Sensitivity Analysis of CO_2 Concentrations as Ventilation Metrics

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ABSTRACT

An approach has previously been developed to estimate space-specific carbon dioxide (CO_2) levels that can serve as metrics for the adequacy of outdoor ventilation rates. These metrics are based on the CO_2 concentration expected in a space given its intended or expected ventilation rate, volume, and occupant information (i.e., the number of occupants, their CO_2 generation rates, and duration of occupancy). This expected concentration can then be compared to a measured value to assess whether the actual outdoor air ventilation rate of the space is consistent with a design value, the requirement in a standard, or other recommended ventilation rate. A measured concentration higher than the expected value may indicate that the target ventilation rate is not being achieved. However, the occupant characteristics that impact the rate at which they generate CO_2 (sex, age, body mass, and level of physical activity) are difficult to know with precision, which impacts the uncertainty in the expected concentration.

This study involved a sensitivity analysis of the calculated CO_2 ventilation metric. Occupant characteristics impacting the CO_2 generation rate (body mass, ratio of male-to-female occupants, and metabolic rates) were varied by about +/- 20 % to evaluate the impact on two metric values of interest (the CO_2 concentration 1 hour after full occupancy and the steady state concentration). In addition, the space ventilation rate was varied by +/- 20 % to allow comparison to the variations associated with the other three inputs. The analysis employs the airflow and contaminant transport tool CONTAM to predict these concentrations over the range of inputs using factorial analysis. The sensitivity analysis employs a two-level full factorial design and a 10-step exploratory data approach (EDA) to identify the factors that have the most significant impacts. The result shows that outdoor ventilation rates and metabolic rates have the most significant effects on the CO_2 ventilation metric values. Varying these two parameters by +/- 20 % results in variations in the CO_2 concentrations of about 20 % to 35 %.

KEYWORDS

carbon dioxide, ventilation, metabolic rates, sensitivity analysis, CONTAM

1 INTRODUCTION

Indoor air quality (IAQ) researchers and practitioners have used indoor carbon dioxide (CO_2) concentrations to evaluate IAQ and building ventilation performance for many years (Persily, 1997), in many cases without a full understanding of the technical bases of the methods employed and the assumptions involved (ASHRAE 2022). The use of CO_2 monitoring for ventilation assessment has become more common in response to the COVID-19 pandemic given the importance of ventilation in managing the risks of infection (Persily and Oke, 2022). Many of these monitoring efforts involve the use of a single value of the CO_2 concentration for all indoor spaces, often in the range of 800 ppmv to 1000 ppmv*. However,

* In this work, CO_2 concentrations are expressed in µL/L, which is equivalent to ppmv.

using a single CO_2 concentration for all indoor spaces ignores important differences between indoor spaces, such as their size, intended use, and occupant characteristics (Persily, 2022). These differences impact the CO_2 generation rates, the timing of the concentration measurements relative to the occupancy schedule, and the outdoor air ventilation rates required by ventilation standards and building codes, which in turn influence the indoor CO_2 concentrations. An approach for analyzing space-specific ventilation rates allows users to identify CO_2 ventilation metrics based on these factors (Persily, 2022). An online tool, QICO2, is available to facilitate the application of this approach (Persily and Polidoro, 2022). However, the calculation of CO_2 concentrations as ventilation metrics involves assumptions for several quantities that are inherently uncertain, such as occupant-related characteristics, and the impact of these uncertainties on the metrics is not known.

This study aims to investigate the uncertainties associated with the CO_2-based ventilation metrics proposed previously. We consider a range of values for the occupant characteristics (ratio of males to females, body mass, and level of physical activity) and outdoor ventilation rates. We use the CONTAM airflow and contaminant transport model (Dols and Polidoro, 2020) to predict CO_2 concentrations over the range of input values, with results being evaluated using factorial analysis. This analysis is intended to help practitioners understand the uncertainties associated with the indoor CO_2 concentrations used as ventilation metrics.

