A simulation study on correlation between indoor volatile organic compounds and carbon dioxide concentration in Beijing, China

Weihui Liang
School of Architecture and Urban Planning, Nanjing University, Nanjing, China
liangwh@nju.edu.cn

Abstract. Indoor air quality (IAQ) plays a significant role to human health. There are many pollutants have been identified indoors. Volatile organic compounds (VOC) are one of the most ubiquitous pollutants with proved adverse health effects. Carbon dioxide (CO2) has a long history of being used as an indicator for IAQ. The VOC sensors are generally expensive and their accuracy are not as good as CO2 sensors. Whether CO2 could be a good indicator for VOC is important to determine ventilation control strategy in engineering application. In this study, indoor CO2 and formaldehyde concentrations in a Beijing’s bedroom was simulated for a whole year by the Monte Carlo method. When emission rate of CO2 was constant, strong positive correlation was identified between CO2 and formaldehyde. CO2 could be a good indicator for formaldehyde when emission rate of formaldehyde (mg/h) divided by the emission rate of CO2 (L/h) was smaller than 0.14. When emission rate of CO2 was changing, CO2 could not be used as an indicator for formaldehyde in general.

1. Introduction
Indoor air quality (IAQ) plays a key role to human health [1]. Carbon dioxide (CO2) has long been used as a surrogate indicator for IAQ [2]–[4]. Under typical circumstances where the odors and pollutants are mainly metabolic, CO2 is a good indicator. However, the dominant indoor source of volatile organic compound (VOC) is building material. The emission characteristics of them is quite different from that of CO2 exhalation. Moreover, the on-line quantitative and qualitative measurement of indoor VOC is difficult to perform and the instruments are very expensive currently. Thus, dynamic IAQ controlled based on the VOC sensor is not quite applicable nowadays. Whether indoor CO2 is a good indicator of VOC in rooms is still unknown.

To answer the aforementioned question, the concentrations of indoor CO2 and VOC were simulated in mechanical ventilation scenario for a whole year by using the stochastic method. Pearson correlation analysis were performed between each pair of the concentrations to identify whether these two kinds of pollutants vary consistently.

2. Materials and Method

2.1. The simulation framework
There are many factors influencing indoor CO2 and VOC concentrations. The diversity of room volume, applied areas and emission characteristics of different building materials, room occupancy, ventilation rate, and indoor environmental conditions may result in different indoor CO2 and VOC concentrations. To achieve a comprehensive result, the mathematical models of CO2 and VOC were coupled with MC method. The framework of this study is illustrated in Figure 1.
To achieve a comprehensive result, the mathematical model was combined with the Monte Carlo (MC) method. Given the distributions and value of relevant input parameters in the mathematical model, the one-dimension MC simulation was used to obtain the one-year variability in indoor CO$_2$ and VOC concentrations. For each scenario, 3000 computations of CO$_2$ and VOC concentrations were conducted. The input parameters were assumed to be independent of each other in the probabilistic simulation.

2.2. Mathematical model

For a single room in residential building, the well-mixed assumption was used. Thus the mass balance equation of CO$_2$ could be expressed as:

$$\frac{dC_{at}(t)}{dt} = AER(t)C_{out}(t) - AER(t)C_{at}(t) + \frac{10^1}{V} \sum_{n=1}^{N_h} E_{CO2}(t)$$

(1)

where $C_{at}(t)$ is the indoor CO$_2$ concentration (ppm); $t$ is time (h); $AER(t)$ is the air exchange rate of the fresh air (m$^3$/h); $C_{out}(t)$ is the outdoor CO$_2$ concentration (ppm); $V$ is the volume of the room (m$^3$); $E_{CO2}$ is the emission rate (L/h). $N_h$ is the number of human in the room at time $t$.

