Evaluation of Uncertainties of Using CO_2 for Studying Ventilation Performance and Indoor Airborne Contaminant Transmissions

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ABSTRACT

The COVID-19 pandemic has raised concerns about indoor ventilation conditions worldwide. Monitoring CO_2 concentrations in rooms has been widely used, but its relationship with outdoor air ventilation rates and ventilation performance is uncertain. Several uncertainties must be quantified, including the location and rate of CO_2 sources, sensor locations, and the dynamics of the surroundings, as well as limitations of existing simulation models, such as well-mixing assumptions. This paper presents field measurements, stochastic modeling, calibrations, and aerodynamics analysis within rooms and contaminant dispersal. Several CO_2 tracer gas tests were conducted in classrooms. Two test setups were used, one for uniformity testing and the other for evaluating ventilation performance. A proposed uniformity index (U_i) is integrated into the tracer decay method to address its limitation due to the well-mixing assumption, thereby improving the air change rate estimation by 22%. As a general rule, the outlet sampling location may represent the average of all locations in mixed-ventilated spaces. Given the small difference in peak CO_2 concentrations (2.6%) and decay periods (15%), 60% of the ventilation capacity should be used instead of the full capacity. As opposed to the instructor's location, the room midpoint yields a 7 percent higher peak CO_2 concentration, which is recommended as a dosing source to estimate air change rates using the tracer decay method. Additionally, novel simulation models have been developed for estimating ventilation air change rates in indoor environments since deterministic approaches cannot incorporate system uncertainties. It has been found that stochastic models, which combine the physical principles of a system with data collected from field measurements, are effective for resolving uncertainties, but they have not been extensively explored in terms of estimating air change rates. Therefore, we also examined the integration of stochastic differential equations (SDEs) and a Bayesian calibration model to evaluate indoor air quality and ventilation conditions in rooms.

KEYWORDS

Decay method; Tracer mixing; CO_2 monitoring; Air change rate; Bayesian calibration

1 INTRODUCTION

Poor indoor air quality (IAQ) often results from insufficient fresh air supply to building occupants. The outbreak of the COVID-19 pandemic has raised public concerns about maintaining a healthy indoor environment and limiting the spread of virus-laden respiratory aerosols. Occupied classrooms in schools, where in-person interactions are frequent, have become one of the vulnerable spaces during this pandemic. Adequate outdoor air ventilation could effectively dilute aerosol concentrations and limit the quantity of inhaled infectious pathogens (Yan, Wang et al. 2023). Thus, ensuring proper ventilation performance in schools has become much more essential than ever before.

Over the years, improving air quality through enhanced ventilation performance has been the subject of various studies (Karava, Athienitis et al. 2012, Qi, Wang et al. 2014, Yuan, Athienitis et al. 2016, Yuan, Vallianos et al. 2018, Hou, Lin et al. 2020, Qi, Cheng et al. 2020). Characterizing ventilation rates (VR) in buildings has been an effective way for people to understand how much fresh air is delivered to the occupants. It should be noted that VR discussed in this study are in terms of the quantity of outdoor air supplied to the occupied areas, which is usually expressed as air volume per unit time (e.g., L/s) or air volume per unit time per person (e.g., L/s/person). For a lecture classroom, the ventilation design standard of the American Society of Heating, Refrigerating, and Air Conditioning Engineers (ASHRAE) recommends a VR value of not less than 4.3 L/s/person (ASHRAE 2019). Until now, few studies have paid attention to understanding the ventilation conditions of Canadian primary or secondary schools. There are several direct and indirect approaches to measuring air change rates (λ), which include airflow measurements, controlled release as well as in-situ monitoring (McNeill, Corsi et al. 2022). The direct flow measurement, which directly measures the air intake at the air-handling unit (AHU), has been widely adopted for determining the air change rate (Damiano 2010). However, this approach only works for mechanically ventilated buildings, while until recently, a large proportion of Canadian schools were naturally ventilated (Karava, Stathopoulos et al. 2006, Cheng, Qi et al. 2018).

