Development of a Bayesian inference model for assessing ventilation condition based on CO₂ meters in primary schools

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Abstract

Outdoor fresh air ventilation plays a significant role in reducing airborne transmission of diseases in indoor spaces. School classrooms are considerably challenged during the COVID-19 pandemic because of the increasing need for in-person education, untimely and incompleted vaccinations, high occupancy density, and uncertain ventilation conditions. Many schools started to use CO₂ meters to indicate air quality, but how to interpret the data remains unclear. Many uncertainties are also involved, including manual readings, student numbers and schedules, uncertain CO₂ generation rates, and variable indoor and ambient conditions. This study proposed a Bayesian inference approach with sensitivity analysis to understand CO₂ readings in four primary schools by identifying uncertainties and calibrating key parameters. The outdoor ventilation rate, CO₂ generation rate, and occupancy level were identified as the top sensitive parameters for indoor CO₂ levels. The occupancy schedule becomes critical when the CO₂ data are limited, whereas a 15-min measurement interval could capture dynamic CO₂ profiles well even without the occupancy information. Hourly CO₂ recording should be avoided because it failed to capture peak values and overestimated the ventilation rates. For the four primary school rooms, the calibrated ventilation rate with a 95% confidence level for fall condition is 1.96±0.31 ACH for Room #1 (165 m³ and 20 occupancies) with mechanical ventilation, and for the rest of the naturally ventilated rooms, it is 0.40±0.08 ACH for Room #2 (236 m³ and 21 occupancies), 0.30±0.04 or 0.79±0.06 ACH depending on occupancy schedules for Room #3 (236 m³ and 19 occupancies), 0.40±0.32,0.48±0.37,0.72±0.39 ACH for Room #4 (231 m³ and 8–9 occupancies) for three consecutive days.

1 Introduction

Airborne transmission of relatively small aerosol droplets plays a dominant role in spreading SARS-CoV-2 (hereafter as COVID-19), especially in indoor spaces (Asadi et al. 2020; Prather et al. 2020). School classrooms pose a considerable challenge because of the increasing needs of in-person learning, relatively lower and delayed vaccinations compared to other spaces, large occupant density, and uncertain ventilation conditions of concern (Zhang 2020). For example, in Quebec province, Canada, a partial lockdown was in effect for non-essential business, with many offices closed, whereas primary and secondary schools open. The weekly school-related COVID-19 cases in Quebec Canada at the end of August 2020 showed that schools accounted for 20% of the province's COVID-19 cases, while students and staffs account for about 18% of Quebec's population (Remiorz 2020). Statistical data shows that 1,781 schools had been observed with at least one positive case in Quebec since the beginning of the pandemic (Covid Écoles Québec 2020). Therefore, the rate of COVID-19 transmission in schools was higher than the community transmission, and mitigation

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measures must be implemented in classrooms to reduce the infection risk.

Several studies revealed the significant impact of ventilation rate in reducing or preventing airborne transmission of diseases in indoor environments (Du et al. 2020). There are different recommendations for the minimum required ventilation rate in indoor spaces to achieve an acceptable indoor air quality or prevent indoor airborne transmission. To name a few among many, the US Centers for Disease Control and Prevention (CDC) and World Health Organization (WHO) recommended a minimum ventilation rate of 12 air changes per hour (ACH) to prevent airborne transmission in healthcare facilities (Sehulster and Chinn 2003; Atkinson et al. 2016). The Harvard-CU Boulder Portable Air Cleaner Calculator (Allen et al. 2020) suggests a total of five ACH as a good ventilation condition for reducing airborne transmission risk in classrooms. While these recommendations are based on the ventilation rate, it has been challenging to quantify the outdoor air ventilation rate in a room. Therefore, indoor air CO_2 concentration is often considered a surrogate/indicator for air quality and ventilation conditions. For example, the Montreal school board (Centre de services scolaire de Montreal) stated in an open letter: "Establishments without a mechanical ventilation system should apply the window opening guidelines to ensure frequent air changes in our premises"; "Always to ensure good indoor air quality, we have also started measuring carbon dioxide (CO_2) in our establishments since November. In addition to this initiative, there are the CO_2 tests that must be carried out by all school service centers in Quebec. The level of CO_2 is a good indicator of the supply of fresh air in a room. Thus, following these tests, corrective measures will be put forward, if necessary." (Québec 2020).

As a result, many schools and teachers started to measure CO_2 levels concerning ventilation conditions and safety in their classrooms. In an unofficial study by the teachers in Montreal's 25 classrooms, one-day CO_2 levels were recorded randomly throughout the day (Wilton 2020) by CO_2 meters. More recently, the ministry of education of Quebec, Canada, purchased 90,000 CO_2 meters to be installed in the schools across the province when more than 600 schools had reported COVID-19 cases, which was more than twice the 2020 fall semester (Lofaro 2021). However, it remains a question of how to interpret the CO_2 readings regarding classroom ventilation conditions. Meanwhile, these data are not continuously recorded but randomly measured during a day under variable student numbers, schedules, and indoor and outdoor conditions (temperature, pressure, and background CO_2 levels). The investigation of these combined parameters will need a scientific approach to consider the stochastic/random nature of the problem. Persily (2015) reviewed the relationship of indoor CO_2 concentration to ventilation

rates, applications of indoor CO_2 levels to controlling outdoor air ventilation, and the role of indoor CO_2 levels in IAQ standards. It is stated that indoor CO_2 concentrations are related to ventilation rate, but the relationship is complicated. In the literature, several studies used a transient CO_2 mass balance method and measured CO_2 levels to calculate the ventilation rate in different indoor environments such as classrooms and university libraries (Penman 1980; Mumovic et al. 2009; Batterman 2017). Batterman (2017) estimated the CO_2 generation rate based on age and assumed activity level for CO_2 calculation in mechanically ventilated classrooms. They then used the whole-day data to estimate the ventilation rate. Many of the previous analyses were deterministic without sensitivities and uncertainties identified. In summary, due to various factors affecting CO_2 levels, such as variable occupant numbers, different CO_2 generation rates based on age and sex, and dynamic surrounding environment, especially when opening windows, is it possible to relate CO_2 concentrations to ventilation rates? If the answer is yes, how could we quantify the uncertainties? The answers to these questions center around the uncertainties and associated sensitivity analysis of parameters. Sensitivity analysis (SA) and calibration methods such as Bayesian Markov Chain Monte Carlo (MCMC) method (Strawderman 2000) can be used along with measured indoor CO_2 concentrations to find the dominant parameters for the CO_2 levels, such as ventilation rate, which may then be calibrated to understand the ventilation condition in a room.

Bayesian MCMC is a calibration technique proposed in the twentieth century. Its application to the computer models' calibration was systematically illustrated by Kennedy and O'Hagan (2001). Bayesian inference calibration has been widely utilized, such as environment (Steel 2001; Van Oijen et al. 2005; Arhonditsis et al. 2008; Lehuger et al. 2009), hydrology (Kuczera et al. 2010; Hall et al. 2011; Xu and Valocchi 2015), transportation (Van Hinsbergen et al. 2009), and medicine research (Whyte et al. 2011). One of the early building applications was conducted by Heo et al. (2012) for building energy model calibrations. In a recent review on Bayesian inference calibration, Hou et al. (2021) indicated that Bayesian inference incorporates uncertainties into real systems' approximations by propagating parameters using probabilistic analysis. Combining multiple sources of information at different scales and with different reliabilities, the inadequacy of a model, revealed by the discrepancy between the predictions and observed data, can be calibrated. It was also found that (1) Bayesian calibration results are more stable and reasonable than conventional deterministic methods, especially when the measurements are qualitatively/quantitatively insufficient. This is because in the Bayesian process, the uncertainties of calibration parameters and

measurements were considered in prior distributions and the likelihood function. (2) Bayesian inference calibration interprets results with a degree of belief by conducting quantitative stochastic analysis. And with more data availability, Bayesian inference is capable of aligning the posterior distributions of calibration parameters to actual conditions. These features are required for the calibration of CO_2 readings and the understanding of ventilation conditions in classrooms.