For VOC simulation, the emission/sorption of multiple building materials, the effects of temperature on material emissions are considered. The VOC simulation is based on the PACT-IAQ simulation tool. The mass balance equation for VOC simulation in both natural and mechanical ventilation could be expressed as:

$$\frac{dC_{at}(t)}{dt} = AER(t)C_{out}(t) - AER(t)C_{at}(t) + \frac{1}{V} \sum_{n=1}^{N_h} E_{N}(t)$$

(2)

Figure 1. The simulation framework of this study
where $C_{in}(t)$ is the indoor VOC concentration (mg/m$^3$); $C_{out}(t)$ is the outdoor VOC concentration (mg/m$^3$). $E_0$ and $R_s$ is the emission rate and sorption rate of building materials (mg/h). $N_E$ is the number of emission sources in the room.

To solve the mass balance equations of 1 and 2, the emission rates of indoor sources need to be estimated first. It is assumed that the human exhalation is the only indoor CO$_2$ emission sources. Human CO$_2$ generation rate from Chinese people was calculated by the equation proposed by Qi et al. [5].

For VOC emission sources, there are different emission models were used for different types of materials. For dry building materials, such as wood floor, furniture and door, the one-phase mass transfer model was used [6]. The initial emittable concentration ($C_0$), diffusion coefficient ($D_m$) and partition coefficient ($K$) are key parameters determining the emission strength of the materials. The effect of temperature was also analyzed by our previously developed model [7]. The coefficients of the correlations between initial emittable concentration and temperature are key parameters in this occasion [8], [9]. For wet materials or material assembly, the one-exponential empirical model was used [10]. The initial emission rate ($E_1$) and first-order decay constant ($k_1$) are key parameters of the model. There are many kinds of VOC have been identified indoors. The emission parameters of different VOC would vary even for the same building product. Given that formaldehyde is the most common identified indoors VOC species with proved carcinogenic effect, it is used as a representative of VOC in this study.

2.3. Input parameter collections

2.3.1 The room and source parameters. The rooms in the residential buildings, such as bedroom, living room, kitchen and bathroom, are of function diversity. The presence of human being, the window opening behavior, the building material types and areas are different from room to room. Bedroom is the place people spend most of their time on the residence, which is the target room in this study. The reference bedroom developed by Liu et al [11] based on 1500 homes survey in Beijing was used. The input parameters of the model, such as ventilation rate, room area, building material types and areas, are different for different cities and rooms. But they can follow the same procedures as this study and the concentrations could also be estimated as long as the input parameters have been given.

The area of the floor, door, and furniture are given in the reference bedroom [11]. The distribution of the emission parameters of the building materials were obtained based on the emission database developed by the Shenzhen Institute of Building Research Ltd. The emission parameters are lognormal distributed. The human weight and height of adults in Beijing are normal distributed according to the survey conducted by Duan [12]. The room occupancy in Beijing’ residences was obtained by the online investigation conducted by Cheng [13]. The input parameters of the models is illustrated in Table 1.

| Parameter | Value/ Probabilistic distribution | Reference or comment |
|-----------|-----------------------------------|----------------------|
| Room information | | |
| Floor area $A_f$ (m$^2$) | $\ln (A_f) \sim N(2.75, 0.38)$ | [11] |
| Room height $h$ (m) | 2.6 | [11] |
| Human characteristics | | |
| Human weight $W$ (kg) | $W \sim N(68.22, 11.6)$ | [12] |
| Human height $H$ (m) | $H \sim N(1.68, 0.1)$ | [12] |
| Emission area and thickness of building material | | |
| Wood floor area $A_f$ (m$^2$) | $\ln (A_f) \sim N(2.75, 0.38)$ | [11] |
| Door area $A_d$ (m$^2$) | 1.8 | [11] |
| Load ratio of furniture $L_f$ (m$^2$/m$^3$) | $\ln (L_f) \sim N(-0.86, 0.81)$ | [11] |
| Load ratio of wall paint $L_w$ (m$^2$) | $L_w \sim N(1.75, 0.19)$ | [14] |
| Composite material area $A_{com}$ (m$^2$) | $A_d + L_f/A_f \times h$ | Estimated |
| Thickness of the wood floor $T_{wf}$ (m) | 0.012 | |


| Thickness of the furniture board $T_f$ (m) | 0.018 | Average value based on the materials in the database |
| Thickness of the wood door $T_d$ (m) | 0.03 |

