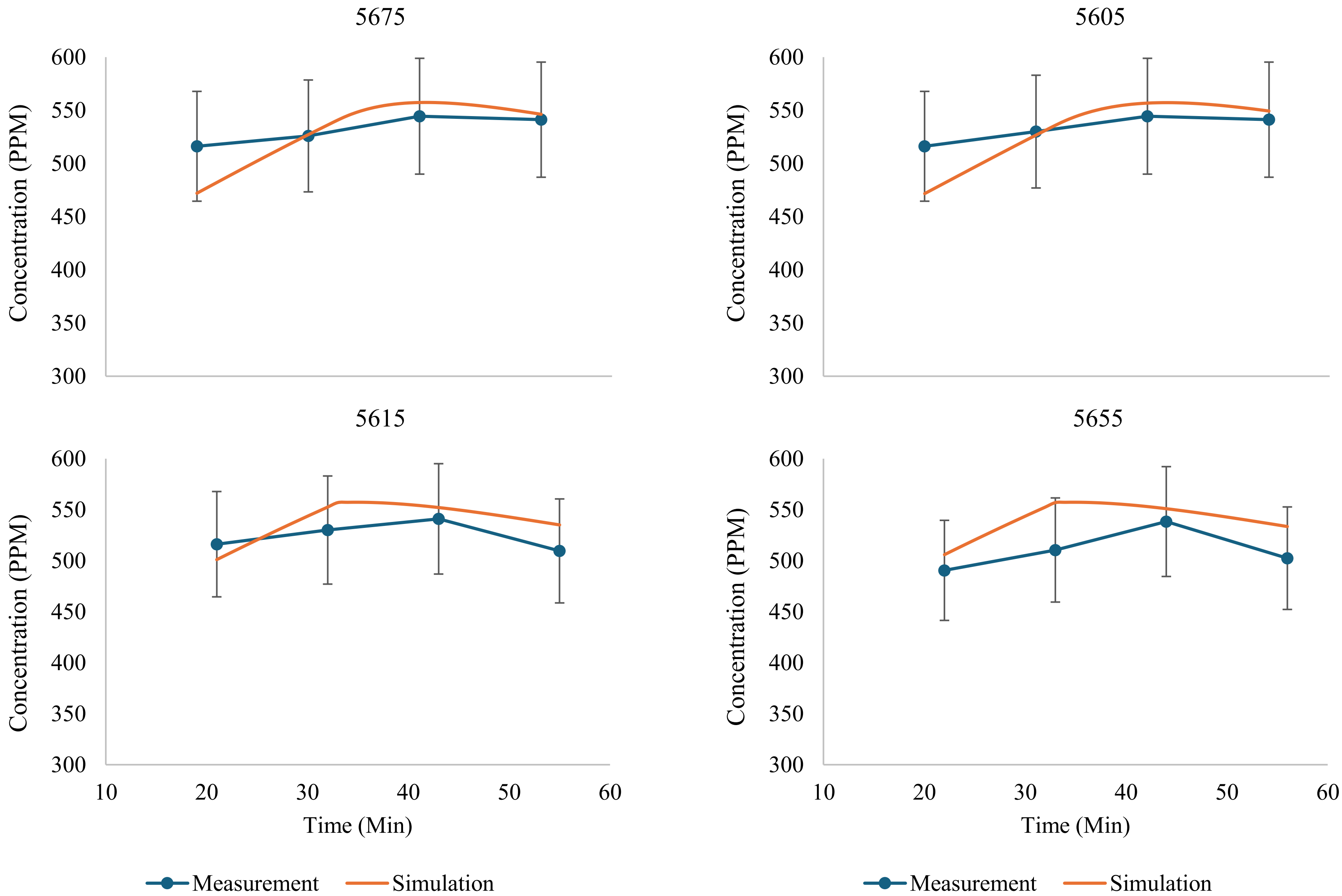


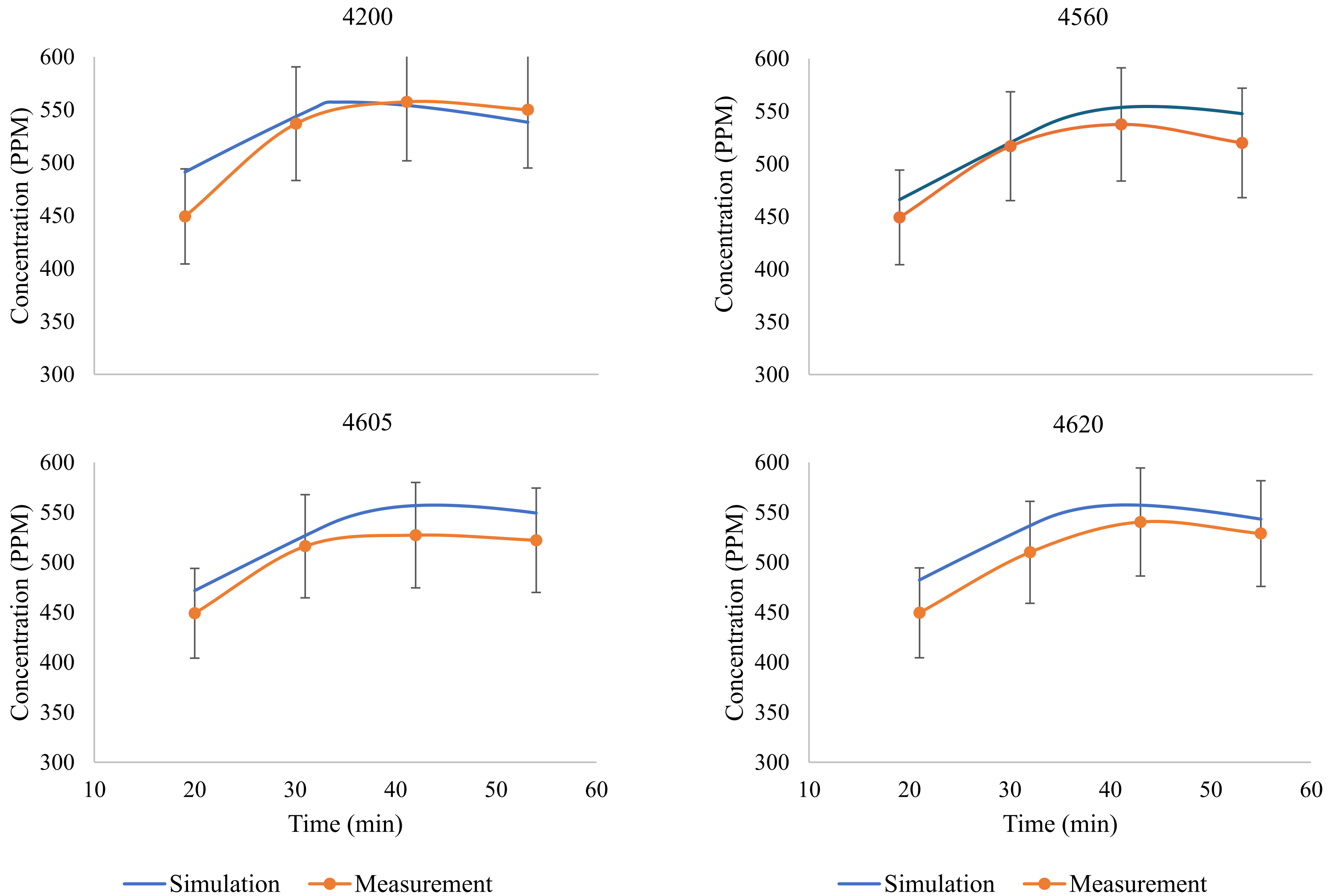
Figure 14. GA Results for Room-to-Floor test

B. Floor-to-Floor Tests

The Floor-to-Floor tests revealed critical insights into the transport of CO_2 between floors via shared spaces and mechanical ventilation. Using the GA, the model parameters were fine-tuned to better replicate the observed vertical dispersion patterns. This process effectively captured non-linear interactions between parameters that influenced cross-floor contaminant transport.

Figure 15 compares simulated and observed CO_2 concentrations for monitored zones on the 5th floor (corner rooms) after ENKF calibration.