The controlled release approach, which has been widely known as the tracer-gas technique, usually releases a designated amount of tracer gas (a single release, constant release, or controlled release) and then observes its decay with time. Due to its simplicity and less dosing volume of tracer, various studies used the concentration decay method to evaluate ventilation performance and estimate indoor air change rate. However, this method often assumes the well-mixing condition between tracer and air. In reality, the non-uniform mixing is unavoidable that caused by either short-circuiting of the inlet to the outlet or stagnant regions. Therefore, the decay method tends to underpredict λ (Van Ryswyk, Wallace et al. 2015). To fill this research gap, it is important to interpret the results of tracer gas tests in the context of a reliable mixing model.

Selecting tracer gas is important in this method e.g., CO_2 is one of the commonly used tracer gases as it appears to be safe and environmentally friendly, and its concentration could be easily measured with inexpensive sensors. In this approach, CO_2 is also an ideal choice since humans would also become the generation source, and the concentration may indicate room occupancy. In order to estimate λ using measured CO_2 concentrations in Canadian schools, traditionally, the tracer-gas mass balance equations would be used for deterministic predictions. However, during the measurement process, uncertainties would exist due to measurement noises, influence from the outdoor environments, etc., which would be ignored in the deterministic estimations. In the meanwhile, sometimes, the adoption of input parameters may be unreasonable, which would result in a large prediction bias. The stochastic grey-box model (Macarulla, Casals et al. 2018), which combines the physical principles of a system and the information generated from field measurements data, is shown to be promising in dealing with the uncertainties, whereas they have not been investigated in depth to be applied to the estimation of air change rates based on CO_2 measurements in rooms. Meanwhile, the key parameters, including room occupancy and occupant CO_2 generation rates, are often unavailable and lead to significant uncertainties, whereas these parameters may be estimated from Bayesian calibrations based on CO_2 measurements (Hou, Wang et al. 2023). These approaches help deal with uncertainties and disturbances that happen during the ventilation interpretation progress.

To address the research gaps presented above, in this study, we aim to deal with uncertainties coupled with CO_2 field measurements, mass-balance equation modeling, parameter estimations, as well as the well-mixing of tracers and airflows in reality. Although the numerical analysis was focused on single-zone cases, the extensions to multi-zone simulations were also discussed.

2 METHODOLOGIES

2.1. Field measurements in mechanically ventilated classroom

In August 2022, several CO_2 tracer tests were carried out in a classroom on the 5th floor of a 16-story institutional high-rise building (Longueuil Campus, Université de Sherbrooke, Montreal, Canada). The classroom has a volume of 266.3 m^3 (8.9×8.8×3.5 m) measured using a laser meter. The entire building is served by a centralized air conditioning system controlled by a building automation system (BAS). A mixed-ventilation system is used consisting of 4 supply air ceiling diffusers (0.6×0.6 m), 6 linear slot diffusers (1.2×0.1 m), and 3 return air ceiling grilles (0.6×0.3 m). Two test setups were built. Setup (I) is designed to quantify the spatial uniformity of CO_2 concentrations by monitoring 16 locations at the breathing level (1.5 m from the floor) using the mid-point as a CO_2 source. On the other hand, setup (II) is arranged to evaluate the effect of three levels of air change rates, two source locations (mid-point and instructor desk's location), and two-door modes (opened and closed) on ventilation performance. Eight sampling locations are monitored at heights of 1.1 and 1.7 m from the floor. For both setups, the inlet (S) and the outlet (R) were also monitored.

Details regarding the tracer tests conducted using CO_2 are presented in Table 1, which is a suitable tracer as recommended by ASTM E741 (ASTM 2017). Test 01 is specified for quantifying the spatial uniformity of CO_2 concentrations, while tests 02-06 are carried out for assessing ventilation performance. Tests 02, 03, and 04 are compared to examine the effect of the air change rates. Tests 04 is compared with Tests 05 and 06 to investigate the effect of door mode and source location on ventilation performance. The BAS system was used to control the ventilation conditions, wherein the air change rate was measured (λ_{eff}) using a balometer device. Meanwhile, the CO_2 injection was controlled using a mass controller, keeping the peak concentration less than 1000 ppm.

Table 1 History of conducted CO_2 tracer tests.