**Emission parameter of wood floor**

| Initial emittable concentration $C_{0,\text{wf}}$ (mg/m$^3$) | Ln ($C_{0,\text{wf}}$)~N(8.94, 0.64) |
| Diffusion coefficient $D_{m,\text{wf}}$ (m$^2$/s) | Ln ($D_{m,\text{wf}}$)~N(-29.26, 0.86) |
| Partition coefficient $K_{m,\text{wf}}$ | Ln ($K_{m,\text{wf}}$)~N(7.70, 0.76) |

**Emission parameter of door**

| Initial emittable concentration $C_{0,\text{d}}$ (mg/m$^3$) | Ln ($C_{0,\text{d}}$)~N(8.59, 1.45) |
| Diffusion coefficient $D_{m,\text{d}}$ (m$^2$/s) | Ln ($D_{m,\text{d}}$)~N(-27.86, 1.25) |
| Partition coefficient $K_{m,\text{d}}$ | Ln ($K_{m,\text{d}}$)~N(7.37, 0.82) |

**Emission parameter of furniture**

| Initial emittable concentration $C_{0,\text{f}}$ (mg/m$^3$) | Ln ($C_{0,\text{f}}$)~N(10.24, 1.25) |
| Diffusion coefficient $D_{m,\text{f}}$ (m$^2$/s) | Ln ($D_{m,\text{f}}$)~N(-29.68, 1.06) |
| Partition coefficient $K_{m,\text{f}}$ | Ln ($K_{m,\text{f}}$)~N(8.86, 1.39) |

**Emission parameter of wall paint**

| Initial emission rate $E_{0w}$ (mg/m$^2$/h) | Ln ($E_{0w}$)~N(-1.71, 1.38) |
| Decay constant $k_w$ (h$^{-1}$) | Ln ($k_w$)~N(-3.8, 0.88) |

**Emission parameter of other composite materials**

| Initial emission rate $E_{0c}$ (mg/m$^2$/h) | Ln ($E_{0c}$)~N(-3.6, 0.98) |
| Decay constant $k_c$ (h$^{-1}$) | Ln ($k_c$)~N(-9.03, 0.89) |

2.3.2 Ventilation schedule and AER. The mechanical ventilation system is assumed to run continuously throughout the year. The minimum ventilation rate for mechanical ventilation system was recommended by the national building code in China, in which the value is depended on the per-capita living space of the residence. The ventilation rate of the mechanical ventilation system is assumed to be a constant value of 0.5 h$^{-1}$ when the system is operated accordingly.

2.3.3 The outdoor concentrations. According to the data of the Shangdianzi (40°39 N, 117°07 E) global atmospheric watch (GAW) station in Beijing, the atmospheric CO2 concentration varied between 370–400 ppm. The monthly-averaged outdoor CO2 concentration was adopted from the data of Xia [16]. A lognormal distribution was used to describe the variation of the monthly outdoor CO2 concentrations. Standard deviations were taken as 20% of the means.

According to a two years outdoor formaldehyde measurement by Zhang [17], the outdoor formaldehyde concentration was highest in summer and lowest in winter in Beijing. The lognormal distribution is also assumed for outdoor formaldehyde concentration. The mean and standard deviation of outdoor formaldehyde concentration in spring, summer, autumn and winter seasons are 6.6±3.7 ug/m$^3$, 10.2±4.2 ug/m$^3$, 8.3±5.8 ug/m$^3$ and 4.3±3.3 ug/m$^3$, respectively.