Therefore, we proposed a Bayesian calibration approach and demonstrated it to estimate CO_2 levels and ventilation rates in four primary schools located in Montreal, Canada. All the CO_2 meters have been carefully calibrated in the lab. The field measurement CO_2 readings were used as calibration and validation data for the transient CO_2 estimation model. A sensitivity analysis was conducted to find the most dominant parameters for indoor CO_2 levels. The Bayesian MCMC method was then developed to calibrate the dominant parameters and quantify the uncertainties. Then we discussed the key parameters of the calibration performance, including the student occupancy schedule and numbers and the CO_2 reading frequencies, which could inform schools how to use a CO_2 meter in daily operations and interpret the readings during the pandemic. Other researchers can apply the proposed Bayesian inference approach to understand better the relation of real-world CO_2 levels and room ventilation conditions.

2   Methodology

This section presents the procedure of Bayesian inference calibration for building indoor air quality models (Figure 1). Details about steps such as indoor CO_2 concentration model, sensitivity analysis, CO_2 sensor calibration, the Bayesian inference calibration method are demonstrated. Also,

performance metrics used to estimate the model predictions are shown.

2.1   Indoor CO_2 concentration model

A transient mass balance model is solved to calculate CO_2 concentration in the room.

$$V\frac{dC_{CO_2}}{dt} = G_s + \lambda_1 C_{oa} - \lambda_1 C_{CO_2} \tag{1}$$

where V is the room volume (m³); C_{CO_2} is the indoor air CO_2 concentration (mg/m³); t is the time duration (s); G_s is the CO_2 generation rate by all occupants (mg/s), which depends on the age, activity level, and occupancy level; λ_1 is the total outdoor air ventilation rate (m³/s); and C_{oa} is the outdoor air CO_2 concentration (mg/m³). The transient mass balance of Eq. (1) applies to solving arbitrary occupancy patterns and generation rates in classrooms. The solution of Eq. (1) is:

$$C_{CO_2} = \frac{G_s}{\lambda_1}\left(1 - e^{-\frac{\lambda_1}{V}t}\right) + \left(C_{CO_2,0} - C_{oa}\right)e^{-\frac{\lambda_1}{V}t} + C_{oa} \tag{2}$$

where $C_{CO_2,0}$ is the observed initial CO_2 concentration at each occupancy phase, e.g., during a class or break session.

2.2   Sensitivity analysis model

Estimating CO_2 levels in rooms include many uncertainties, such as ventilation and emission rates. These parameters may impact the results and should be calibrated by measurement data. Ideally, with sufficient measurements and computing resources, all the uncertain parameters should be included in the numerical calibration parameters. In reality, limited by data quality/quantity or computer
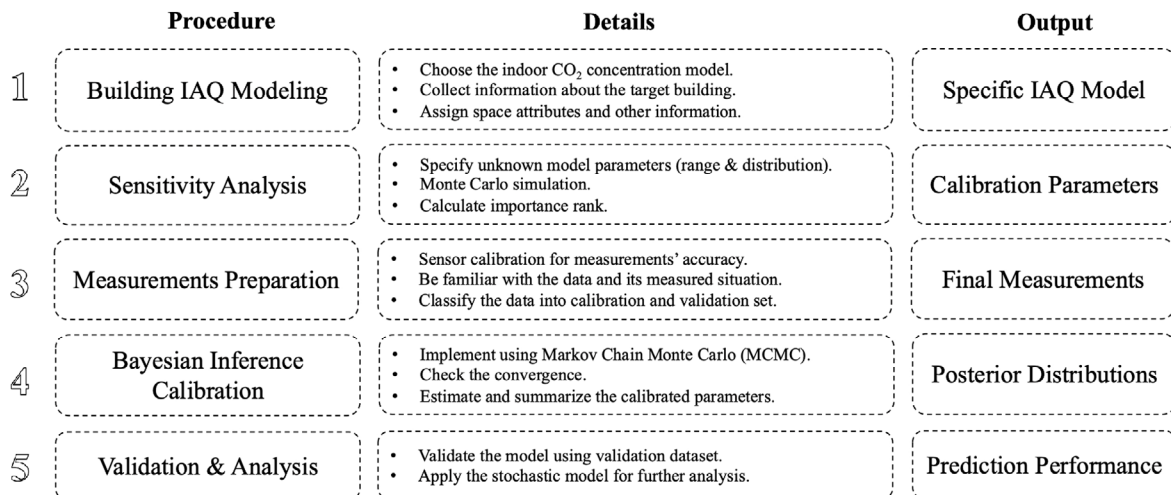
Procedure	Details	Output
1 Building IAQ Modeling	• Choose the indoor CO_2 concentration model. • Collect information about the target building. • Assign space attributes and other information.	Specific IAQ Model
2 Sensitivity Analysis	• Specify unknown model parameters (range & distribution). • Monte Carlo simulation. • Calculate importance rank.	Calibration Parameters
3 Measurements Preparation	• Sensor calibration for measurements' accuracy. • Be familiar with the data and its measured situation. • Classify the data into calibration and validation set.	Final Measurements
4 Bayesian Inference Calibration	• Implement using Markov Chain Monte Carlo (MCMC). • Check the convergence. • Estimate and summarize the calibrated parameters.	Posterior Distributions
5 Validation & Analysis	• Validate the model using validation dataset. • Apply the stochastic model for further analysis.	Prediction Performance

Fig. 1 Procedure of Bayesian calibration for building IAQ models

resources, we may consider only a few parameters. Many parameters and inputs could also manifest different uncertainty and significance levels on simulation outputs. For several parameters, their impacts are slight or even can be ignored. While for certain key parameters, an imperceptible change can cause a considerable transformation of model outputs. So, it is impracticable and unnecessary to calibrate all parameters but for dominant parameters. Calibrating only for critical model parameters makes it more practical in reality with limited data and computing costs. Identifying these dominant parameters cannot merely rely on arbitrary parameter selections from modelers' knowledge but should be based on a scientific process, i.e., a sensitivity analysis.

To conduct a sensitivity analysis process, prior distributions and ranges of selected unknown parameters should be assumed according to design code/standard, physical conditions, or modeler's knowledge. Then Monte Carlo (MC) simulation is employed to conduct parametric simulations by using Latin hypercube sampling (LHS) method (Li et al. 2016), which achieves the convergence of parameter space with relatively fewer samples. The obtained input–output dataset is then employed to identify the dominant model parameters that strongly affect the outputs. The importance ranking results may vary with different combinations of sensitivity methods and outputs depending on the variety of fundamental algorithms and conditions of each sensitivity analysis method (Menberg et al. 2016). To avoid the potential inconsistency caused by the variety of algorithms and conditions of each sensitivity analysis method, the sensitivity analysis method, sensitivity value index (SVI), was applied (Lim and Zhai 2017). Equation (3) defines the SVI by the normalization and aggregations for different sensitivity analysis methods.

$$\sum_{l=1}^{m} \frac{\sum_{j=1}^{k} \left(\dfrac{V_{i,j}}{\sum_{i=1}^{n} |V_{i,j}|} \right)}{m \cdot k} \times 100 = \text{sensitivity value index(SVI)(\%)}$$

(3)

where $V_{i,j}$ is the value of a sensitivity analysis method, i is a parameter, n is the total number of the parameters, j is a sensitivity method, k is the total number of sensitivity methods, l is the target output, and m is the total number of target outputs.