2 METHODS

The analysis presented in this paper involved single-zone CONTAM simulations of CO_2 concentrations in several space types. A two-level, full factorial design that was analyzed with a 10-step exploratory data (EDA) approach to identify the most important factors impacting the calculated CO_2 concentrations (NIST/SEMATECH e-Handbook of Statistical Methods). This approach allows the assessment of the impact of each input value on the calculated concentrations as well as the interactions between the input values. The analysis focused on four factors: metabolic rate, ratio of male to female occupants, body mass, and outdoor airflow rate into the space. The calculated CO_2 concentrations reveal the sensitivity to these factors after 1 hour of occupancy and at a steady state.

2.1 Single-zone simulation model

The calculation of these ventilation metrics employs a single-zone mass balance of CO_2 in each space, which is expressed in equation (1):

$$V\frac{dC}{dt} = Q\,[C_{out} - C(t)] + G \tag{1}$$

where V is the volume of the space being considered, C is the CO_2 concentration in the space, C_{out} is the outdoor CO_2 concentration, t is time, Q is the volumetric flow of air into the space from outdoors and from the space to the outdoors, and G is the CO_2 generation rate in the space. We ignore air density differences between the indoors and outdoors by using the same value of Q for the flow into and out of the space. In addition, the single-zone model does not account for concentration differences within and between the building zones or for CO_2 transport between zones. The solution to equation (1) is expressed in equation (2):

$$C(t) = C(0)\,e^{-\frac{Q}{V}t} + C_{ss}\left(1 - e^{-\frac{Q}{V}t}\right) \tag{2}$$

where C(0) is the indoor concentration at t = 0, and C_{SS} is the steady-state indoor concentration, which is given by:

$$C_{ss} = C_{out} + \frac{G}{Q} \quad (3)$$

Note that the indoor concentration will only achieve steady state if Q and G are constant for a sufficiently long period of time, which may not occur in some spaces depending on the occupancy schedule. We used the factorial capabilities in CONTAM simulations by varying the inputs as described below to estimate the indoor CO_2 concentrations at 1-minute intervals over 24-hours.

2.2 Model Inputs

The inputs investigated in the sensitivity analysis include the following: metabolic rate of the occupants, which is a function of their level of physical activity; the ratio of male to female occupants (MF ratio); body mass of the occupants; and the outdoor airflow rate into the space. We investigated several space types from the commercial/institutional building spaces covered by ASHRAE Standard 62.1 (ASHRAE 2022). Each building space is assumed to be at an indoor temperature of 23 °C and an initial CO_2 concentration of 400 ppmv. Table 1 shows the baseline values for the occupant-related characteristics and the space ventilation rate. For the lobby, we investigated two levels of physical activity of the occupants, referred to as “active” and “mellow,” where the former is associated with a higher met rate. Also, in institutional spaces such as classrooms and lecture rooms, we examined scenarios with either a male teacher or a female teacher. The body mass values in the fourth column contain two values corresponding to the male and female occupants, respectively.

Table 1: Baseline input values for the occupant characteristics for CO_2 concentration calculations

Space type	**Occupant density (#/100 m^2)**	**MF ratio**	**Body mass M/F (kg)**	**Metabolic rate (met)**	**Ventilation rate (m^3/h)**
Classroom (5 y to 8 y)	25	12 : 12 (1 adult Teacher)	Students: 26.4 / 25.8 Teacher: 93.4 / 79.6	Student: 1.5 Teacher: 2.1	185
Lecture classroom	65	32 : 32 (1 adult Lecturer)	Students: 83.6 / 73.7 Lecturer: 93.4 / 79.6	Student: 1.7 Lecturer: 2.1	277
Restaurant dining room	70	Customer: 33:33 Workers: 2 : 2	93.4 / 79.6	Customer: 1.7 Server: 2.2	356
Conference meeting room	50	25 : 25	93.4 / 79.6	1.7	155
Office space	5	2.5 : 2.5	93.4 / 79.6	1.9	42.5
Active Lobby	150	75 : 75	93.4 / 79.6	2.2	405
Mellow Lobby	150	75 : 75	93.4 / 79.6	1.9	405
Retail	15	7.5 : 7.5	93.4 / 79.6	2.1	117

