Healthy Buildings 2017 Europe
July 2-5, 2017, Lublin, Poland

Paper ID 0240 ISBN: 978-83-7947-232-1

Steady State and Dynamic Indoor Ozone Estimation Model with Indoor Ozone Source

Jialei Shen[1], Zhi Gao[1,*]

[1] Nanjing University (NJU), Nanjing, China

[*] *Corresponding email: zhgao@nju.edu.cn*

SUMMARY
The indoor ozone concentration estimations are present based on a single zone mass balance model considering indoor ozone sources, which both steady state and dynamic ozone concentration can be predicted. Values of γ of totally 54 common indoor materials are compiled from literatures. Field measurements are conducted to validate the estimation model in steady state and dynamic conditions. The estimated results are consistent with the measured data, which means it is useful for predicting indoor ozone concentration levels and then taking strategies to control ozone exposure. The estimations of indoor ozone concentration levels are of great significance for occupants' health. Particularly, knowledge of the dynamic indoor ozone concentration levels is useful in terms of the time required for occupants to safely return to the building after the disinfection.

KEYWORDS
Indoor ozone estimation; Indoor/outdoor ratio; Ozone source; Dynamic ozone concentration; Field measurement

1 INTRODUCTION

Ozone is a reactive gas that can have negative health effects on human (Jerrett et al., 2009). Indoor residential ozone exposure accounts for more than 50% of the total ozone exposure (Zhang and Lioy, 1994) since people spend almost 90% of their time indoors. Therefore, quantitative estimations of indoor ozone concentration levels contribute to taking strategies to control indoor ozone exposure.

In the absence of indoor sources, indoor concentrations of ozone are generally lower than outdoor due to irreversible reactions with indoor materials. The rate of ozone removal at indoor surfaces can be characterized by the deposition velocity (v_d) which is specific to each indoor environment and each material. Using a mass balance model in a well-mixed room, the indoor ozone concentration can be then estimated when indoor environment, materials and outdoor ozone concentration are known. Shair and Heitner (1974) discussed a ventilation model of indoor ozone levels in relation to outdoor values in details. Grøntoft and Raychaudhuri (2004) developed the IMPACT model to make predictions of indoor concentration levels of some pollutant gases (O_3, SO_2 and NO_2) in museums. Walker and Sherman (2013) estimated residential ozone levels using a single zone model. Weschler has provided one of several strong scientific reviews of ozone in indoor environments (Weschler, 2000), including the possibility of an indoor emission source in the basic model equation. Indoor ozone sources are common in residential and public buildings, e.g. laser printers, photocopiers and ozonolysis air cleaning devices.

This paper develops a mass balance model tool to estimate indoor ozone concentration levels considering indoor ozone sources, which both steady state and dynamic ozone concentration can be predicted. The predictions of indoor ozone concentration levels are of great significance for occupants' health. Particularly, knowledge of the dynamic indoor ozone concentration levels is useful in terms of the time required for occupants to safely return to the building after the disinfection (Poppendieck et al., 2007). The estimation model is then validated by the field measurement in a dormitory in Nanjing.

2 METHODS

Theoretical

The indoor ozone level estimations are based on a single zone mass balance model that depends on air flows in and out of the buildings (Walker and Sherman, 2013). The following equation is used to describe the rate of change of indoor ozone concentration with time,

$$\frac{dC}{dt} = \lambda C_o + \frac{S'}{V} - \lambda C - \sum v_{d,i} A_i \frac{C}{V} \tag{1}$$

where C is the indoor ozone level (mg/m^3), C_o is the outdoor ozone level (mg/m^3), S' is the ozone emission rate of indoor source (mg/h), V is the building volume (m^3), λ is the air change rate (h^{-1}), $v_{d,i}$ is the deposition velocity of the ith building surface material (m/h) and A_i is the area of the ith building surface (m^2). Steady state analysis requires that $dC/dt = 0$. The ozone deposition velocity to a surface encompasses the transport of ozone to the surface and the reactivity of a surface with ozone, which can be calculated by (Cano-Ruiz et al., 1993)

$$\frac{1}{v_d} = \frac{1}{v_t} + \frac{1}{v_s} = \frac{1}{v_t} + \frac{4}{\gamma \langle v \rangle} \tag{2}$$

where v_d is the deposition velocity (m/h), v_t is the transport-limited deposition velocity (m/h), v_s is the reaction-limited deposition velocity (m/h), γ is the reaction probability (-), which is the ozone removal rate divided by the ozone collision rate, and $\langle v \rangle$ is Boltzmann velocity for ozone ($\langle v \rangle = 3.60 \times 10^4$ cm/s).