2.3 Experimental calibrations of CO_2 meters

In this study, two CO_2 meters, Temtop M2000C Monitor (handheld unit) and HOBO MX1102A CO_2 logger (wall mount unit), were employed and experiemtanlly calibrated by two approaches in the calibration chamber, one with a reference meter Vaisala GMP252, and the other with the ISO certified calibration gas. Details are summaried in Table 1. The Temtop monitor is an off-the-shelf multi-functional air quality monitor with a Non-Dispersive Infrared (NDIR) CO_2 meter and RH, PM, and temperature sensors at a price range of a few hundred dollars. The HOBO logger has an NDIR CO_2 meter and RH and temperature sensors at a higher price range. The Temtop monitor allows the manual calibration to the zero level with a resolution of 1 ppm and a maximum level of 5000 ppm. The HOBO logger has the same maximum measurement range and the claimed accuracy of ±50 ppm. It has manual zero calibration and automatic calibration functions. The auto-calibration means the logger is set to the background CO_2 level of 400 ppm automatically based on the three lowest measurements during the 24-hour or 8-day time period when applicable. That is to say, once

Table 1 Basic information and calibration conditions about the CO_2 meters

Model	Temtop M2000C	HOBO MX1102A
Type	Handheld	Wall mount
Used for	Rooms #1–#3	Room #4
Features	• CO_2 meter with RH, PM, and temperature • Lower price • Range: 0–5000 ppm • Manual calibration	• CO_2 meter with RH and temperature • Higher price • Range: 0–5000 ppm • Manual and automatic calibration
Calibration condition		
Chamber temperature	22.1–25.3 °C	22.1–25.3 °C
Chamber indoor pressure	1013.3–1014.1 hPa	1013.3–1014.1 hPa
Flow rate	3 LPM	2 LPM
Average CO_2	Measurements in last 10 min	Measurements in last 30 min
Calibration method	Reference meter (Vaisala GMP252) & ISO certified calibration gas	
Accuracy	6%	3%

the logger starts, it will be calibrated after 24 hours and then again after 8 days automatically unless it is manually calibrated.

The experimental calibrations were conducted in the Indoor Air Quality group at National Research Council Canada (NRC). The calibration chamber conditions were recorded to be between 22.1–25.3 °C and 1013.3–1014.1 hPa. For the reference meter, the time-averaged levels were recorded every 10 seconds for the last 10 minutes of the test. For the HOBO CO_2 calibrations, the flow rate was set to be 2 LPM, and then the chamber pressure was increased to 1013 hPa to ensure a slight positive pressure compared to the ambient environment. Each test ran for an hour in total, allowing the CO_2 concentration to be stabilized in the 1st thirty minutes and the last thirty minutes for calculating the averages of the CO_2 concentration. For the Temtop calibrations, the flow rate was 3 LPM, and the last 10 minutes were averaged for the CO_2 concentrations with all other conditions the same as the HOBO meters. Figure 2 shows the calibration results for both CO_2 meters compared to the reference meter and ISO calibration gas cylinders. All meters show good linearities, whereas the Temtop has an average accuracy of 6% and the HOBO has 3%. In comparison, the reference meter has an accuracy of 1%. All three meters show the underestimations of the calibration gas.

2.4 Bayesian calibration and Markov Chain Monte Carlo (MCMC) models

As the footstone of all Bayesian statistics, Bayes' theorem was first proposed by Reverend Thomas Bayes in his doctoral dissertation (Bayes 1763) and can be described as:

$$\text{Posterior} = \frac{\text{Probability of the data} \times \text{Prior}}{\text{Average probability of the data}} \quad (4)$$

The probability of an event is inferred based on the prior knowledge of conditions related to the event. Bayesian inference is one application of Bayes' theorem and can be written as:

$$p(\theta|y) = \frac{p(y|\theta) \cdot p(\theta)}{p(y)} \propto p(y|\theta) \cdot p(\theta) \quad (5)$$

where $p(\theta|y)$ is the posterior distribution of the unknown parameter θ based on known observation y. $p(y|\theta)$ is the likelihood function of observation conditional on the unknown parameter. $p(\theta)$ is the prior distribution of the unknown parameter which is the marginal probability that means it is irrespective of the outcome of another variable, and $p(y)$ is the probability of the observation that is marginal as well to normalize $p(y|\theta)$. Therefore, the posterior probability is proportional to the product of the prior probability and the likelihood.

Implementing the Bayesian inference for all possible scenarios in a solution domain is impractical because the likelihood's integrals can be computationally expensive or sometimes impossible to calculate. MCMC is a versatile approach to solve the parameter estimation problem with two components. One is the well-known Monte Carlo method. It is a computational algorithm to solve statistically challenging problems relying on repeated random samplings and approximate the target value (e.g., mean value) using the independent samples' results. The other is the Markov Chain method for solving a sequence of possible events. The probability of each event depends only on the state attained in the previous event. By combining MCMC and Bayesian inference, it is guaranteed that a series of samples can be generated from the posterior distribution efficiently to represent the features of the posterior distributions. Different MCMC algorithms can be classified into either a "random walking" group or a gradient-based group according to the acceptance-rejection criterion. This study applied the Hamiltonian Monte Carlo (HMC) sampling method (Betancourt 2017) for the MCMC. HMC is a typical representation of gradient-based approaches that use the
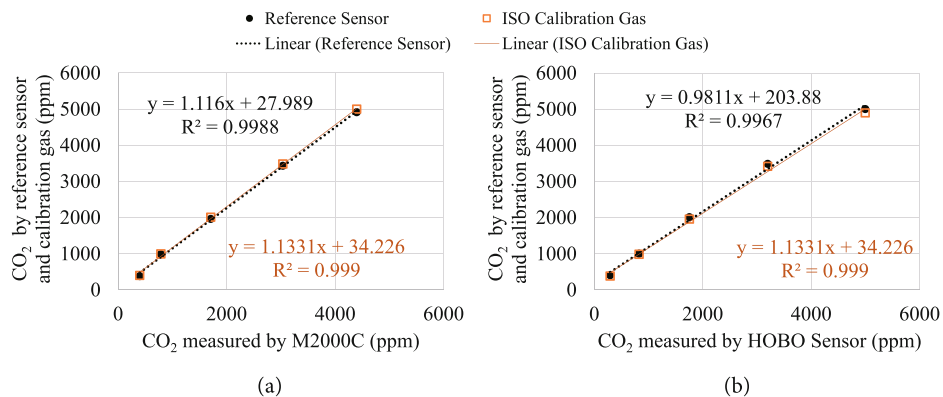

Fig. 2 Calibrations of CO_2 meters: (a) Temtop M2000C and (b) HOBO MX1102A

first-order gradient information to determine how to move in the right direction quickly. A Gaussian distribution was assigned to the likelihood function. The output of the indoor CO_2 concentration model was used to estimate the mean value of the Gaussian distribution. The posterior distribution of the calibration model parameters can be generated during the HMC process by absorbing the information from measurements. Five thousand steps of the HMC algorithms on each of four separate chains were explored in this study to make a total of 20,000 samplers. We used one thousand samples during the "warming-up" stage to move chains toward the highest density area and tune sampler hyperparameters. For each room, the first 2/3 of measurements are used for the calibration, which means that the measurements are employed in the Bayesian calibration process to calculate the calibration parameters. While the remaining are used for model validation, which means the values of the calibration parameters determined during the calibration process are set in the indoor CO_2 concentration model to simulate the CO_2 levels. Then the output CO_2 concentrations are compared to the last 1/3 CO_2 measurements to calculate the performance metrics for the accuracy assessment. At each time step, t, the measurement of $(t-1)$ time step is used as the initial value of the CO_2 concentration model. The information such as occupancy level, outdoor weather condition, and indoor air temperature of the current time step was used. The "rolling-window" approach was found to perform better than that using the first measurement as the initial value for all time steps.

2.5 Performance metrics

To assess the performance of the models, we consider two criteria: (1) the Accuracy of prediction compared to the measurements (Alavi et al. 2020), and (2) the mean absolute percentage error (MAPE) (Taheri and Razban 2021). The Accuracy of a prediction is computed as the percentage of the predicted values that fall within the confidence interval around the measurements, and the confidence interval was set to be ±(30 ppm + 5% × reading) (Yasuda et al. 2012;

Alavi et al. 2020). MAPE is a performance metric based on the percentages of errors:

$$\text{MAPE} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{y_i - \hat{y}_i}{y_i}\right| \times 100 \qquad (6)$$

where $\hat{y}_i$ is a predicted variable value for period i, y_i is an observed value for the time i, and N is the sample size. Different MAPE values indicate the performance of a prediction: <10% for an accurate forecast, 11% to 20% for a decent forecast, 21% to 50% for a fair forecast, and >50% for a poor model (Ahmadi et al. 2021).