To estimate the CO_2 generation from building occupants, we utilized an approach based on the basal metabolic rate (BMR) and the level of physical activity (M) (Persily and de Jonge, 2017). The BMR is influenced by sex, age, and body mass, and when multiplied by the physical activity level, provides the rate of energy expenditure. Based on that approach, the CO_2 generation, V_{CO2}, of an individual is estimated by equation (4):

$$V_{CO2} = \mathrm{BMR} \cdot \mathrm{M} \left(T/_{P}\right) 0.000179 \quad (4)$$

where M is the metabolic rate, BMR is the basal metabolic rate (MJ/day), and T and P are the air temperature (K) and pressure (kPa), respectively. We estimated the volumetric flow of air into and out of the space using the Ventilation Rate Procedure in ASHRAE Standard 62.1 (ASHRAE 2022), which requires ventilation rates as the sum of a *People Outdoor Air Rate*, R_p (L/s·person) and an *Area Outdoor Air Rate*, R_a (L/s·m^2) using equation (5):

$$V_{bz} = R_p \times P_z \times R_a \times A_z \quad (5)$$

where P_z is the number of people in the space, and A_z (m^2) is the net occupied floor area.

Body mass values were derived from the 2015-2018 National Health and Nutrition Examination Survey (NHANES), a comprehensive anthropometric survey representing various age groups and demographics in the United States (Fryar et al., 2021). For the adult population in all spaces, we assumed the occupants were in the range of 30 to 60 years old. The number of occupants in each space was based on the default occupant density values in ASHRAE Standard 62.1 (ASHRAE 2022) and remained constant during each simulation. Metabolic rates were calculated based on the values for activities from published literature for adults (Ainsworth et al., 2011) and youths (Butte et al., 2018).

2.3 Sensitivity Analysis

Two settings were selected for each input in the two-level design, represented as “-1” or “+1” to indicate lower and higher values, respectively. The simulations encompassed all possible combinations of high/low levels for each of the inputs. The number of simulations equals 2^k, where k is the number of factors. In this analysis, with k = 4, the total number of simulations was 16. The primary advantage of employing a full factorial design is that it allows for estimating both main effects and interactions among the factors. For simulation purposes, the baseline values of the studied inputs were varied by +/- 20 %. The 20 % range is not based on specific data or analyses, but rather is intended to represent a realistic range of variation. The 10-step analysis of the results of the simulations produces graphical output that provides insights into the results. For this analysis, the steady-state CO_2 concentration and the concentration at 1 hour were selected as the outcomes or response factors.

Although the 10-step analysis generates 10 plots, we will focus on the ordered data plot and main effects plot as these are most relevant to this study (interaction effects were negligible and the plots related to fitting a model are not applicable). The ordered data plot, shown in Figure 1, shows the output values from smallest to largest for all combinations of input level for the steady-state CO_2 concentration for the classroom. This plot shows which combination of input settings yields higher or lower indoor CO_2 concentrations.

The main effects plot, shown in Figure 2, shows the mean response value for all data at a given level of a factor. For example, the "-" column for MF ratio plots the mean of all the data which have a "-"setting for MF ratio while the "+" column plots the mean of all data which have a "+" setting for MF ratio. The difference between the means for the "-" and "+" setting is the effect size for that factor (this is shown as "|Effect|" on the plot. The plot also shows the relative effect (i.e., the overall mean of the response variable divided by the effect size expressed as a percentage). The values of the effect sizes indicate the relative importance of the factors. This plot demonstrates that the outdoor ventilation rate and metabolic rate have the most significant effect, body mass has some effect (about half the size of metabolic rate and outdoor Ventilation Rate) and MF ratio has very little effect.