The figures show that the Root Mean Square Error (RMSE) decreased by approximately 25%, particularly in zones with complex airflow patterns. The method demonstrates its efficiency in refining parameters such as initial indoor CO_2 levels. ENKF proved effective for rapid adjustments, making it well-suited for cases requiring near-real-time calibration.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Concentration (PPM)
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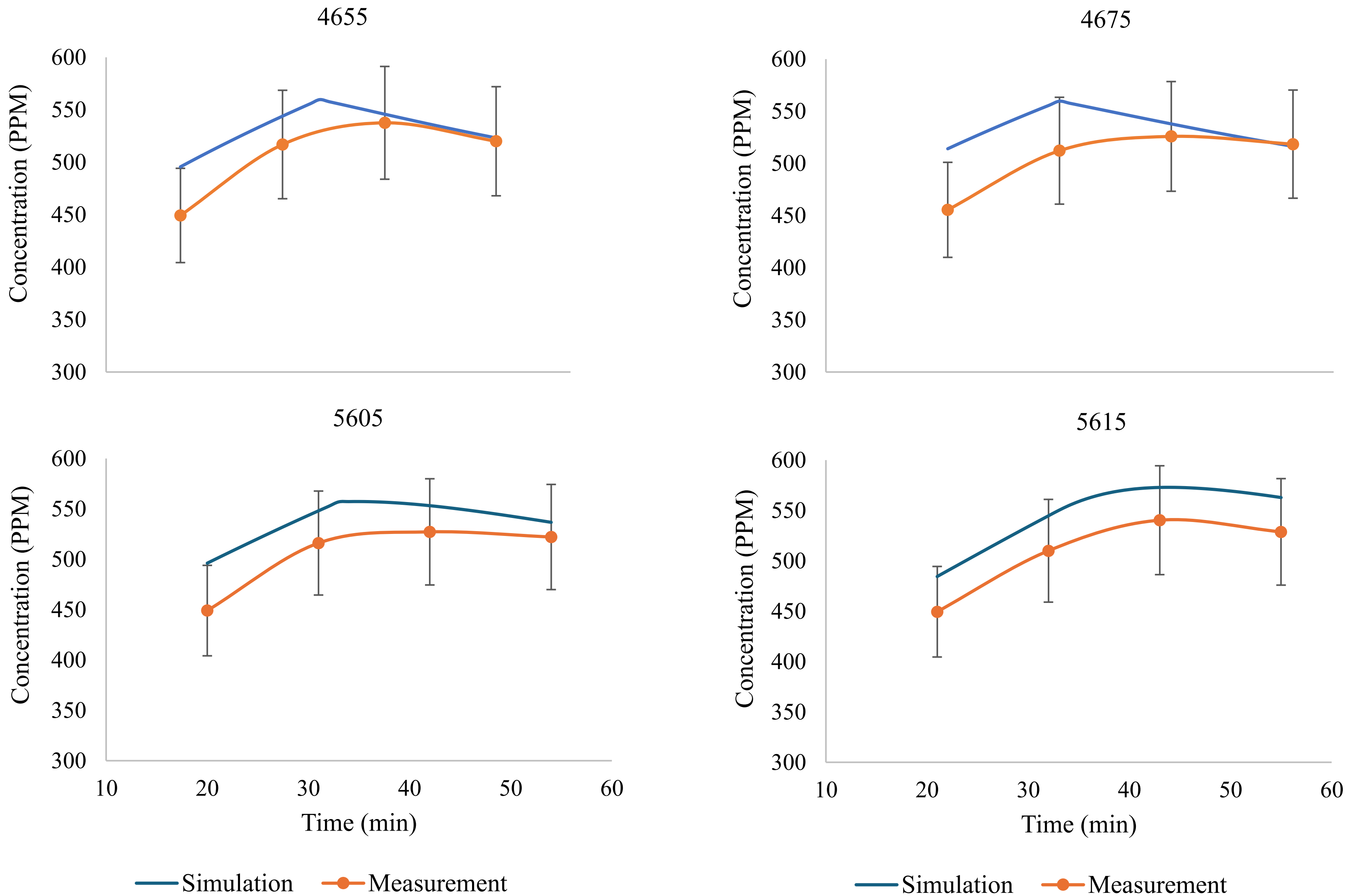
Time (min)
Simulation
Measurement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Concentration (PPM)
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Time (min)
Simulation
Measurement