Field measurement

The estimated results of the model are validated by the field measurements conducted for a period of 37 days (July 15, 2015 to August 31, 2015) in a student dormitory in Nanjing University without any indoor ozone source. Both indoor and outdoor ozone concentrations are measured at 1min interval by using the ozone monitors (2B Technologies, POM and Model 202). Air exchange rate (λ) of the room was evaluated according to the concentration decay of SF_6, which measured by Innova 1412i Lumasense gas monitor. As shown in Figure 1, the volume of the research room is 45m^3 (3m*5m*3m). The floor and ceiling are wooden and latex painted, respectively. All the walls are latex painted, of which two walls are covered with wallpapers. In addition, there are still some wooden furniture and clothes in the room. Both steady state and dynamics ozone concentration are measured and estimated.

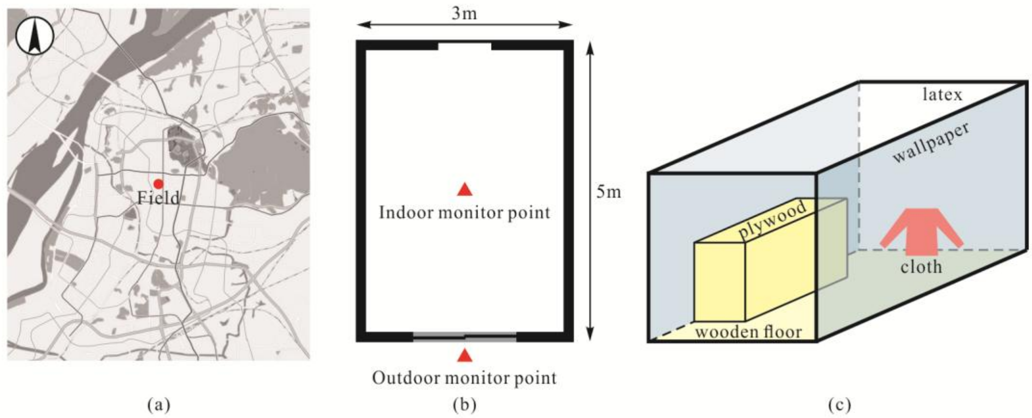

Figure 1. (a) Location of field measurement, (b) monitor points, and (c) indoor materials.

3 RESULTS

Estimation model

Values of v_d, v_t and γ from measurements made both in experimental chambers and in real rooms are reported in the literatures. Table 1 compiles γ of common indoor materials from previous studies. The experimental results of Hoang et al., (2009), Lamble et al. (2011) and Gall et al., (2013) suggested that the effects of temperature and humidity on γ are not significant. Thus, value of γ of each material is treated as a constant in this paper, which does not vary with temperature and humidity. A similar approach to Grøntoft and Raychaudhuri (2004), value of γ of each material is mean of experimental measurement values from literatures. If the literature values are orders of magnitude different, the most improbable values will be discarded.

Values of γ vary over four orders of magnitude for typical indoor materials, from 10^{-8} (e.g. glass) to 10^{-5} (e.g. carpet and brick). In general, fleecy and porous materials exhibit higher γ than smooth, non-porous surfaces. The materials containing clay tend to consume more ozone, maybe owing to a reaction catalysed by metals present in the clay. Besides, surface treatments (e.g. painted) have great influences on γ of the materials. Values of γ are generally consistent with the values of Grøntoft and Raychaudhuri (2004), while more available indoor materials are compiled in this study.

Table 1. Values of γ for ozone.

Material	γ (-)	Material	γ (-)
Glass[1,4,7,8,14,24]	6.06E-08	Wall plaster, clay[15,17]	2.20E-05
Lucite[1,4]	5.50E-08	Sunflower[23]	3.78E-06
Metal, aluminium[1,4,5,6,7,24]	1.08E-07	Cork[23]	5.67E-06
Metal, stainless steel[1,5]	1.30E-06	Wheat[23]	5.22E-06
Metal, galvanized steel[7,9]	1.10E-06	Nylon[1,4,24]	5.50E-08
Ceramic[23]	4.44E-07	FEP Teflon[1,2]	5.50E-07
Stone material, soft dense[24]	7.82E-06	Rubber[14,15,17]	6.86E-06
Stone material, hard dense[24]	1.67E-08	Neoprene[1,4]	1.90E-06
Floor, wooden[12]	1.20E-06	Polyethylene sheet[1,3,4]	1.10E-06
Floor, finished hardwood[15,17]	2.45E-06	Medium density fibreboard[16]	4.50E-06
Floor, finished bamboo[15,17]	1.95E-06	Particle board[16]	5.00E-07
Porcelain clay tile[15,17]	1.02E-06	Plywood[1,4,7,24]	5.80E-07
Resilient tile[15,17]	1.11E-06	Bamboo[23]	4.44E-07
Ceiling tile, perlite[15,17,18,19]	1.02E-05	Cedar[14]	5.20E-06
Ceiling tile, mineral fiber[15,17]	4.65E-05	Woodwork, fine, hard[24]	5.59E-07
Ceiling tile, fiberglass[15,17]	3.74E-05	Woodwork, course, soft[24]	4.16E-06