3 Case study

In this study, four typical classrooms, each from different primary schools in Montreal, Canada, were measured for the CO_2 levels. Three classrooms were monitored during a typical pandemic day (November 6–10, 2020) by the Temtop M2000C Monitor (Group 1), while one school was monitored for three consecutive pandemic days (September 21–23, 2020) by the HOBO MX1102A CO_2 logger (Group 2). The Group 1 measurements were provided from a source with the name withheld and with recorded student ages and numbers, ventilation system status (if any), and window status (open/close). The Group 2 data were obtained from our previous research project (Wang and Shu 2021), where the student information and window status were not recorded, and indoor conditions were available from the meters. Please note that the measurement data from Group 1 represent the realistic scenario that random, discrete, and limited CO_2 readings were collected by school teachers, whereas more continuous data from Group 2 were obtained from our project for research purposes with more readings available. Both scenarios are considered to cover what may happen in reality at different levels of uncertainty. We have continuously monitored CO_2 levels in six schools with more than 18 classrooms for 2020–2022. This study selected only Group 2 data to demonstrate the proposed Bayesian inference method. The summary of the measured information is shown in Table 2 and Figure 3.

Table 2 Basic information about the measured classrooms

Groups	Room No.	Date	Volume (m³)	MV	NV	Occupancy recording	Student age	CO_2 data points	Measured resolution	Case study
	#1	Nov. 10, 2020	165	Y	Y	Y	7	14	Random	Section 4
1	#2	Nov. 6, 2020	236	N	Y	Y	11	14	Random	Section 4
	#3	Nov. 9, 2020	236	N	Y	Y	7	12	Random	Sections 4 & 5.1
2	#4	Sept. 21–23, 2020	231	N	Y	N	7	73×3	5 min	Sections 4 & 5.2

Notes: MV = mechanical ventilation; NV = natural ventilation; Y=yes; N=no.

Fig. 3 (a) CO_2 concentration measurements, (b) occupancy level profiles, (c) outdoor air temperatures, (d) outdoor air pressures, and (e) indoor temperatures

The ASHRAE Standard 62-2001 (ANSI/ASHRAE 2001) recommended a CO_2 level of 1000 ppm for acceptable indoor air quality. Similarly, the ASME Standard D6245-18 (ASTM 2018) recommended the same 1000 ppm level based on the perception of body odor to be acceptable for at least 80% of unadapted persons (visitors) in a room when the outdoor CO_2 level is 350 ppm. The National Institute for Occupational Safety and Health (NIOSH) recommended a CO_2 level of 600–1500 ppm for schools and workplaces but only considered comfort and working efficiency (NIOSH 2020). In this study, Room #1 was equipped with a mechanical ventilation system, and the windows were opened too for more outdoor air. So the measured indoor CO_2 level was between 500 and 1000 ppm (Figure 3(a)), which was below the level of the previously stated requirements. The rest of the rooms were only with natural ventilation from windows, so the CO_2 concentrations were higher. Especially for Room #4, the CO_2 reached up to 2200 ppm. The outdoor air pressure and temperature data were extracted from the datasets from Environment and Climate Change Canada (ECCC 2020) for Rooms #1–#3. For Room #4, the outdoor air temperature was measured by a local weather station (Wang and Shu 2021). Other parameters required for the CO_2 calculation, such as CO_2 generation rate, outdoor air ventilation rate, and CO_2 levels, are not available and need to be calibrated. Indoor air temperatures were calibrated for Rooms #1, #2, and #3 since they were not measured.

The occupancy patterns of Room #1 and Room #2 were recorded, but for Room #3, only one people number was recorded in the morning. Therefore, in the next section, the

reported occupancy levels were used in the calibration process for Room #1 and #2. For Room #3, the occupancy level was unknown, so two different patterns were investigated and compared: one constant occupancy of 19 persons (occ1) and the other with variations (occ2), which was based on the recorded information in the morning and the trend of CO_2 measurements during the day. Specifically, for the first two measured CO_2 readings, the trend is increasing. Therefore, the occupancy level was assumed as 19 at the first two time step accordingly. For the third and fourth measured points, the occupancy level was assumed as zero since the indoor CO_2 levels decreased. From the fourth point to the last point, the occupancy level was assumed as 19 except for the sixth time step since from the fifth point to the sixth point, the CO_2 concentrations increased slightly. For the sixth time step, the occupancy level were assumed as 0. For the generation of occupancy schedule occ2, we referred to the relationship between indoor CO_2 concentration and occupancy level in Room #1 and Room #2, where the occupancy schedule was recorded by teachers. The comparison of the impacts of these two occupancy schedules was discussed. For Room #4, the daily averaged constant occupancy level was calibrated.

4   Results

In this section, the sensitivity analysis was conducted to find the dominant parameters for calculating CO_2 concentrations. Then we use the Bayesian MCMC calibration to estimate the time-averaged ventilation rate using 2/3 of the CO_2 measurement data and occupancy patterns. We validated the calibrated CO_2 model by 1/3 of the measurement data. The impacts of the assumptions on occupancies and the measurement frequencies on the estimations were discussed in Section 5.

4.1 CO_2 model sensitivity analysis

Outdoor/indoor pressure, outdoor/indoor air temperature, occupancy level, room volume, outdoor air ventilation rate, and CO_2 generation rate are input parameters to predict CO_2 concentration. The ranges of selected model inputs/parameters were defined according to the references, codes, and standards available for the sensitivity analysis. Then LHS, one of Monte Carlo sampling methods, was applied to sampling from the ranges. According to Matala's suggestion (Matala 2008), a total of 440 sampling sets was determined and used as the inputs to calculate the indoor CO_2 concentration. The input–output datasets were employed to calculate the SVI value and the importance rank. Table 3 shows the parameters with their sensitivity importance rankings: a smaller number indicates a more important/sensitive parameter.

The result showed that the most dominant parameters affecting classroom CO_2 levels are outdoor air ventilation rate, CO_2 generation rate per person, number of occupants, and outdoor CO_2 concentration. Specifically, the outdoor air ventilation rate's SVI is more than twice the CO_2 generation rate. For Group 1 classrooms, because occupant number, outdoor temperature, and pressure were measured, they do not need to be calibrated. We selected outdoor air ventilation rate, CO_2 generation rate, outdoor CO_2 concentration, and indoor air temperature for the next step model calibration. For Room #4, the occupant number was unknown, so all relevant parameters were calibrated.

4.2   Calibration and validation

For the calibration of the CO_2 model by the Bayesian inference method, during an occupancy phase (e.g., between every two measurements), we applied the "rolling window"

Table 3 Sensitivity analysis with importance ranking for indoor CO_2 concentration

Parameters	Symbol	Range	Reference	Sensitivity analysis method				
				SRC	Random forest	T-value	Sensitivity value index	Rank
Outdoor air ventilation rate (ACH)	λ_1	0.01–2 (natural); 1–5 (mechanical)	ANSI/ASHRAE 2019	0.32	27.8	7.3	42.1	1
CO_2 generation rate per person (L/(s·person))	G_1	0.002–0.01	Batterman 2017; Persily and de Jonge 2017	0.18	10.1	4.1	20.2	2
Number of occupants (#)	N_{tot}	10–30	Measured	0.06	4.6	1.4	7.5	3
Outdoor CO_2 (ppm)	C_{oa}	396–416	Batterman 2017; McGee 2016	0.08	2.3	1.7	7.4	4
Outdoor pressure (kPa)	P_{oa}	100.5–102.5	ECCC 2020	0.05	0.7	1.2	4.6	5
Indoor pressure (kPa)	P_{in}	100.5–102.5	ECCC 2020	0.02	4.3	0.4	4.2	6
Indoor air temperature (°C)	T_{in}	18–25	ECCC 2020	0.04	1.9	0.8	4.0	7
Outdoor air temperature (°C)	T_{oa}	10–20	ECCC 2020	0.01	1.82	0.2	1.6	8

concept so that the first measurement of every measurement interval was used as the initial CO_2 level for that interval in Eq. (2). Figure 4 and Table 4 showed the posterior distributions of the Bayesian inference. In each subplot, the red dash lines represent the parameters' prior distributions in Table 4, and the posterior distributions are indicated by the shaded areas. A high peak value of the probability density function (PDF) from the *Y*-axis shows a high chance of the calibrated parameter value. Figure 4 clearly shows that the outdoor air ventilation rates, CO_2 generation rates for all rooms, and occupancy level for Room #4 illustrate higher peak values after the calibrations, meaning a higher chance of these calibrated parameter values to occur in reality than before the Bayesian analysis.