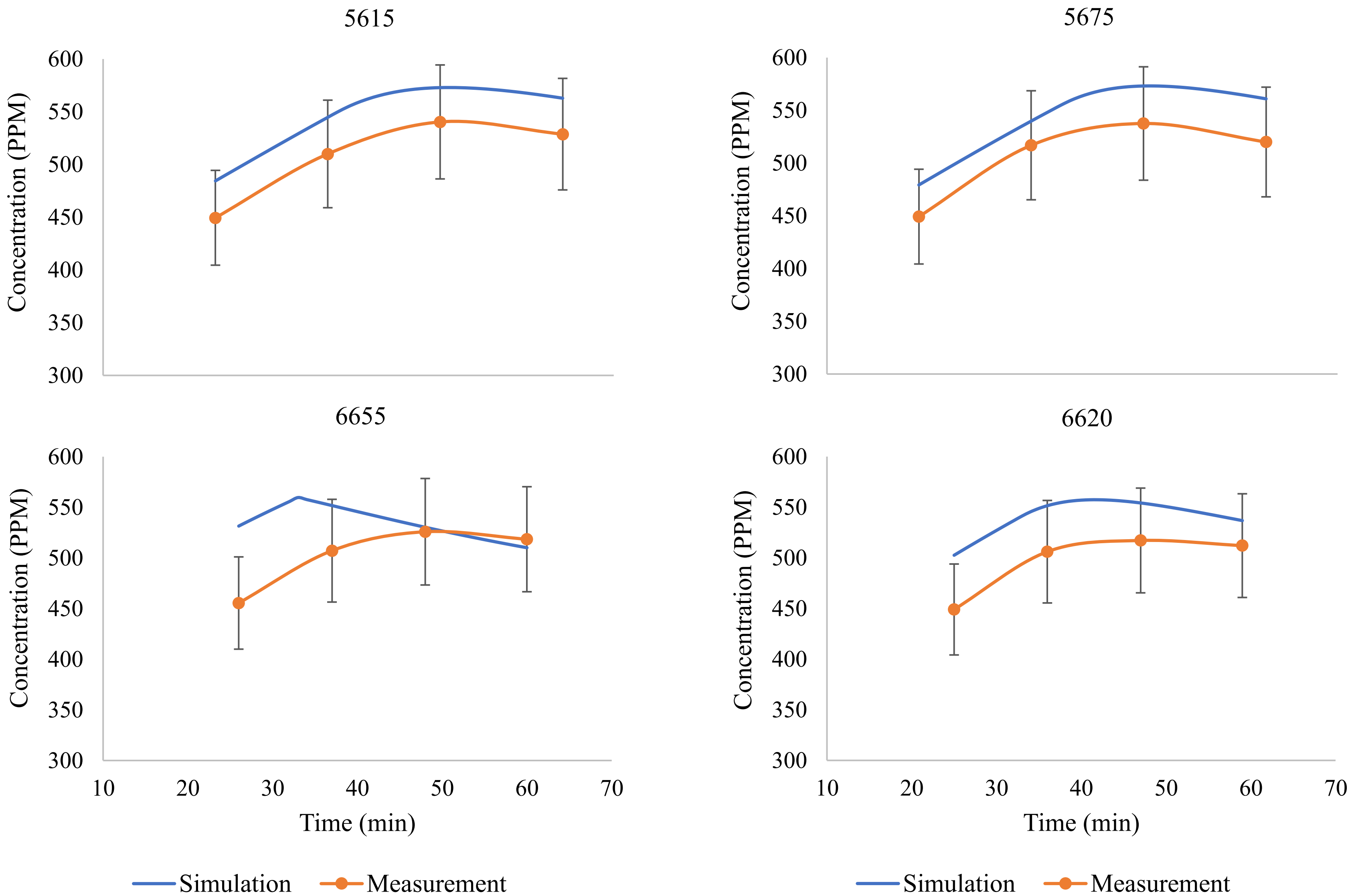

Figure 15. GA Results for Floor-to- Floor test

5.4.3 Discussion

The CONTAM model's calibration using the ENKF and GA approaches revealed essential insights into the role of critical parameters in accurately predicting CO_2 dispersion within the building. By refining parameters such as occupancy count**,** CO_2 generation rate**,** and initial indoor CO_2 concentration, the calibrated models demonstrated significant improvements in replicating the observed data.

Initial conditions played a critical role in influencing the early stages of CO_2 dispersion. Calibration efforts adjusted these values to match better observed starting concentrations, ensuring accurate CO_2 decay and transport behaviour simulation. This parameter particularly impacted the ENKF calibration, as iterative updates refined its value during each forecast cycle.

Table 5 shows the RMSE, CVRMSE, and NMBE for the ENKF and GA values, and Table 6 shows the values of the calibrated parameters against their actual Values.

Table 7. Error Metrics for the ENKF & GA Results

Room Number	Ensemble Kalman Filter (ENKF)			Genetic Algorithm		
	RMSE	NMBE	CVRMSE	RMSE	NMBE	CVRMSE
4200	54.11	9.72%	10.05%	22.06	1.57%	4.15%
4560	33.08	6.01%	6.14%	18.23	3.08	3.49
4605	36.26	6.53%	6.73%	23.77	4.28%	4.52%
4620	23.48	4.36%	4.43%	23.88	4.28%	4.51%
4655	33.08	6.01%	6.14%	27.22	4.02%	5.16%
4675	25.60	4.82%	4.85%	38.23	5.45%	7.19%
5605	36.33	6.53%	6.75%	32.11	5.61%	6.02%
5615	23.48	4.36%	4.43%	34.14	6.29%	6.31%
5655	25.60	4.82%	4.85%	25.56	4.82%	4.84%
5675	33.08	5.01%	6.14%	33.02	5.01%	6.13%
6620	44.13	4.92%	8.19%	43.24	5.19%	7.47%
6655	26.79	5.06%	5.07%	44.38	5.49%	8.36%
6675	31.81	4.82%	5.91%	45.29	4.52%	8.53%

Table 8. Comparison between the calibrated and the actual values of the injection flowrate

Parameter	ENKF Calibrated Value	GA Calibrated Value	Actual Value
CO2 Injection Flowrate (L/min) (Room-to-floor test)	24.75	24.63	25
CO2 Injection Flowrate (L/min) (Floor-to-floor test)	29.81	29.74	30