Concrete, course[24]	9.65E-06	Cloth, <1 year old[24]	8.99E-06
Concrete, fine[24]	4.20E-06	Cloth, >1 year old[24]	7.06E-07
Wallpaper[7,8,14,24]	4.28E-06	Linoleum[24,27]	7.89E-07
Fabric wall covering[15,17]	5.30E-06	Linen[1,4,24]	6.30E-07
Paint, latex[7,8,15,17]	1.47E-06	Carpet, recycled[15,17,18,19]	3.20E-05
Paint, clay[15,17]	5.65E-05	Carpet, fabric-backed[15,17]	2.30E-05
Paint, water-based[14]	4.90E-06	Carpet, nylon[10,17,20]	1.38E-05
Paint, oil-based[14]	6.10E-06	Carpet, olefin[10,17,20]	1.01E-05
Paint, collagen[15,17]	3.15E-06	Carpet, wool[24]	1.06E-05
Gypsum board, painted[17,18,19,24,25]	4.72E-06	Brick[24]	1.59E-05
Gypsum board, untreated[24]	1.73E-05	Activated carbon cloth[13,17,19,24]	2.24E-05

References:
[1] Cano-Ruiz et al., 1993; [2] Simmons and Colbeck, 1990; [3] Sutton et al., 1976; [4] Sabersky et al., 1973; [5] Mueller et al., 1973; [6] Cox and Penkett, 1972; [7] Liu and Nazaroff, 2001; [8] Reiss et al., 1994; [9] Morrison et al., 1998; [10] Morrison and Nazaroff, 2000; [11] Coleman et al., 2008; [12] Lin and Hsu, 2015; [13] Grontoft, 2002; [14] Ito, 2007; [15] Lamble et al., 2011; [16] Poppendieck et al., 2007; [17] Darling et al., 2016; [18] Gall et al., 2013; [19] Cros et al., 2012; [20] Morrison and Nazaroff, 2002; [21] Wang and Morrison, 2006; [22] Wang and Morrison, 2010; [23] Hoang et al., 2009; [24] Grontoft and Raychaudhuri, 2004; [25] Kleno et al., 2001.

Values of v_t are determined by the indoor air flow condition, which depend on specific experimental or measured conditions. Values of v_t in an apartment were measured ranged from 0.1cm/s to 0.7cm/s (Morrison et al., 2003). Gall et al. (2013) measured values of v_t in a room-scale chamber (5.5m*4.6m*2.7m) with different mixing conditions. Values of v_t range between 0.33cm/s for low mixing condition and 0.70cm/s for high mixing condition. Grøntoft and Raychaudhuri (2004) set values of v_t in the range between 0.1cm/s and 0.75cm/s in the IMPACT model. This paper sets v_t in the range between 0.1cm/s and 0.7cm/s. Values of v_t are estimated according to indoor air flow conditions.

Table 2 lists some indoor ozone sources from literatures. Ozonolysis air cleaning devices have potential hazards on human, owing to the high ozone emission rate and long working time. In addition, disinfection with ozone generators, though with potential health hazards, is still quite prevalent in China, particularly in public buildings, e.g. hospitals and primary schools.

Table 2. Ozone emission rate of common indoor sources from the literatures.

Indoor source	Ozone emission rate (mg/h)	Reference
Photocopier	15.5	Hannsen and Andersen, 1986
	6.8-12.9	Wolkoff et al., 1991
	3.0-7.9	Leovic et al., 1996
	1.0-10.0	Wolkoff, 1999
	1.2-6.3	Black and Worthan, 1999
Fruit and vegetable washer	11.4-16.7	Zhang and Jenkins, 2016
Refrigerator air purifier	1.3-12.1	Zhang and Jenkins, 2016
Ozonolysis air cleaning devices	40.2-1114.8	Kissel, 1993
	10	Hanley et al., 1995
	33-312	Dawn, 1998
	0.16-220	Britigan et al., 2006
	4.22-30.5	Yu et al., 2011
	2.12-400	Morrison et al., 2014

Experimental validation

The experimental results show that the air change rate (λ) of the research room is 1.32h^{-1} when the windows are open, and 0.66h^{-1} when the windows are closed. Value of v_d of each material in the room is calculated through Eq. (3) by assuming v_t is 0.5cm/s with the windows open and 0.3cm/s with the windows closed. The steady state indoor and outdoor ozone concentrations of the research room with the windows open and closed are shown in Figure 2(a) and 2(b), respectively. The measured data in Figure 2(a) and 2(b) are mean values of monitoring for 1h, which is therefore considered to be steady state. The measured indoor/outdoor (I/O) ozone concentration ratios are 0.44 and 0.30, respectively. The estimated I/O ozone ratios are highly consistent with the measured ones, i.e. 0.49 and 0.33 respectively.