In Table 4, the calibrated mean value of the outdoor ventilation rate with the confidence level of 95% is 1.96 ± 0.31 ACH for Room #1, 0.40 ± 0.08 ACH for Room #2, and 0.79 ± 0.06 ACH for Room #3 (occ1 by default), 0.40 ± 0.32,

0.48 ± 0.37, 0.72 ± 0.39 ACH for Room #4 in the three consecutive days, respectively. Room #1 was both mechanically and naturally ventilated (i.e., open windows), so its ventilation rate is significantly higher than other rooms with open windows only. For the first three rooms of Group 1, which has a similar number of measurement points, the span of the posterior distribution of Room #1 is more significant because of its wider prior distribution range than the other two rooms. For the parameters of CO_2 generation rate, outdoor CO_2 level, and indoor air temperature, Room #2 is closer to Room #3 than to Room #1 because Rooms #2 and #3 were both naturally ventilated only. In comparison, the uncertainties of calibration parameters (i.e., the standard deviations), such as outdoor air ventilation rate and CO_2 generation rate for Room #4, are greater than the Group 1 rooms. It is also noted that the calibrated outdoor CO_2 concentrations were stable for all Rooms on different days between 401.80 and 414.40 ppm.
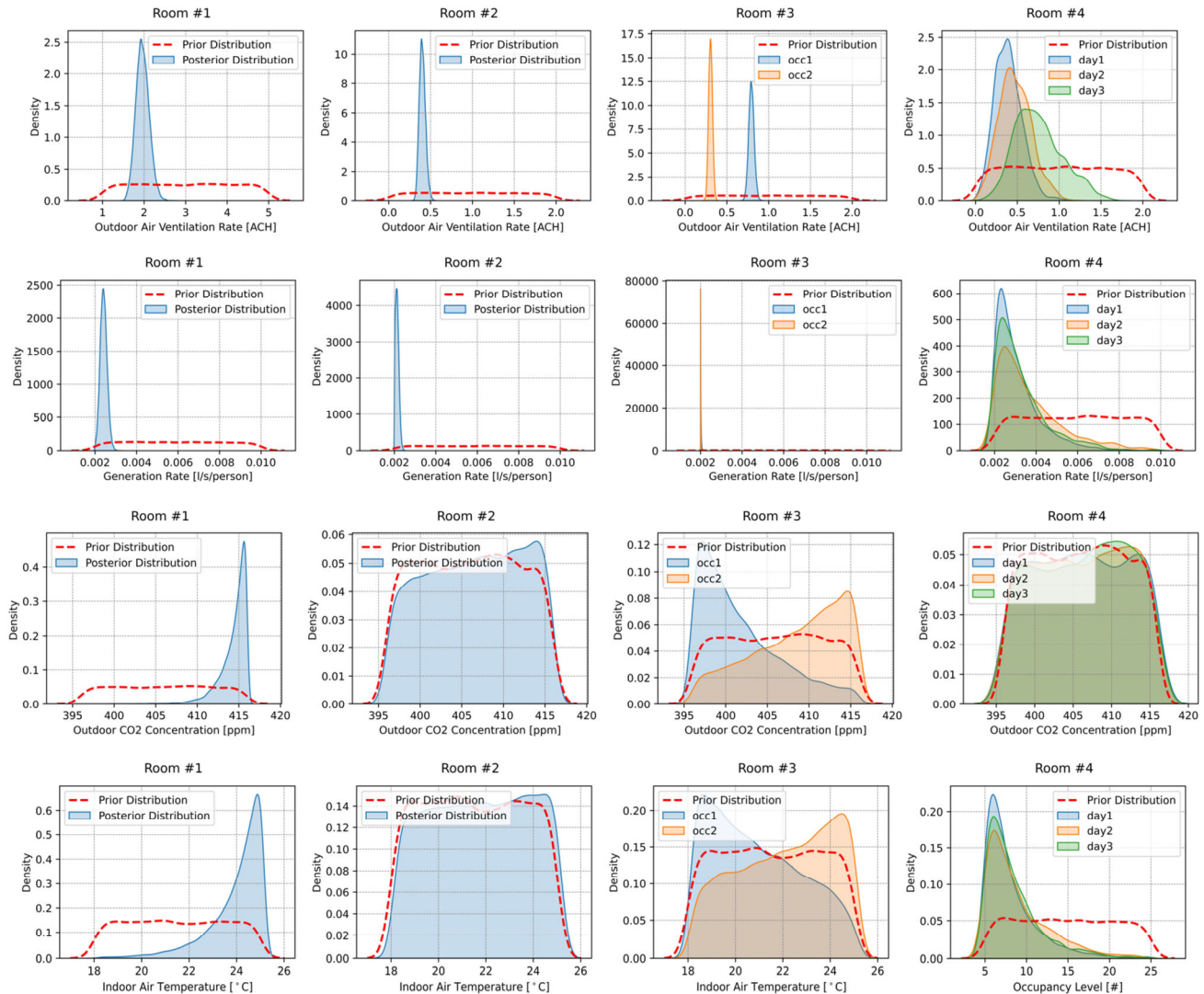

Fig. 4 Distribution of calibrated parameters of the indoor CO_2 model

Table 4 Calibrated parameters of the CO_2 model

Room	Prior distribution Uniform distribution range	Posterior distribution Mean value	Standard deviation	Quantiles (%) 2.5	25	50	75	97.5
Outdoor air ventilation rate (ACH)								
Room #1	(1, 5)	1.96	0.16	1.67	1.85	1.96	2.07	2.29
Room #2		0.40	0.04	0.33	0.38	0.40	0.43	0.48
Room #3 (occ1)		0.79	0.03	0.73	0.77	0.79	0.81	0.86
Room #3 (occ2)	(0.01, 2)	0.30	0.02	0.26	0.29	0.30	0.32	0.35
Room #4 (day 1)		0.40	0.16	0.11	0.27	0.38	0.49	0.73
Room #4 (day 2)		0.48	0.19	0.13	0.34	0.46	0.61	0.89
Room #4 (day 3)		0.72	0.26	0.28	0.54	0.72	0.93	1.35
CO_2 generation rate ($\times 10^{-3}$ L/(s·person))								
Room #1		2.42	0.16	2.12	2.30	2.41	2.52	2.75
Room #2		2.14	0.08	2.01	2.07	2.13	2.19	2.32
Room #3 (occ1)		2.02	0.02	2.00	2.01	2.01	2.03	2.07
Room #3 (occ2)	(2.0, 10.0)	2.01	0.01	2.00	2.00	2.01	2.01	2.04
Room #4 (day 1)		3.00	1.00	2.02	2.30	2.76	3.48	6.00
Room #4 (day 2)		4.00	1.00	2.00	2.47	3.16	4.33	7.80
Room #4 (day 3)		3.00	1.00	2.03	2.36	2.90	3.74	6.63
Outdoor CO_2 concentration (ppm)								
Room #1		414.40	1.62	410.10	413.80	414.90	415.60	416.00
Room #2		406.50	5.72	396.60	401.70	406.90	411.60	415.50
Room #3 (occ1)		401.80	4.89	396.20	397.90	400.40	404.70	414.10
Room #3 (occ2)	(396, 416)	408.50	5.43	397.20	404.50	409.60	413.20	415.80
Room #4 (day 1)		405.91	5.80	396.40	401.01	406.17	411.37	415.66
Room #4 (day 2)		406.16	5.89	396.42	401.06	406.26	411.37	415.60
Room #4 (day 3)		405.98	5.93	396.50	401.11	406.74	411.35	415.62
Indoor air temperature (K)								
Room #1		297.00	1.13	293.80	296.60	297.40	297.90	298.10
Room #2	(291, 298)	294.70	2.03	291.40	293.00	294.80	296.60	298.00
Room #3 (occ1)		293.90	1.92	291.20	292.20	293.60	295.40	297.70
Room #3 (occ2)		295.10	2.00	291.40	293.40	295.30	296.90	298.00
Occupant level								
Room #4 (day 1)		8.00	3.00	5.00	6.00	7.00	9.00	17.00
Room #4 (day 2)	(5, 25)	9.00	4.00	5.00	6.00	8.00	11.00	19.00
Room #4 (day 3)		8.00	3.00	5.00	6.00	7.00	10.00	18.00