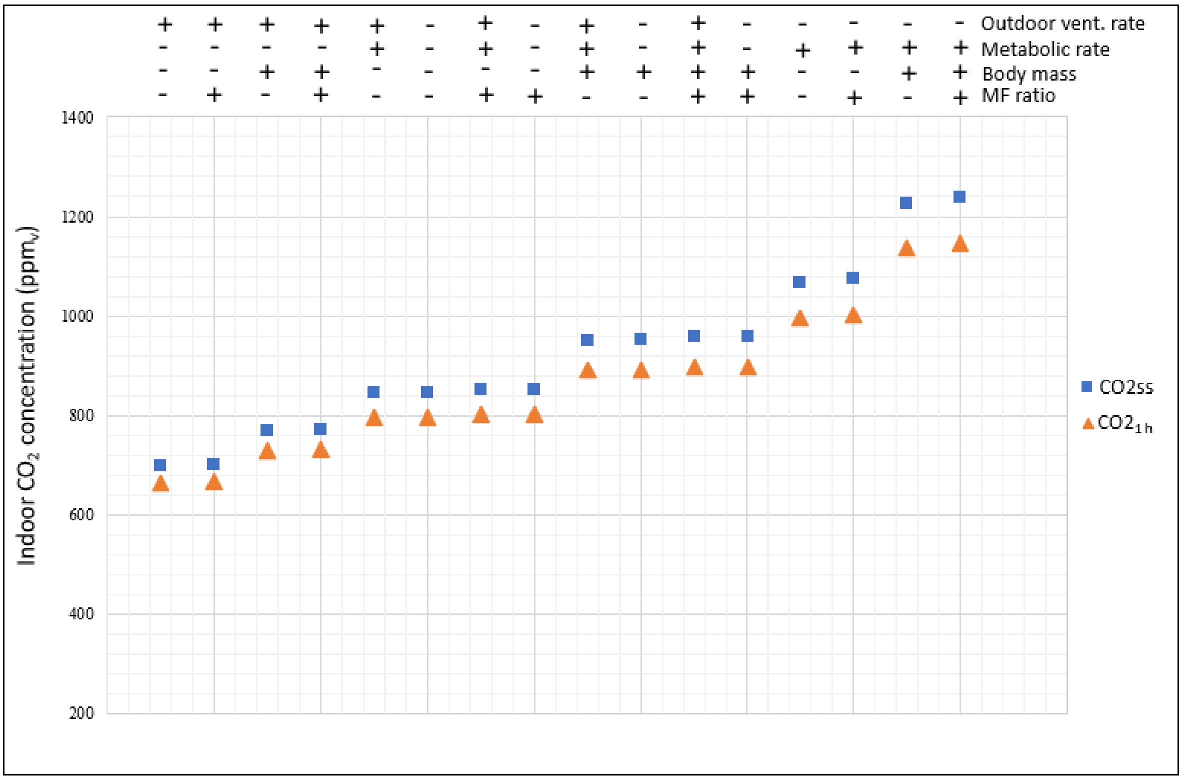

Figure 1: Ordered data plot for steady-state and 1-hr CO_2 concentration in a classroom comprising students aged 5 to 8 with an adult male teacher