Test No.	**Test 01**	**Test 02**	**Test 03**	**Test 04**	**Test 05**	**Test 06**
Test period [min]	108	70	85	75	75	75
Measured air change rate λ_{eff} [/h]	5.35 ± 0.21	8.92 ± 0.31	5.35 ± 0.21	7.25 ± 0.26	7.25 ± 0.26	7.25 ± 0.26
Source location	Mid-point	Mid-point	Mid-point	Mid-point	Mid-point	Instructor desk
Door mode	Closed	Closed	Closed	Closed	Opened	Closed
Number of sensors	18	10	10	10	10	10

2.2. Field measurements in naturally ventilated classroom

Indoor field measurements of CO_2 levels were performed in one of Montreal's primary schools from 2020 to 2021. The selected classroom has a floor area of 9.4 m × 6.6 m, which is naturally ventilated. The MX1102 (SN: 20820982) CO_2 sensor was installed at 1.7 meters height on the west internal wall right above the thermostat (1.5 m height). Table 2 illustrates the measurement information.

Table 2 Measurements information in the classroom

Location	Age (years)	Dimensions (m)	Ventilation mode	Measurement Periods	Maximum Occupancy
Montreal	5-8	9.4 × 6.6 × 3.5	Natural ventilation	2020/06/22 - 2021/06/21	16

2.3. Single-zone ventilation performance evaluation

To estimate the air change rate λ_o, the well-known decay method (Eq. 1) is commonly used. However, this method assumes a well-mixed space, which limits its accuracy. To address this research gap, a uniformity index (U_i) has been proposed (Eq. 2). By integrating U_i into the decay method, the modified decay method (Eq. 3) has been developed to improve the estimation of air change rates. This modified decay method considers the unavoidable non-uniform mixing, which might be caused by stagnant regions or short-circuiting from the inlet to the outlet. The mathematical solution of Eq. 3 was developed according to (Barber 1982, ASTM 2017).

$$\lambda_o = \frac{1}{(t-t_0)} \ln \frac{(C - C_{bg})}{(C_0 - C_{bg})} \tag{1}$$

$$U_i = \frac{C_{min}}{C_{avg}} \tag{2}$$

$$\lambda_m = \begin{cases} \dfrac{1}{U_i(t-t_0)} \ln \dfrac{(C - C_{bg})}{(C_0 - C_{bg})}, & \text{for short} - \text{circuiting when } \lambda_o < \lambda_{eff} \\ \dfrac{U_i}{(t-t_0)} \ln \dfrac{(C - C_{bg})}{(C_0 - C_{bg})}, & \text{for stagnant regions when } \lambda_o > \lambda_{eff} \end{cases} \tag{3}$$

where λ_o is estimated air change rates for uniform mixing [/h]; t and t_o are the final and initial elapsed time [h]; C and C_o are the final and initial tracer concentrations [mg/m^3]; C_{bg} is the background tracer concentration [mg/m^3]; U_i is uniformity index; C_{min} and C_{avg} are minimum and average tracer concentrations [mg/m^3]; λ_m is estimated air change rates for non-uniform mixing [/h]; λ_{eff} is measured air change rates [/h].

Plastic tubings (8 mm ID) were utilized to install the CO_2 injection and sampling systems. The injection flow rate was controlled with a mass controller to keep the peak CO_2 concentration under 1000 ppm. Meanwhile, an automated system monitored the CO_2 concentrations at desired locations online. A vacuum pump operating at 114 L/min continually drew fresh air samples one at a time, which were then supplied to the gas analyzer when the 18-position valve selected them for analysis. A mass spectrometer (UGA-100, Stanford Research Systems) with a quadrupole probe was used. It was also calibrated in one of Concordia's laboratories and in situ. A combination of standard gas concentrations was used for this calibration method (Blessing, Ellefson et al. 2007). According to ASTM E741, the regression curve should be within the 95% confidence level.

2.4. Single-zone air change rate predictions and calibrations

The white-box CO_2 model, which was the traditional deterministic CO_2 mass-balance model at the constant temperature, was shown as follows:

$$V\frac{dC_r}{dt} = -(C_r - C_o) \cdot Q + E \tag{4}$$

where V is the room volume [m^3]; C_r is the CO_2 concentration in the room [ppm]; C_o is the CO_2 concentration of outdoor air ventilation flows [ppm]; Q is the air supply into the room [m^3/h] ; E is the CO_2 generation rate in the room [L/s].