Using the mean values of the calibration parameters, we compared the simulation results and measurements of CO_2 in Figures 5 and 6. The accuracy performance of all scenarios for both calibration and validation process were summarized in Table 5. The calibrated models were able to capture the concentration trends in all cases with various performances at specific time points for different cases. Room #2 and Room #4 are more accurate than other cases, especially Room #4. The time interval of every two

measurements was 33–41 min for Room #1, 17–43 min for Room #2, 24–55 min for Room #3, and 5 min for Room #4. Room #4 had the most data for calibration, so the average Accuracy of the three days was 83% for the calibration step and 89% for the validation step (Figure 6). The highest MAPE of Room #4 is 6%, which is considered an "accurate" forecast (<10%). The accuracy of Room #3 is the lowest due to the constant occupancy assumed (i.e., 19 students) and the longer data intervals (e.g., 55 min maximum) for the
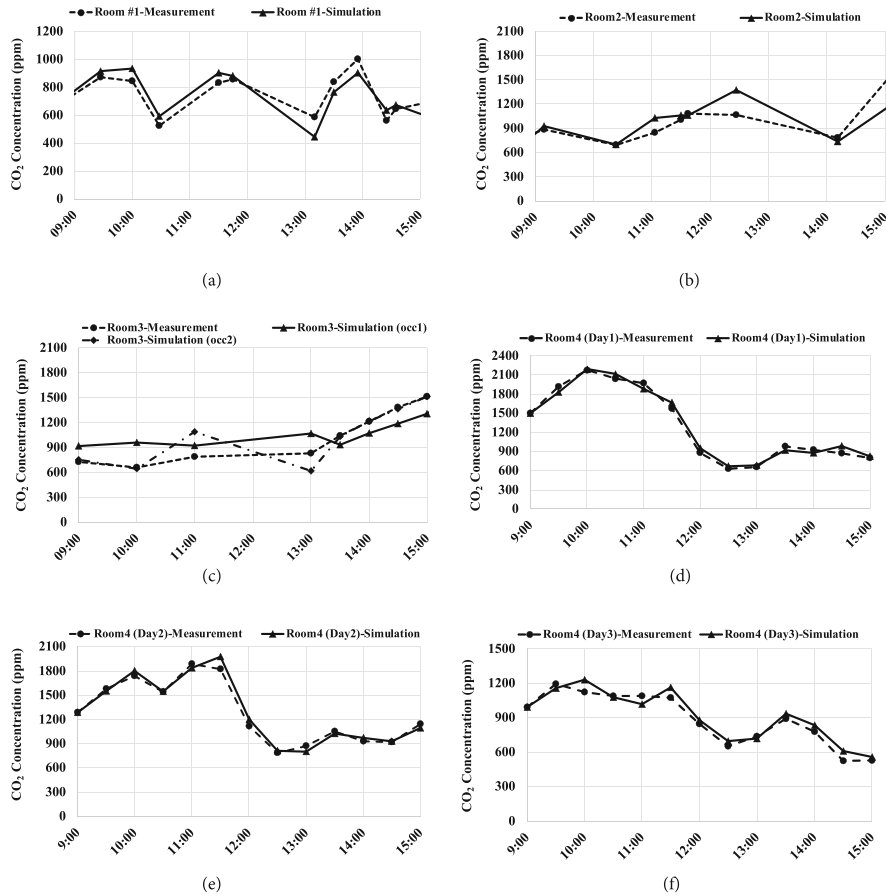
Fig. 5 Comparisons of the simulated and measured CO_2 levels in (a) Room #1, (b) Room #2, (c) Room #3, (d) Room #4 – Day 1, (e) Room #4 – Day 2, and (f) Room #4 – Day 3
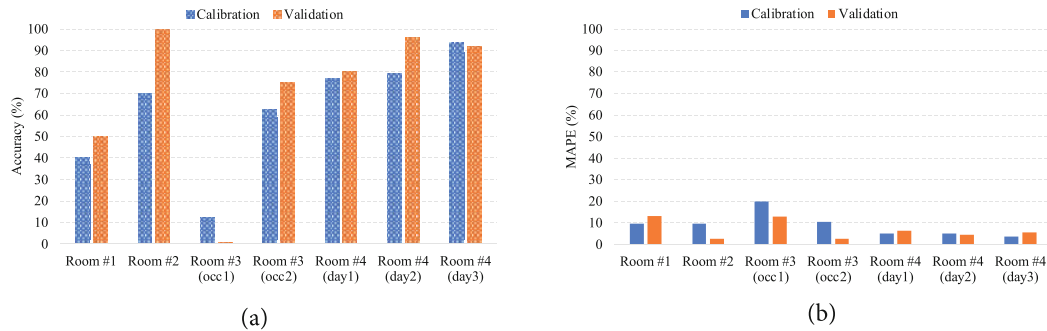

Fig. 6 The performance of the model predictions by (a) Accuracy; (b) MAPE

calibration, especially around the noontime. In comparison, Room #2 performs better as a result of a relatively shorter measurement interval.

5 Discussion

5.1 Occupancy schedule

The sensitivity analysis revealed that occupancy is the third important parameter so we chose Room #3 to investigate the impacts of two occupancy schedules: the default one with the constant people number (occ1, 19 students) throughout the day and the other dynamic schedule estimated by the morning counts of the student number and the CO_2 measurement trend (occ2) as shown in Figure 3(b). Table 4 shows the calibration results for both occupancy schedules. By using occ2, the mean outdoor air ventilation rate decreased from 0.79 to 0.30 ACH with a reduced standard deviation. For the second important parameter, CO_2 generation rate, occ2 also results in a

Table 5 Summary of performance metrics of the studied rooms

Case study			Performance metrics			
			Accuracy (%)		MAPE (%)	
			Calibration	Validation	Calibration	Validation
Room #1			40.0	50.0	9.6	13.2
Room #2			70.0	100.0	9.5	2.5
Room #3	Occ1		12.5	0.0	19.8	12.8
	Occ2		62.5	75.0	10.6	2.4
Room #4	Day 1	5 min	77.1	80.0	5.0	6.4
		10 min	37.5	46.2	10.5	10.0
		15 min	31.3	22.2	16.6	15.6
		20 min	25.0	14.3	20.8	19.3
		30 min	22.2	25.0	28.4	20.1
		60 min	20.0	0.0	47.2	54.4
	Day 2	5 min	79.2	96.0	5.0	4.5
		10 min	40.0	66.7	9.4	6.6
		15 min	29.4	62.5	13.0	8.7
		20 min	23.1	66.7	17.5	12.2
		30 min	22.2	50.0	20.3	13.1
		60 min	20.0	0.0	28.9	34.6
	Day 3	5 min	93.8	92.0	3.7	5.6
		10 min	58.3	41.7	6.7	11.8
		15 min	25.0	25.0	8.9	17.0
		20 min	50.0	33.3	11.9	28.3
		30 min	50.0	25.0	13.8	41.4
		60 min	25.0	0.0	24.6	78.3

reduced standard deviation but no major difference for the mean value. Figure 6 compares the Accuracy and the MAPE for both schedules. The occ2 scenario outperforms the occ1 with an increased Accuracy from 13% to 63% for the calibration step and from 0% to 75% for the validation step. The corresponding MAPE also decreased from 20% to 11% for the calibration and from 13% to 2% for the validation. Therefore, the availability of occupancy count and schedule could become critical, especially when there are not enough measurement data for the calibration. In comparison, when more CO_2 measured data are available, e.g., in Room #4, it is still possible to achieve an accurate prediction without the information of the occupancy schedule: the MAPE values were less than 10% for all three days (Figure 6). In this case, the proposed Bayesian inference method estimated an average number of 8 occupants for Days 1 and 3 and 9 students for Day 2, which were verified by the counted number of 8 students from our research project.