The calibration of the CONTAM model using the Ensemble Kalman Filter (ENKF) and Genetic Algorithm (GA) led to substantial improvements in predicting CO_2 concentrations across monitored zones. To evaluate the performance of these methods, three error metrics—Root Mean Square Error (RMSE), Normalized Mean Bias Error (NMBE), and Coefficient of Variation of RMSE (CVRMSE)—were used to assess accuracy, bias, and relative error, respectively.

Key Observations

1. **RMSE Performance**

   The GA consistently achieved lower RMSE values than the ENKF in most zones, with reductions as high as 59% in spaces like corridors (e.g., Room 4200). This demonstrates GA's effectiveness in minimizing overall prediction errors, particularly in areas where CO_2 transport is primarily influenced by mechanical ventilation and predictable airflow patterns.

2. **Bias Reduction (NMBE)**

   Both methods significantly reduced bias, but GA consistently outperformed ENKF in achieving lower NMBE values. For instance, in high-variability zones like Room 4675, GA maintained NMBE values below 5%, whereas ENKFexhibited slightly higher bias levels. These results highlight GA's ability to deliver accurate and unbiased estimates of CO_2 concentrations under varying conditions.

3. **Relative Error (CVRMSE)**

   GA also excelled in relative error reduction, with CVRMSE values frequently falling below the industry-accepted threshold of 15%. This consistent performance contrasts with ENKF, which occasionally produced higher CVRMSE values, exceeding 7% in certain zones.

These findings indicate GA's superior reliability in capturing relative variations in CO_2 concentrations across multiple zones.

Algorithm Strengths

- **Ensemble Kalman Filter (ENKF):**

  ENKF demonstrated faster convergence and superior error reduction, particularly in zones with predictable airflow dynamics and pressurization conditions. Its iterative assimilation of observational data and parameter refinement made it computationally efficient, achieving high accuracy and low bias.