The grey-box CO_2 model, which was established with the stochastic differential equation (SDE), could be expressed as follows:

$$dC_r = \frac{-(C_r - C_o)\cdot Q + E}{V} \cdot dt + \sigma \cdot dw \tag{5}$$

where σ is the incremental variance in the Wiener process; dw is a Wiener process.

In this study, the Bayesian calibration approach was adopted for the inference of air change rates in the established CO_2 white-box/grey-box model. In Bayesian calibration, the probability of the estimated parameters was inferred based on the prior distributions estimated for them. The likelihood of the estimated parameters given the measured data Y (CO_2 indoor concentration) is demonstrated as follows in Bayes's law:

$$P(Q|Y) = \frac{P(Y|Q)\cdot P(Q)}{P(Y)} \tag{6}$$

where $P(Y|Q)$ is the likelihood probability that measurement data Y (which is measured CO_2 concentration *Cr* in this study) occurs given the prior information of Q, P (Q) is the prior joint probability of Q, and P (Y) is the probability of the measurements results, which is a normalized constant. The prior distributions estimated for models were based on a previous study (Hou, Wang et al. 2023).

2.5. Multi-zone simulations and calibrations

CONTAM software (William and Brian 2015) is one of the most powerful multi-zone simulation tools for indoor air quality analysis. Thus, CONTAM is employed in this study to predict and validate CO_2 concentrations at different locations. For this purpose, the 5th floor of the Longueuil Campus (Montreal, Canada) was modeled (Figure 1). Accurate and real boundary conditions were inputted using the BAS to describe ventilation conditions in addition to considering the measured CO_2 data. Regarding the building envelope parameters, e.g., the infiltration values were obtained from the Quebec code of construction (National Research Council of and Régie du bâtiment du 2022) of 0.25 L/s/m^2. The model considered other different types of infiltration, such as internal wall and door infiltration. CO_2 injection was defined based on the original injection rate that was carried out during the measurements.

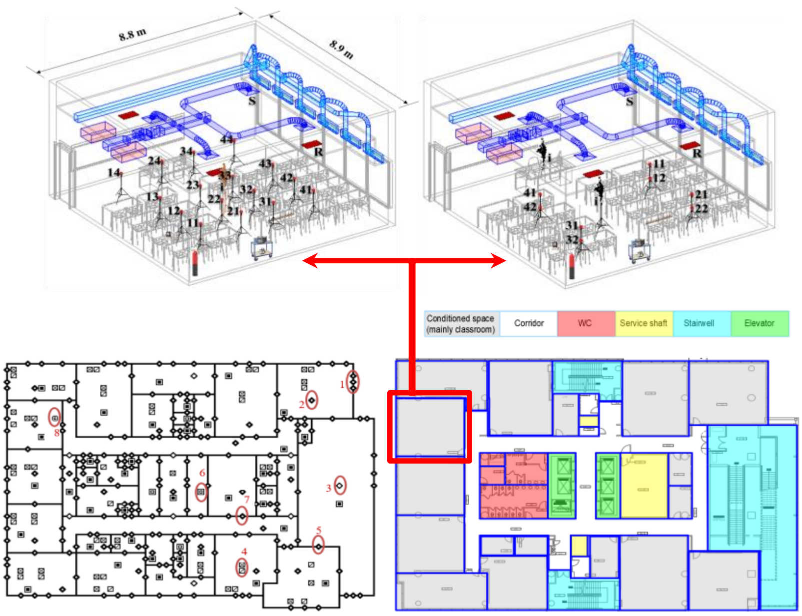


Figure 1 Architectural layout and CONTAM model of the 5th floor, Longueuil Campus, Université de Sherbrooke, Montreal, Canada (1. External wall leakage; 2. Floor leakage; 3. Stair leakage; 4. AHU supply and return; 5. Internal wall leakage; 6. Elevator shaft leakage; 7. Door leakage; 8. CO_2 injection source). Highlighted in red, are 3D views of the selected classroom showing two setups of tracer tests.