Therefore, the discussion here revealed that the performance of a Bayesian inference strongly depends on the amount of measurement information available, and it is always preferable to have as much information as possible to be collected from the field. When there is a lack of occupancy count and schedule information, one of the solutions is to increase the number of CO_2 measurement points, which are relatively easier to collect than occupancy counting. In fact, previous researchers have tried to estimate building/room occupancies based on CO_2 concentrations (Calì et al. 2015; Pantazaras et al. 2018; Han and Zhang 2020). Meanwhile, another question may arise regarding the impact of the CO_2 data points on the prediction accuracy when there is no occupancy information. This is related to the measurement interval of a CO_2 meter to be discussed in the next section.

5.2 Measurement interval

To study the impact of measurement intervals/frequencies on the model calibration accuracy, we investigated Room #4 with variable measurement intervals. Figure 7 compares the time-dependent CO_2 levels for different measurement intervals. A longer interval inclines to create a smoother profile and fails to capture the peak values. Considering that the airborne infection could occur in the order of minutes for close contacts (CDC 2020), especially for the new COVID-19 variants, a longer interval would not capture the short-term impacts. When the measurement interval was set to be 5 min, the time-dependent profiles were well captured at both high and low peak values. Therefore, if the hardware allows, such as the storage memory, it is always preferable to keep the measurement intervals in the order of minutes. The details of calibrated parameters for three days are summarized in Table 6. The observation shows that one of the direct outcomes of a longer interval is the overestimation of the outdoor air ventilation rates. The estimation could be doubled for an interval of 30 or 60 min compared to the case with the 5-min interval. The estimated occupancy level is also significantly higher than what was confirmed by the original researcher of the measurements. Here, a basic knowledge of occupancy, such as daily-averaged number, could be helpful during the evaluation when the detailed occupancy schedule may not be available.

The model prediction performance was also evaluated in Figure 8. The model performance decreased when the interval increased from 5 min to 10, 15, 20, 30, or 60 min. When the indoor CO_2 concentration was measured hourly, the simulation results considerably deviated from the observations with more than 50% MAPE for Day 1 and Day 3 and close to 40% for Day 2. If a MAPE cutoff of 20% for a decent forecast is applied, the time interval of 15 min
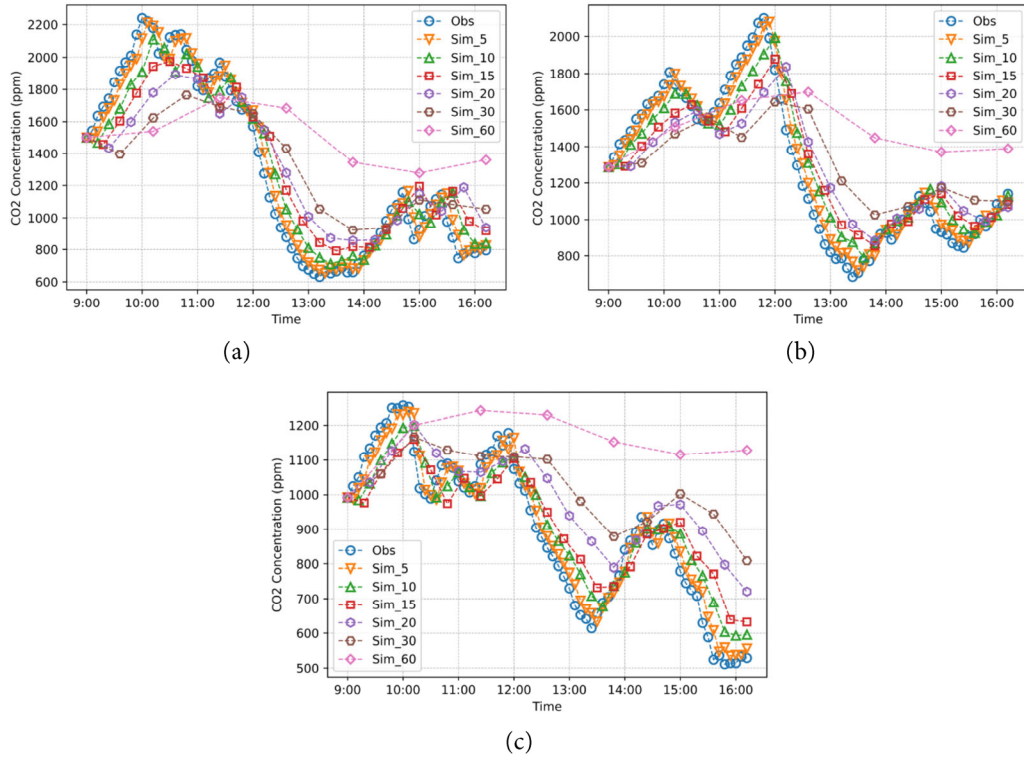
Fig. 7 Comparisons of the model predictions with different measurement frequencies for (a) Day 1, (b) Day 2 and (c) Day 3 of Room #4

Table 6 Calibrated model parameters for Room #4 with different measurement intervals

| Measurement interval (min)	Outdoor air ventilation rate (ACH)		CO$_2$ generation rate ($\times10^{-3}$ L/(s·person))		Outdoor CO$_2$ concentration (ppm)		Occupancy level	
	Mean	Std	Mean	Std	Mean	Std	Mean	Std
Day 1								
5	0.40	0.16	3.00	1.00	405.91	5.80	8.00	3.00
10	0.83	0.41	4.00	2.00	406.00	5.90	11.00	5.00
15	1.08	0.48	5.00	2.00	405.97	5.80	12.00	5.00
20	1.16	0.51	5.00	2.00	405.77	5.75	13.00	6.00
30	1.22	0.52	5.00	2.00	406.11	5.83	13.00	6.00
60	1.18	0.54	6.00	2.00	405.91	5.74	14.00	6.00
Day 2								
5	0.48	0.19	4.00	2.00	406.16	5.89	9.00	4.00
10	0.96	0.44	5.00	2.00	406.13	5.84	12.00	5.00
15	1.15	0.50	5.00	2.00	406.21	5.95	13.00	5.00
20	1.18	0.53	5.00	2.00	405.90	6.02	13.00	5.00
30	1.16	0.54	5.00	2.00	406.00	5.91	14.00	6.00
60	1.13	0.57	6.00	2.00	406.06	5.81	14.00	6.00
Day 3								
5	0.72	0.26	3.00	1.00	405.98	5.93	8.00	3.00
10	1.25	0.44	4.00	2.00	406.19	5.78	11.00	5.00
15	1.33	0.46	4.00	2.00	405.78	5.78	11.00	5.00
20	1.30	0.50	5.00	2.00	405.92	5.78	12.00	5.00
30	1.27	0.53	5.00	2.00	405.89	5.61	12.00	5.00
60	1.16	0.55	5.00	2.00	405.80	5.80	13.00	6.00
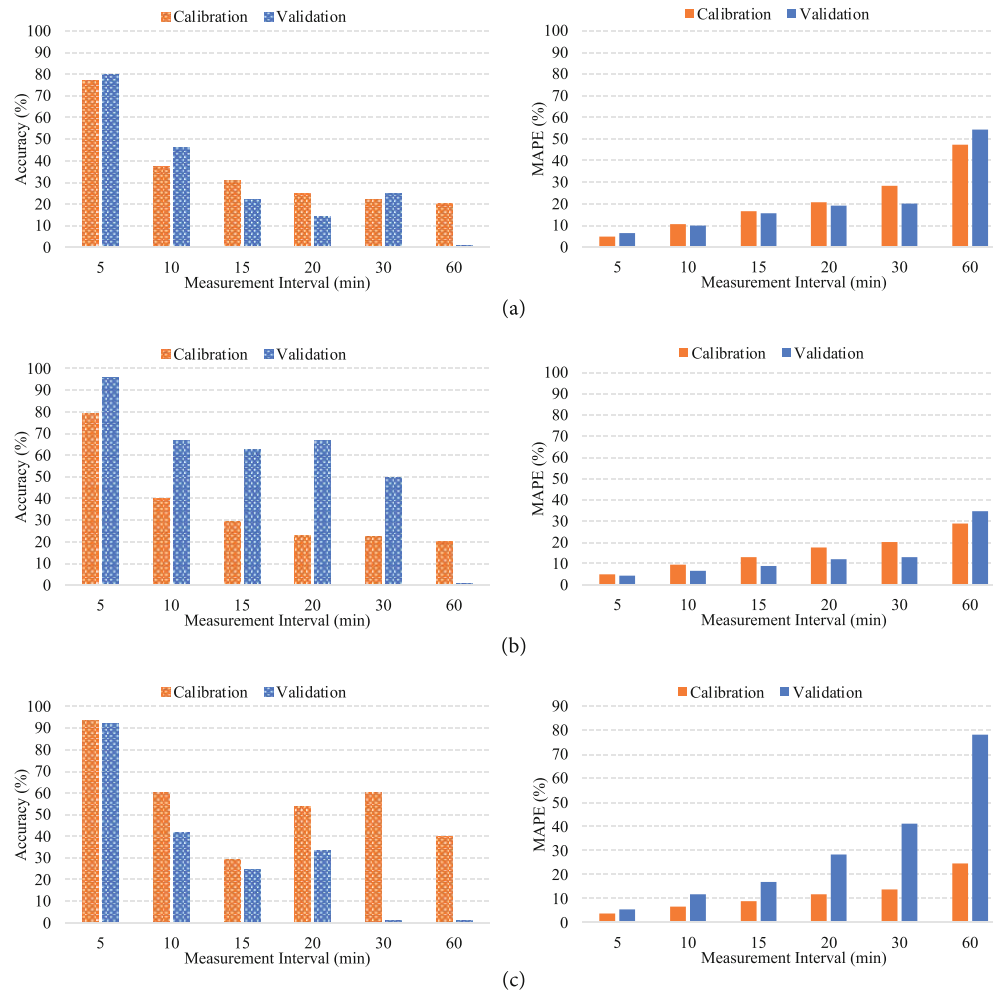
Fig. 8 The comparison of prediction performances of different measurement intervals for (a) Day 1, (b) Day 2, and (c) Day 3 of Room #4