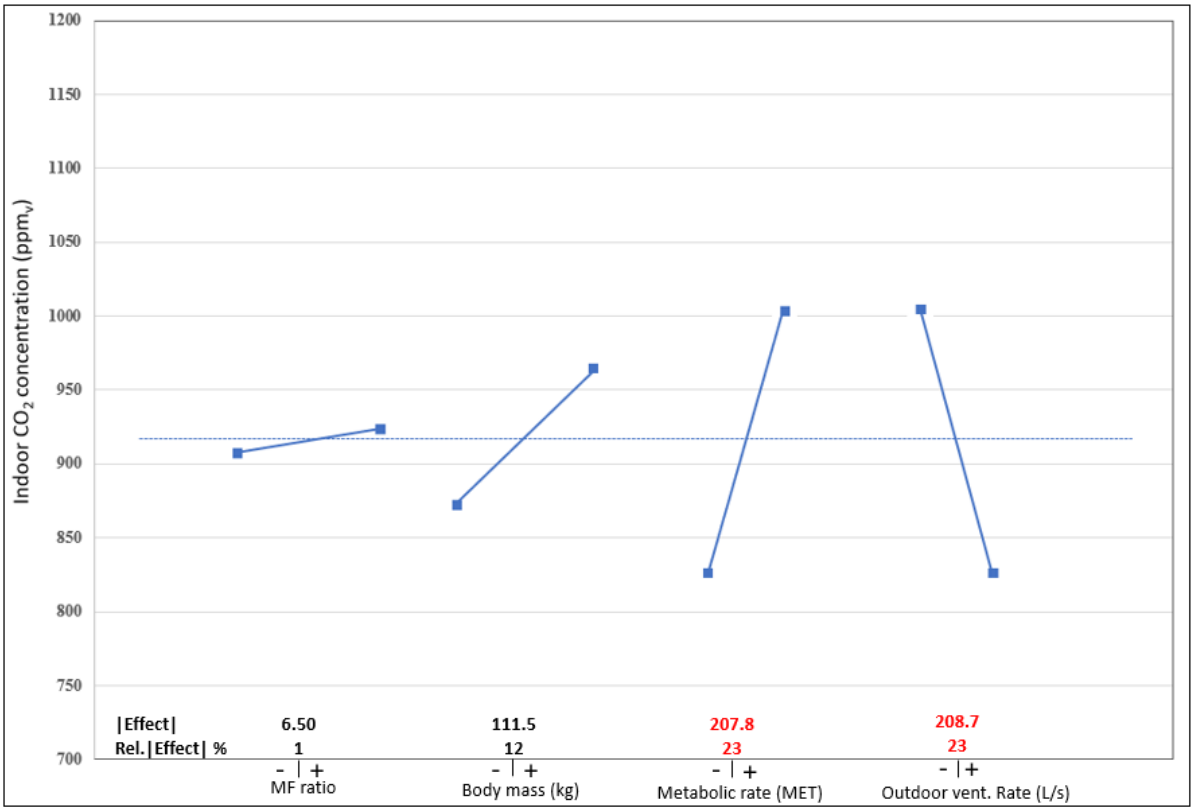

Figure 2: Main Effects plot for the steady-state CO_2 concentration in a classroom comprising students aged 5 to 8 with an adult male teacher

3 RESULTS

Table 2 displays the uncertainty analysis results for the ten spaces considered in this study for the 1-hour CO_2 concentration subject to a +/- 20% variation in each of the four input variables. Table 3 displays the results for the steady-state CO_2 concentrations. The second column of Tables 2 and 3 shows the minimum, maximum, and mean CO_2 concentrations. The remaining columns present the percent difference between the mean concentrations of the lower (–) and upper settings (+) for the four input variables.

Table 2: Percentage difference in 1h concentration for a +/- 20 % variation in the input variable

		Percent difference in 1 h concentration for +/- 20% variation in input variable			
Space type	**Minimum/maximum concentration (mean) ppm_v**	**MF ratio**	**Body mass**	**Metabolic rate**	**Ventilation rate**
Classroom (5 y to 8 y, male teacher)	665/1146 (865)	1	11	21	22
Classroom (5 y to 8 y, female teacher)	659/1129 (855)	1	11	21	21
Lecture classroom (male lecturer)	1175/2825 (1846)	3	21	33	31
Lecture classroom (female lecturer)	1171/2812 (1838)	3	21	33	31
Restaurant dining room	1134/2509 (1700)	3	15	31	31
Conference meeting room	1380/3312 (2170)	4	16	35	33
Office space	595/953 (742)	2	9	17	18
Active Lobby	2146/5456 (3504)	5	18	35	35
Mellow Lobby	1855/4520 (2952)	5	17	33	35
Retail	761/1546 (1074)	7	13	28	25

Table 3: Percentage difference in steady state concentration for a +/- 20 % variation in the input variable

		Percent difference in steady-state concentration for +/- 20% variation in input variable			
Space type	**Minimum/maximum concentration (mean) ppm_v**	**MF ratio**	**Body mass**	**Metabolic rate**	**Ventilation rate**
Classroom (5 y to 8 y with a male teacher)	697/1237 (922)	1	12	23	23
Classroom (5 y to 8 y with a female teacher)	691/1217 (910)	1	12	22	22
Lecture classroom (with a male lecturer)	1245/3043 (1976)	3	21	34	32
Lecture classroom (with a female lecturer)	1241/3030 (1968)	3	21	34	32
Restaurant dining room	11165/2598 (1755)	3	15	31	31
Conference meeting room	1561/3849 (2496)	4	17	36	34
Office space	889/1783 (1257)	4	14	26	27
Active Lobby	2246/5745 (3682)	5	18	36	36
Mellow Lobby	1938/4755 (3098)	5	17	33	35
Retail	954/2160 (1435)	8	14	32	29