- **Genetic Algorithm (GA):**

  GA excelled in scenarios involving complex, non-linear parameter interactions. It achieved competitive RMSE values in zones with intricate airflow dynamics, though it required more iterations and computational resources to converge. Its ability to explore a broader parameter space made it particularly valuable in addressing unpredictable parameter relationships.

Recommendation

Based on the calibration results, GA is recommended for most multizone airflow scenarios due to its computational efficiency, rapid convergence, and consistent reduction in RMSE, NMBE, and CVRMSE. ENKF's iterative approach ensures reliable and accurate predictions, especially in systems where airflow dynamics and pressurization conditions are well understood.

5.5 Case Study

This case study focuses on analyzing the distribution of quanta, which represent infectious particles, within a multizone-building model. Quanta was introduced into Room 4610 to simulate the release of contaminants, and the study varied two critical parameters to evaluate their impact on quanta dispersion:

1. Fresh Air (FA) Supply**:** The fresh air supply rate was incrementally adjusted, ranging from 10% to 100% of the total airflow. This variation allowed for an assessment of how increased FA rates influence the dilution and removal of quanta within the affected zones.
2. Stairwell Pressurization**:** The stairwell was alternately pressurized and left non-pressurized to determine its role in controlling the quanta's vertical and horizontal transport.

   This analysis's objective was to evaluate the combined effectiveness of increased FA supply and stairwell pressurization as strategies for mitigating the spread of quanta to adjacent zones and floors. The findings provide insights into ventilation and pressurization practices that could help reduce the risk of airborne transmission in multizone buildings.

5.5.1 Methodology

Quanta was continuously introduced into Room 4610 to simulate a localized source of airborne contaminants, with an injection rate calibrated at 65 quanta per hour. This rate reflects the typical exhalation of an infected individual based on standard infectious particle generation rates. The CONTAM model was utilized to analyze two distinct scenarios:

1. Scenario 1**:** The fresh air (FA) supply varied incrementally from 10% to 100% of the total airflow in four steps without activating stairwell pressurization.

2. **Scenario 2:** FA supply was maintained at the levels used during regular building operation, with stairwell pressurization activated to assess its effect on quanta distribution.

For both scenarios, quanta concentrations were monitored in adjacent rooms, such as 4610 and 4655, and on upper and lower floors. The analysis focused on three key metrics:

- Quanta Concentration: Average concentration levels and decay rates were evaluated for each zone to assess the effectiveness of FA supply and pressurization in reducing airborne contaminants.
- Cross-Zone Transport: The movement of quanta into adjacent rooms and shared spaces was analyzed to understand horizontal dispersion patterns.
- Cross-Floor Transport: The spread of quanta to upper and lower floors was assessed, with particular attention to the stairwell's role in facilitating or mitigating vertical transport.

This study aimed to quantify the effectiveness of increased FA supply and stairwell pressurization in controlling the spread of airborne contaminants. It provided insights into strategies for enhancing indoor air quality and reducing infection risks in multizone buildings.

5.5.2 Results

The following section presents the results of the quanta distribution analysis conducted in a multi-zone building model. This study investigates the effects of varying fresh air (FA) supply rates and stairwell pressurization on the spread and dilution of quanta, a proxy for airborne infectious particles, across different zones and floors. The results are organized to illustrate trends in quanta concentration over time in critical rooms, both adjacent to and distant from the source (Room 4610), under different experimental scenarios.

This analysis provides insights into optimal ventilation and pressurization strategies for minimizing airborne contaminant transmission in multi-zone environments. The results regarding quanta concentration trends, mitigation effectiveness, and implications for building ventilation design are discussed.

Figure 16 shows the quanta distribution for the 4 different rooms discussed above. The analysis shows the rise and decay of the quanta after the injection at 8 a.m.