An automatic calibration method should be proposed due to the challenges involved in manually calibrating multiple parameters. To perform this, several steps should be taken. The initial step is to conduct a parametric simulation, which includes testing all possible ranges of various simulation parameters with different combinations to obtain a reasonable simulation result. To generate various combinations, a uniform distribution for all parameters was chosen using ContamFactorial 1.0, along with the necessary flagged and value files for creating different project files. A Python code was developed to execute the extracted data files and convert the simulation results into a spreadsheet format for exporting the results. Table 3 displays the parameter ranges utilized in this parametric analysis. Sampling was needed first to minimize the number of simulations. Sampling is often used to select the combinations that could be used to cover the whole range of these combinations. There are different kinds of available sampling methods. In this study, the Sobol method is used as it could be used in capturing the linear and non-linear correlations between the inputs and outputs when performing the sensitivity analysis, as discussed later. By utilizing sampling techniques, the total number of simulation cases can be reduced to 1152, which is significantly less than the millions of cases. Then, sensitivity analysis is proposed to evaluate the importance of each parameter in the results. Sobol variance-based method (Saltelli, Annoni et al. 2010) was used to evaluate the correlations between the different input parameters and output results. A sample file was first created that has all the possible combinations of the input parameters. Then, the Monte-Carlo integration was used to calculate the sensitivity index (SI) based on both the sample files and the results.

Table 3. Utilized parameter ranges for parametric analysis

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 CO_2 concentration	396 – 416	ppm
Initial indoor CO_2 concentration	400 – 700	ppm
Indoor CO_2 generation rate	0.002 – 0.01	L/s/ person
Occupancy	0 – 40	Number

3 RESULTS AND DISCUSSION

3.1.Single-zone measurements and simulations, calibrations

Figure 2a shows measured CO_2 concentrations at various locations with peak difference values ranging from 213 to 331 ppm. The outlet location has a peak CO_2 concentration (272 ppm) close to the average of all distributed 16 sensors at the breathing level (278 ± 33 ppm). Therefore, the outlet location is a good sampling representative of interest in this mixed-ventilated zone. Integrating the proposed uniformity index (U_i = 0.77) in the decay equation succeeded in decreasing the error caused by the well-mixed assumption at the outlet and the average locations from 25% to 3% (Figure 2b).

Both peak CO_2 concentration and decay period inversely correspond to increasing the air change rate (Figure 2c). When the maximum air change rate of 9 /h decreases to the minimum value of 5 /h, the peak CO_2 concentration and decay period both decrease by 39% and 63%, respectively. On the other hand, when comparing the maximum air change rate of 9 /h with the frequent operating air change rate of 7 /h, there were only minor differences observed in both the peak CO_2 concentration (2.6%) and decay period (15%). As a result, it is suggested to operate the space at 60% of its full ventilation capacity (7 /h). Opening the door reduces exposure to peak CO_2 concentration and decay period by 34% and 56%, respectively. The mid-point location is recommended as the dosing source for estimating the air change rate, rather than the instructor's desk location, as it resulted in a 7% higher peak CO_2 concentration.

Figure 3 shows (a) the measured CO_2 level in different seasons and (b) an example for evaluating the modeling approach on a selected day. During school hours (9:00 – 16:00), measurement data from 9:00 to 13:00 and 13:00 – 16:00 were used for predicting the estimated parameters and evaluating the prediction performance, respectively. The single-zone simulated CO_2 concentration with parameters estimated from the white-box and grey-box model is shown in Figure 3c. The rolling-window approach was applied for the simulation of indoor CO_2 levels (Hou, Wang et al. 2023). Results suggest that the grey-box model tends to have a better prediction performance than the white-box model. The mean average error (MAE) is 97.4 for the white-box model ppm and 48.6 ppm for the grey-box model (Table 4). This indicates that the grey-box model gives more reasonable predictions for this selected day. The results evaluated from other indices also indicate a similar trend, as shown in Table 4.