seems to be reasonable for all three days, which corresponds to four readings per hour. Figure 7 also confirms that an interval of 15 min would generally capture the trends and peaks of the concentration profiles in all cases. In comparison, hourly measurements should be avoided if possible, and the 5-min interval already provides one of the best performances (MAPE <10%), so it would be unnecessary to go with shorter intervals for the current cases. On the other hand, because CO_2 meters would have become more accepted as a proxy of ventilation and indoor air quality conditions in buildings, these conclusions should be further evaluated and confirmed by more data from the field. This study proposed the Bayesian inference approach and demonstrated the analysis procedure necessary for conducting more research on this topic.

On the other hand, it is noted that, according to its definition mentioned in Section 2.5, the performance metric of Accuracy is based on the counting number of the prediction values that fall within the confidence interval around the measurements. The difference between predictions and measurements, however, is not directly considered. This can result in some acceptable predictions may be mis-counted in the calculation of the Accuracy when the points are quite close to the confidence interval bounds. For example, in Figures 7(c) and 8(c), the points 6, 9, and 12 of the interval of 15 min were not counted, but they were only with a small difference of 2.90, 5.92, and 2.40 ppm from the 95% confidence interval. This results in a lower "Accuracy" for the 15 min than the 20 min result (Figure 8(c)). The Accuracy (the orange bar for the calibration step of the 15-min in Figure 8(c)) would increase from 29.4% to 47.05% if these three points are counted. This also shows when measurement data are limited, the impact of each point becomes significant on the final result, so more data points are always preferred to avoid the randomness and uncertainty from a specific point.

6 Conclusion

This study focused on a few important aspects of using CO_2

meters in primary schools in terms of the key parameters contributing to their readings and the exploration of the possibility of estimating outdoor air ventilation rate based on these readings. The study conducted a sensitivity analysis and proposed a Bayesian inference calibration approach using measured indoor CO_2 profiles in four primary schools to identify the relations between CO_2 levels and ventilation rates. The impacts of the occupancy schedule and measurement intervals on the proposed Bayesian inference performance were also discussed. The main findings are as follows:

a. The sensitivity analysis revealed that the outdoor ventilation rate, CO_2 generation rate, and occupancy level are the top three most significant parameters for indoor CO_2 concentrations.

b. For the top parameters determining the indoor CO_2 level, the outdoor ventilation rate is more than double as important as the CO_2 generation rate, which is then more than double as important as the occupant number in a school context.

c. The proposed Bayesian inference approach was shown to be able to capture the trends and time-dependent CO_2 profiles accurately when enough measurement data points are available. For example, the MAPE of the case with the 5-min measurement interval is less than 10%, indicating an accurate prediction of the CO_2 level on different days.

d. We demonstrated the possibility and explained the procedure of using Bayesian inference to estimate outdoor ventilation rates and occupancy levels. For example, the corresponding outdoor air ventilation rate with a 95% confidence level is 1.96 ACH for Room #1 with mechanical ventilation and fully open windows and 0.3–0.79 ACH for other rooms with only windows open. The estimated occupant number in one of the school rooms was 8–9 (Room #4), which was confirmed after the calibration was completed.

e. This study evaluated the importance of the occupancy schedule when there is a lack of CO_2 measurement data. As one of the major uncertainties, the dynamic occupancy schedule is critical for the CO_2 level estimations, especially when limited CO_2 data are available during a calibration.

f. This study also evaluated the importance of CO_2 reading intervals when there is a lack of occupancy information. For an accurate estimation, hourly CO_2 recording should be avoided because it smoothes the measurement profiles, fails to reflect the peak CO_2 values, and could overestimate the outdoor ventilation rates in the room. A 15-min measurement interval can capture both the trends and peak CO_2 values in the rooms of interest with a MAPE of less than 20%. It is preferable to go with shorter durations if possible, whereas a 5-min reading

seems adequate to reach an acceptable level of the estimation with a MAPE of less than 10%.

A few limitations of this study are noted and can be explored further in the future:

▪ The transient CO_2 model in Eq. (1) assumes a well-mixed environment and no neighbor zones or neighbor zones with the same concentration as the outdoor. So it could be improved to consider the non-well-mixing conditions in which the locations of the CO_2 meters could become important, as illustrated by the previous studies (Emmerich and Persily 2001; Rackes et al. 2018; Pantelic et al. 2020). The neighbor zone impacts could also be incorporated by installing extra CO_2 meters in these zones, the effect of which may be in doubt since the surrounding CO_2 level is at a lower rank than other key parameters, such as occupancy schedule. A future dynamic model to consider both the non-uniformity and neighboring impacts can be explored further.

▪ This study relied on the measured CO_2 data for the model's validity, whereas the actual ventilation rate in the room was not measured directly. As mentioned previously, it is quite challenging to quantify the ventilation rate in a real-world situation due to the many uncertainties, especially for naturally-ventilated spaces, even with well-developed techniques such as tracer gas tests. However, if two tracer gases were used, one with CO_2 and the other with another tracer gas, e.g., SF_6, the proposed model could be further tested by comparing the predicted ventilation rates.

On the other hand, although the actual ventilation rates in this study were not measured, we demonstrated that the CO_2 levels in four primary school classrooms can be reasonably predicted when many uncertainties were involved. Therefore, others could apply the proposed Bayesian inference model and procedure to (1) estimate/forecast indoor CO_2 levels for advanced demand control ventilation and (2) to explore the potential of using CO_2 meters as indicators of indoor air quality and proxies of ventilation conditions in other buildings. When more CO_2 and other air quality meters are expected to be employed in the near future, it is possible to develop relatively simple correlations of ventilation rates as a function of indoor CO_2 levels so the public can use them directly without the need for knowledge of Bayesian calibrations, once a Bayesian inference model is calibrated and validated.

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