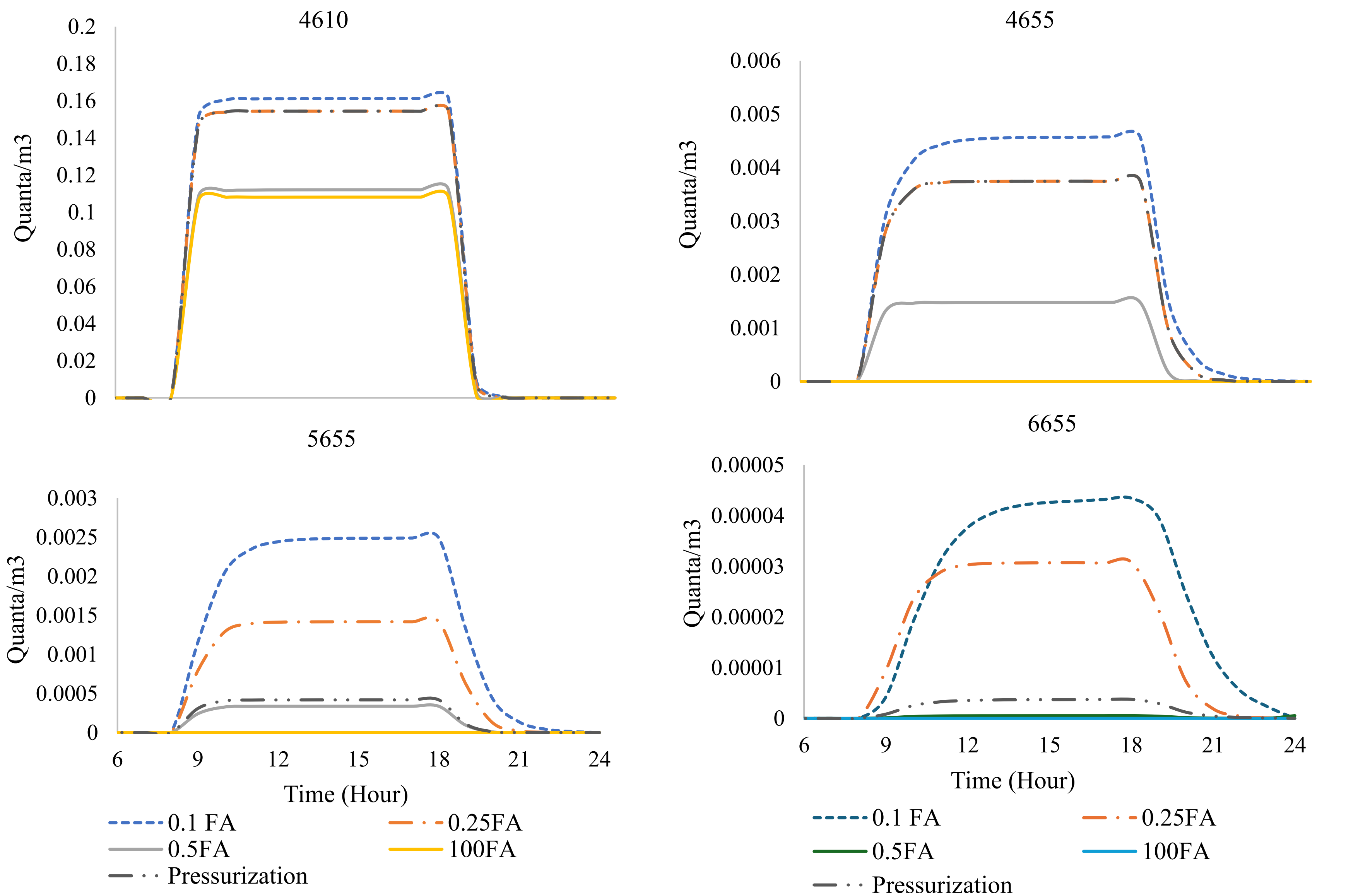

Figure 16. Results of the different measures using the calibrated model

5.5.3 Discussion

The results shown above show that across all rooms (4610, 4655, 5655, and 6655), the quanta concentrations followed a similar decay pattern, influenced by the fresh air (FA) supply and stair pressurization level. Concentrations started at zero, rose quickly after the injection began, and then decayed over time as fresh air and pressurization affected the transport and dilution of contaminants.

At lower FA levels, quanta concentrations remained higher and persisted for extended periods across all rooms. For instance:

- In Room 4610, concentrations peaked at approximately 0.0045 quanta/m3 at time step 15 (3 PM), with significant residual levels even at later time steps.
- In Room 6655, a remote room on an upper floor, low FA levels led to noticeable quanta concentrations, with a peak of 0.000043 quanta/m3 at time step 18 (6 PM). This demonstrates the limited effectiveness of low FA in diluting contaminants, even in distant rooms.

Increasing FA to 25%- 50% reduced quanta concentrations across all rooms. The decay rate was faster, particularly in nearby zones such as Room 4655, where concentrations dropped by over 50% compared to the 10% FA case at similar time steps.

At 100% FA, quanta concentrations were almost eliminated in all rooms after the initial peaks. For example, in Room 5655, quanta levels were effectively zero throughout the simulation, reflecting the high dilution capability of maximum fresh air supply.

In the Pressurization scenario, quanta concentrations were consistently lower in remote rooms, particularly those connected by the stairwell. For example:

- In Room 4610, concentrations were nearly halved compared to the non-pressurized scenarios at low FA levels, indicating reduced contaminant transport.
- In Room 6655, concentrations remained below 0.00001 quanta/m3 throughout the simulation, demonstrating the effectiveness of stair pressurization in minimizing vertical transport of quanta to upper floors.

Due to their proximity to the source, adjacent rooms, such as Room 4655, experienced higher quanta concentrations than distant zones (e.g., Room 6655). This trend was evident across all FA and pressurization scenarios.

Vertical transport was significantly reduced with high FA and pressurization, as seen in Room 6655, where concentrations were negligible in the pressurized scenario, even at low FA rates.

The results emphasize the critical role of fresh air supply and stair pressurization in controlling quanta distribution within multi-zone buildings:

1. Fresh Air Supply: Increasing FA supply consistently reduced quanta concentrations across all zones, with maximum FA (100%) proving the most effective strategy for mitigating contaminant buildup and transport.
2. Stair Pressurization: Pressurizing the stairwell further minimized cross-floor contaminant transport, complementing the effects of increased FA supply.
3. Combined Strategy: The combination of high FA and pressurization offered the most effective mitigation, ensuring rapid dilution of contaminants near the source and preventing significant transport to adjacent or distant zones.