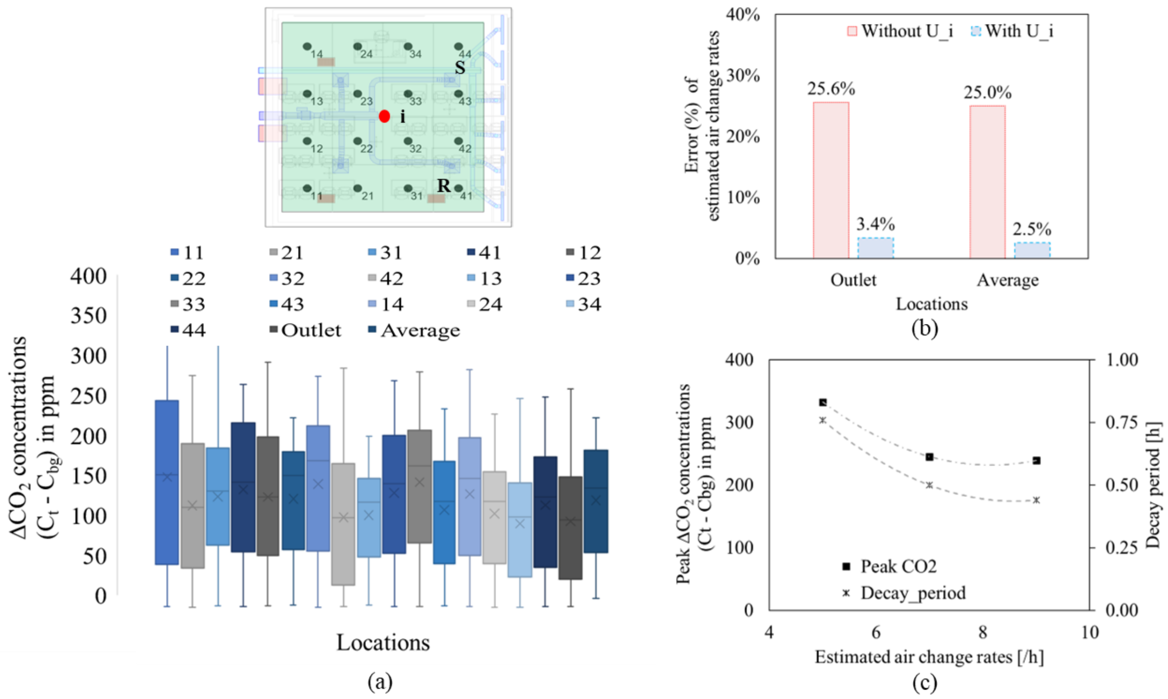
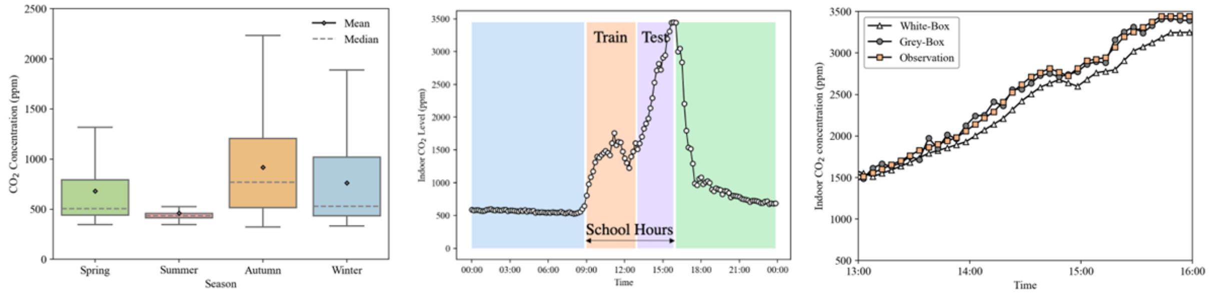


Figure 2 (a) Measured CO_2 concentrations at 16 different sampling locations in addition to the inlet and outlet. (b) Comparing the error percentage of estimated air change rates at the outlet and the average of all 16 locations at the breathing level. (c) Peak CO_2 concentrations and decay periods at various air change rates.

Table 4 Evaluations for the modeling performance

Model	**MAE (ppm)**	**MAPE (ppm)**	**MSE (ppm)**	**RMSE (ppm)**	**R^2**
White-Box	97.4	4.8	12791.2	113.1	0.99
Grey-Box	48.6	2.6	3361.9	58.0	0.99



(a) (b) (c)

Figure 3 Measured CO_2 concentration in the classroom for different seasons (a) and for one selected day (b) Simulated CO_2 concentration with parameters estimated from the white-box/grey-box model (c).