3. Results and discussion

The mean concentrations of indoor formaldehyde and CO2 are presented in the left figure in Figure 2. Due to the constant AER, there is no difference of CO2 concentration in different seasons. While formaldehyde concentration decreased with time.
Figure 2. The mean (left) and Person correlation coefficient (P-value) (right) of indoor formaldehyde and CO$_2$ concentration in the mechanical ventilation scenario.

The right figure in Figure 2 presented the day-averaged medium Person correlation coefficient variation with time. The p-value is smaller than natural ventilation. Moreover, only at weekend (corresponded to the peaks in the figure), the strong positive correlations are presented. This is because of the home occupancy at the weekend don’t vary much at different time period. Thus, the CO$_2$ emission rate from human exhalation is relatively stable, which is consistent with the variation pattern of the formaldehyde emission sources.

Figure 3 presents the demand for fresh air to ensure the concentrations of CO$_2$ and formaldehyde below the threshold limits for 90% residences in Beijing based on this study. The demand for fresh air was highly depended on the emission rate of room. As the emission rate of CO$_2$ changed in weekly cycle, the demand for AER varied in the same pattern, the maximum AER requirement was 1 h$^{-1}$ when two occupants stayed in room (fully occupied). The demand for fresh air for formaldehyde was decreasing. At the time of 438 h, the demand for formaldehyde was the same as the maximum AER requirement of CO$_2$. Thus, the fresh air was sufficient to dilute formaldehyde concentration after that if the room was fully occupied. CO$_2$ could be a good indicator for formaldehyde. However, if the emission rate of CO$_2$ was changing, the demand for ventilation from CO$_2$ perspective could be smaller than that for formaldehyde. CO$_2$ is hard to be used as an indicator for formaldehyde in engineering application.

Figure 3. The demand for fresh air for CO$_2$ and formaldehyde control

4. Conclusion
To verify whether CO$_2$ could be used as an indicator for VOCs from engineering project, the concentrations of CO$_2$ and formaldehyde in Beijing’s residences were simulated by MC method. There were some conclusions.

(1) Pearson correlation analysis showed that poor correlation presented between CO$_2$ and formaldehyde from long-term perspective.
(2) Strong correlation presented between CO₂ and formaldehyde in the short-term when emission rate of CO₂ was constant. CO₂ could be used as a good indicator for formaldehyde if emission rate of formaldehyde (mg/h) divide emission rate of CO₂ (L/h) was smaller than 0.14.

(3) When the emission rate of CO₂ was changing, poor correlation presented. CO₂ could not be used as an indicator for formaldehyde in this occasion.

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References
[1] Wolkoff P 2018 International J Hygiene Environ. Health.
[2] Hung IF 1989 J. Environ. Sci. Heal. Part A Environ. Sci. Eng. 24 4
[3] ASHRAE standard 2007
[4] British Standards Institution BS EN 15251 2007 3
[5] Qi M, Li X, Weschler B and Sundell J 2014 Indoor Air 24 6
[6] Huang H and Haghighat F 2002 Build. Environ. 37 12
[7] Liang W, Lv M and Yang X 2016 Proc. Indoor Air 2016 Gent, Belgium
[8] Liang W, Lv M and Yang X 2016 Build. Environ. 98
[9] Huang S, Xiong J and Zhang Y 2015 Environ. Sci. Technol. 49
[10] Dunn JE 1987 Atmos. Environ. 21
[11] Liu W, Zhang Y and Yao Y 2013 Chinese Sci. Bull. 58
[12] Duan X 2013 Ministry of Environmental Protection of People’s Republic of China,
[13] Chen P 2018 Ph.D. Thesis, Tsinghua University
[14] Shi S, Chen C and Zhao B 2017 Environ. Pollut. 220
[15] Xia L 2013 Ph.D. Dissertation Nanjing Information Engineering University
[16] Zhang Y, Mu Y, Liu J and Mellouki A 2012 J. Environ. Sci., 24