Chapter 6

6. Conclusion

The research presented in this thesis focuses on the development and application of advanced calibration techniques for multi-zone indoor air quality (IAQ) models, specifically leveraging Genetic Algorithms (GA) and the Ensemble Kalman Filter (EnKF). Integrating these methodologies with CONTAM modeling software addresses critical challenges in model calibration, parameter uncertainty, and real-world applicability. This study's findings hold significant implications for designing, operating, and optimizing building ventilation systems.

6.1 Summary of Key Findings

This research demonstrates the effectiveness of GAs and EnKF in enhancing the accuracy and reliability of multi-zone IAQ models. The sensitivity analysis revealed the influence of critical parameters, including occupancy count, generation rates, and initial indoor CO_2 concentration, on model performance. The application of GAs enabled calibration optimization through iterative convergence across generations, while EnKF provided robust real-time updates using observational data. Both methods improved the fidelity of CONTAM models, particularly in replicating experimental data from room-to-floor and floor-to-floor tracer gas tests.

The comparative analysis showed that while both algorithms improved model accuracy, they exhibited distinct strengths. EnKF excelled in handling dynamic, real-time data, whereas GAs demonstrated superior performance in exploring complex parameter spaces and identifying global optima. These findings validate the complementary nature of these techniques and their potential for integration into hybrid calibration frameworks.

6.2 Contributions to the Field

The thesis makes several key contributions:

1. Development of a comprehensive calibration methodology integrating GAs and EnKF, tailored for CONTAM-based IAQ modeling.
2. Advancement of sensitivity analysis techniques to prioritize influential parameters and improve model calibration efficiency.
3. Validation of calibration methods through extensive experimental data, covering diverse test scenarios such as room-to-floor and floor-to-floor airflow analyses.
4. Exploration of GAs' and EnKF's strengths and limitations, providing insights into their respective applications for IAQ and energy modeling.

6.3 Practical Implications

The results of this thesis have far-reaching implications for improving building performance. The calibrated models can inform the design of energy-efficient ventilation systems, optimize airflow distribution, and enhance occupant health and comfort by mitigating exposure to indoor pollutants. The methodologies developed in this study apply to various building types, including healthcare facilities, schools, and commercial spaces, where IAQ is critical.

Furthermore, integrating data-driven calibration techniques with CONTAM models bridges the gap between theoretical modeling and practical implementation. This enables building operators and engineers to make informed decisions based on accurate, real-time data, ensuring optimal ventilation performance under varying conditions.

6.4 Future Directions

While this thesis addresses significant challenges in IAQ modeling and calibration, it also opens avenues for further research. Future studies could:

- Explore the integration of IoT-enabled sensors and machine learning algorithms to enhance real-time calibration and data assimilation.
- Investigate hybrid calibration frameworks that combine GA and EnKF with other optimization techniques, such as Bayesian Inference or Machine Learning-based surrogate modeling, to leverage their complementary strengths.
- Expand the scope of the calibration methodology to include other IAQ factors, such as particulate matter and volatile organic compounds.
- Conduct longitudinal studies to assess calibrated models' long-term stability and performance under evolving environmental conditions and occupancy patterns.

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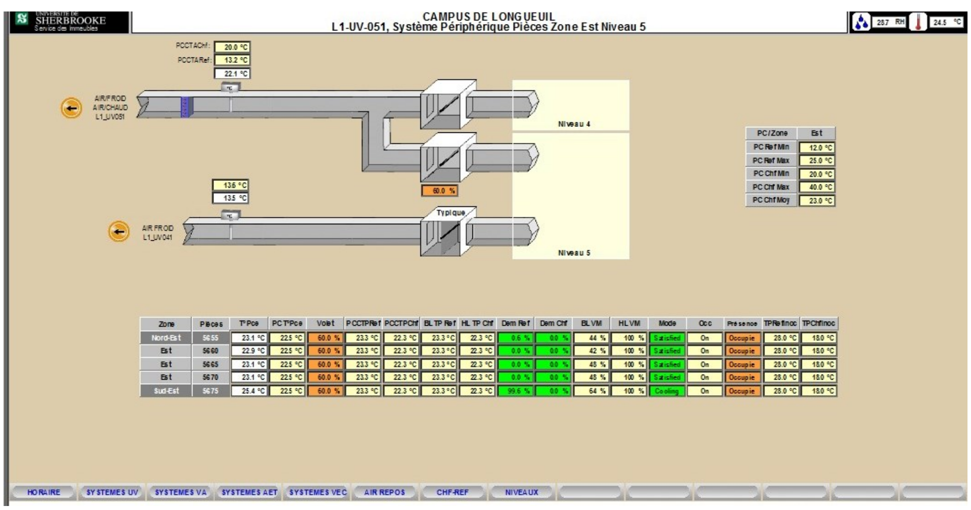
8. Appendix