3.2.Multi-zone simulations and calibrations

The baseline model was first validated against the measurement data. Figure 4 shows the difference in CO_2 concentration relative to the initial concentration for one sample room within the building. The results are shown for the whole measurement time, including a pre-injection period in the beginning, an injection period, and then decay. These results suggest that there has been a considerable deviation between the measurements and the simulation due to the uncertainties of the input parameters. Initially, manual calibration was explored to determine if it was feasible to adjust the input parameters based on the results. It was found that a calibration technique is necessary when dealing with such issues, particularly when there are a large number of input parameters that would make it difficult to modify each parameter individually or manually.

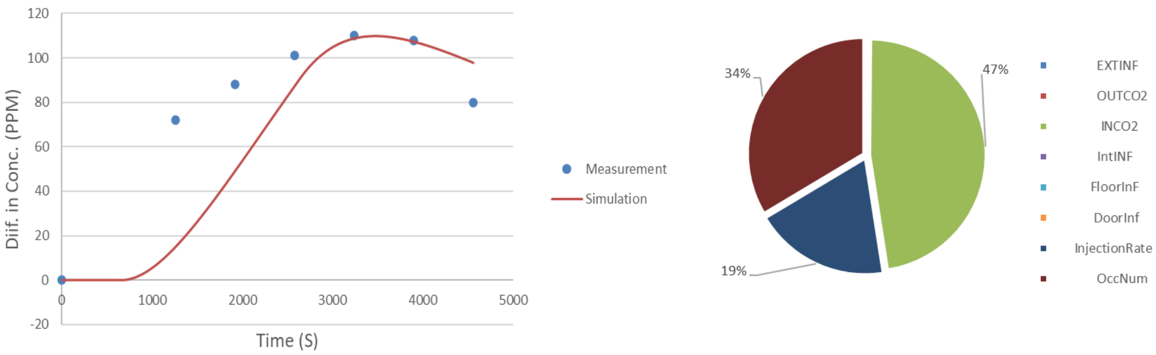


Figure 4 CO_2 concentration difference versus time (left) and sensitivity index of the input parameters (right).

After performing the parametric simulations and extracting the results, the sensitivity analysis was performed to evaluate the importance ranking of every input parameter on the output results. Figure 4 (right) shows the sensitivity Index (SI) for all the input parameters. The results suggest that the initial CO_2 concentration within the room, the occupancy, and the CO_2 generation rate are the main parameters that shall be calibrated for each zone. The other parameters will be assigned with their mean value as their influence is almost negligible. It should be noted that the proposed methodology is expected to work for the other buildings but the results may be different.

4 CONCLUSIONS

This study quantifies inevitable uncertainties coupled with monitoring and modeling CO_2 concentrations to assess ventilation performance, i.e., quantify air change rates and mitigate aerosol viral transport in buildings. A proposed uniformity index (U_i) is integrated into the decay method to reduce its limitation on uniform mixing only. Later, the effect of air change rate, source location, and door mode on ventilation performance is experimentally evaluated.

In addition, stochastic modeling and calibrations were carried out to investigate other significant factors (CO_2 injection rate and the dynamics with the surroundings). The grey-box CO_2 model was integrated with the Bayesian calibration method to support the evaluations of indoor air quality and air change rates in Canadian classrooms. By taking uncertainties from different sources into consideration, this approach would effectively estimate the air change rate from in-situ CO_2 monitoring. Additionally, this study presents a novel approach for calibrating multi-zone CO_2 simulations, which helps to identify the key parameters to be calibrated.

The following conclusions were researched through this study: The proposed uniformity index succeeded in decreasing the error caused by the well-mixed assumption from 25% to 3%. The grey-box model could give reasonable predictions for CO_2 monitoring. Three main parameters that need to be calibrated are the initial CO_2 concentration, occupancy, and CO_2 generation rate, as they have a significant impact on the accuracy of the air change rate estimation.

Future studies should be directed to developing an algorithm that can assign values to the parameters requiring calibration by utilizing measurements to minimize the error between the measurements and the simulation. Additionally, investigating the possibility of applying the same methodology to other contaminants and different ventilation systems would be beneficial.

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