These tables show that outdoor ventilation and metabolic rates impact the 1-hour and steady-state CO_2 concentrations more than body mass and MF ratio. This trend holds across all the spaces examined, although the percentage difference in CO_2 concentration varies across the different space types. For example, in the 5 y to 8 y classroom with an adult male teacher, changing the outdoor ventilation and metabolic rates by +/- 20 % leads to a 22 % and 21 %

shift in the 1-hour CO_2 concentration, respectively (Table 2). At steady state, the same adjustments result in approximately 23 % variation in the CO_2 concentrations, as shown in Table 3. For the office space, varying the outdoor ventilation and metabolic rates by +/- 20 % results in 18 % and 17 % changes in the CO_2 concentration after 1 hour of occupancy, respectively, which increases to 27 % and 26 % percent differences in the CO_2 steady-state concentration.

Body mass and MF ratio have lesser impacts on the calculated CO_2 concentration. In the 5 y to 8 y classroom with an adult male teacher, the +/- 20 % variation in body mass and MF ratio results in 11 % and 1 % shifts in the 1-hour CO_2 concentration. At steady state, the +/- 20 % percent in body mass results in a 12 % change in the CO_2 concentration, while the MF ratio yields a 1% change (Table 3). For the office space, the same variation in body mass and MF ratio resulted in 9 % and 2 % changes in the CO_2 concentration after 1 hour of occupancy and 14 % and 4 % changes in the CO_2 steady-state concentration (Table 3).

4 CONCLUSIONS

In support of the use of CO_2 concentrations as ventilation metrics, a sensitivity analysis was conducted to understand which inputs to the calculations of these metrics were most important and to estimate the impact of their variation on the calculated concentration values. This analysis involved single-zone CONTAM simulations of seven spaces using ventilation rates and default occupant density levels from ASHRAE Standard 62.1 and other parameters impacting CO_2 generation rates based on Persily (2022). The inputs of body mass, male-female ratio for some occupancies, level of physical activity or met rate, and the outdoor air ventilation rate, were all varied by +/- 20 %. The simulations employed a two-level, full factorial design that was analyzed with a 10-step EDA described above. The results showed that ventilation and met rates impact the CO_2 ventilation metric values more than the male-female ratio and body mass, with a range of 20 % to 35 % for the +/- 20 % variation in these inputs. Variations in body mass impacted the CO_2 metrics by 10 % to 20 %, and the male-female ratio variation was closer to 1 % to 8 %.

These results will help users of the CO_2 ventilation metric approach better understand the precision in the calculation of those metrics. In practice, when applying this approach, the ability to determine the required inputs will vary. In cases where one is calculating CO_2 metric values for generic space types, e.g., offices, rather than a specific office, one can only estimate the number of occupants and their characteristics that impact CO_2 generation rates. The target ventilation rate should be known with a higher degree of confidence based on the standard or guidance value one is attempting to verify, though the value may also depend on the number of occupants, as it does in ASHRAE Standard 62.1. Nevertheless, the results of this sensitivity analysis clarify the potential range in the CO_2 metric values in relation to the uncertainty in the concentration measurement. If one is evaluating a specific, existing space, they should have a better idea of the male-to-female ratio, but estimating body mass will be more difficult, requiring characterization of the occupants of the space. The met rate for the space is inherently difficult to determine as the values in the literature are based on specific activities but do not address met levels for occupied spaces, which generally are associated with a range of activities of varying durations. Therefore, the uncertainty in the CO_2 metric values associated with variations in met rates need to be explicitly acknowledged and quantitatively considered.

Additional work is planned to consider other space types, occupancy details, and other times for the CO_2 concentration calculations (as suggested in Persily 2022) to better understand the uncertainties inherent in the CO_2 ventilation metric approach. Also, developing guidance on the use of the CO_2 ventilation metric based on this work that targets practitioners is being considered.

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