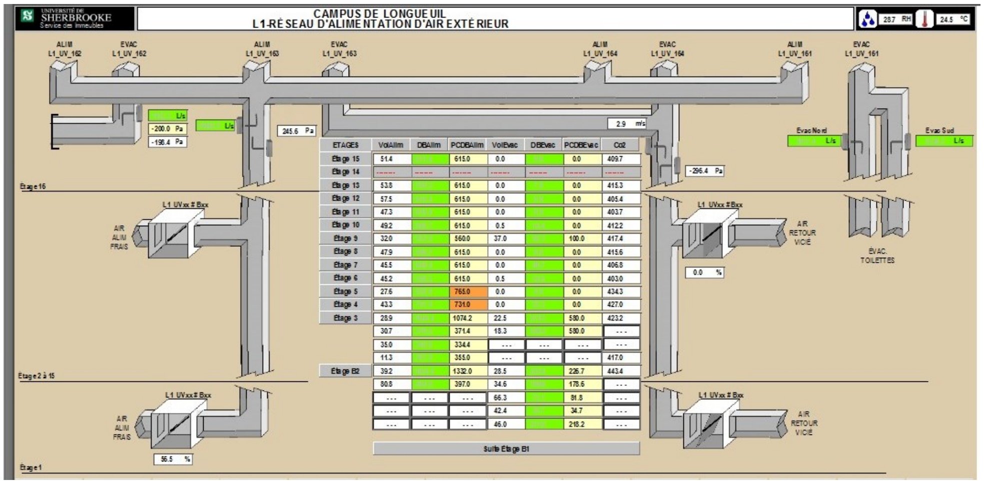
Appendix 1: Photos taken during the measurement

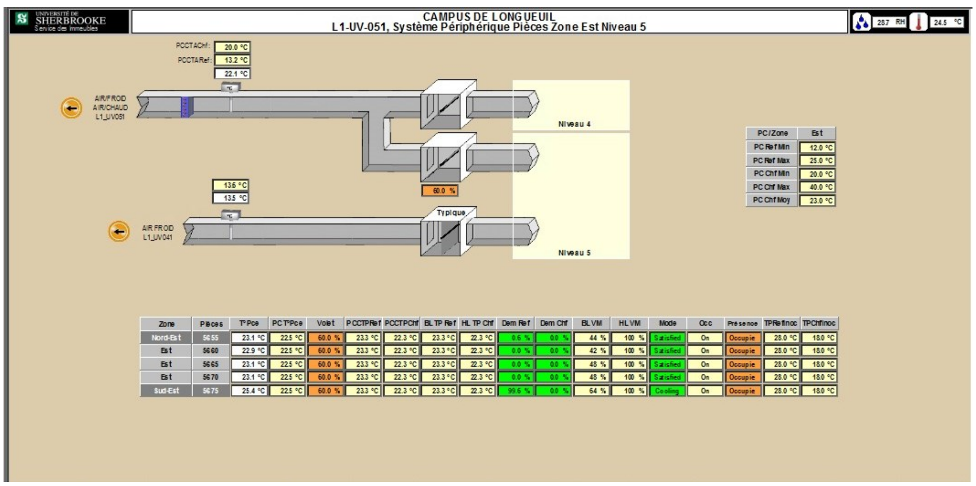
The accompanying images illustrate key elements of the experimental setup used during the CO_2 measurement process. The CO_2 cylinders, visible in the photographs, served as the source for injecting gas into the building to simulate contaminant dispersion. Sampling tubes, shown extending throughout the building, were strategically placed to collect air samples from various rooms and transfer them to the Universal Gas Analyzer (UGA) for detailed analysis.

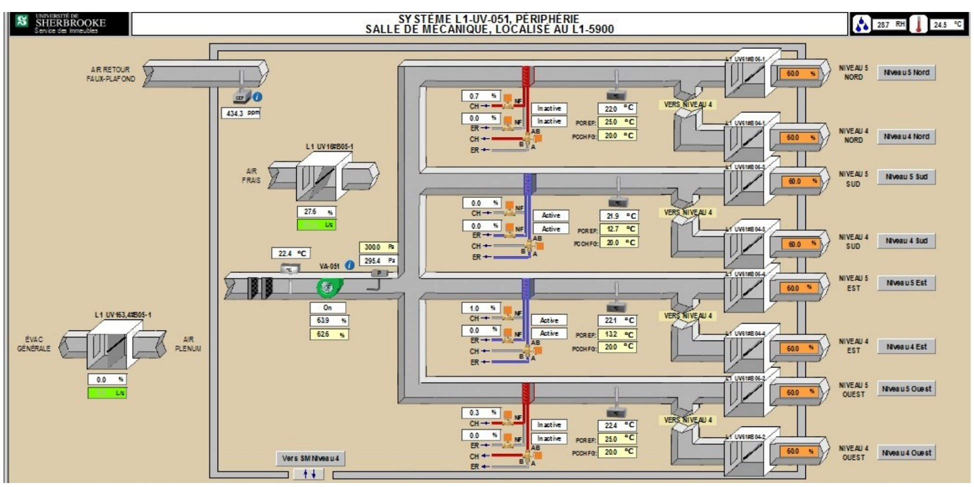
To ensure accurate and consistent measurements, the sampling tubes were securely fixed at the required locations using tripods. This setup allowed precise monitoring of CO_2 concentrations across different zones, facilitating a comprehensive assessment of airflow and contaminant transport within the building.

Appendix 2: Screenshots from the BAS System









Screenshots from the BAS system show the operating conditions for the 5th floor and the fresh air unit for the whole building.