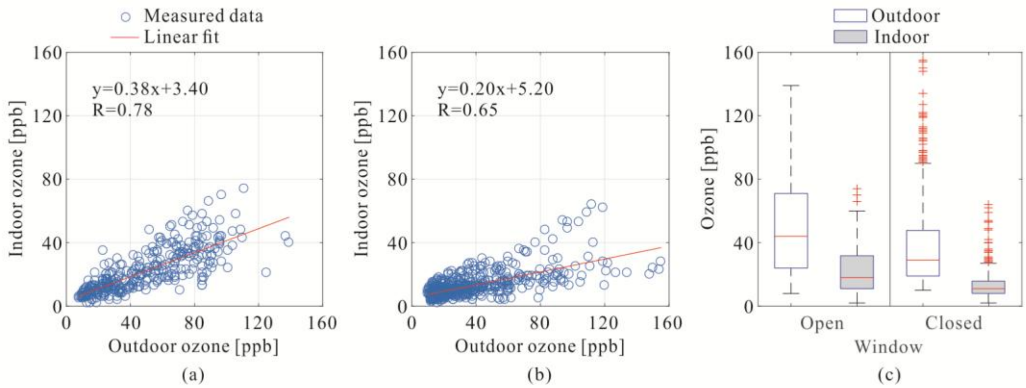

Figure 2. The measured indoor and outdoor ozone concentrations of the research room with the windows (a) open and (b) closed. (c) Boxplots of measured ozone levels.

Figure 3(a) shows the dynamic indoor ozone concentrations during the initial 60min after closing the windows. The initial (t = 0min) indoor ozone concentration is 40ppb, and the average outdoor ozone concentration is 80ppb. The estimated ozone concentrations are generally consistent with the measured concentrations. Figure 3(b) shows the estimated dynamic indoor ozone concentrations assuming that there is an indoor ozone source (S' = 500mg/m^3) disinfecting the research room for 30min with the windows closed. After the disinfection, the indoor ozone concentrations are estimated under two ventilation conditions. The condition with the windows open are favourable to indoor ozone removal compared to the condition with the windows closed, which spends less 21min for indoor ozone concentration to fall below the hazardous level (140ppb in China). Knowledge of the dynamic indoor ozone concentration levels are useful in terms of the time required for occupants to safely return to the building after the disinfection. However, this paper doesn't conduct experiments to validate the dynamic indoor ozone concentration with an indoor ozone source.

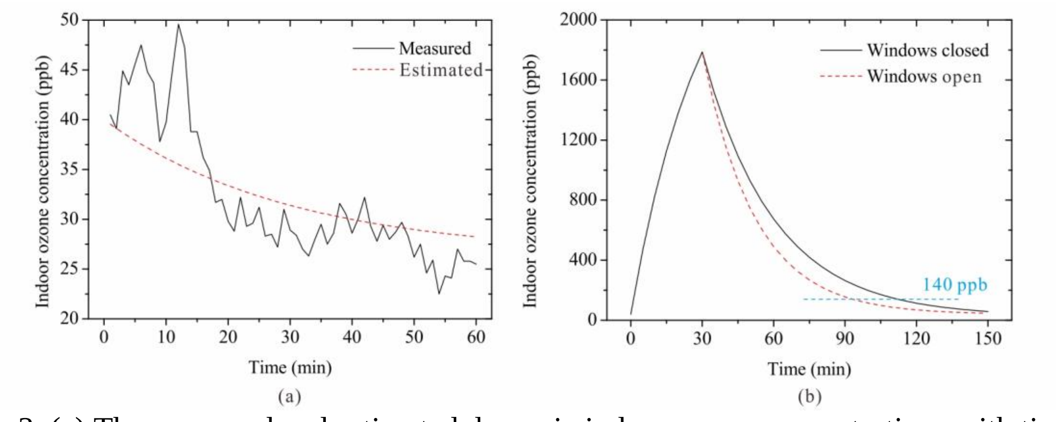

Figure 3. (a) The measured and estimated dynamic indoor ozone concentrations with time. (b) The estimated dynamic indoor ozone concentrations with an indoor ozone source.

4 DISCUSSION

The estimated results have a good consistency with the measured data. The estimation model in this paper is useful for predicting indoor ozone concentration levels and then taking strategies to control ozone exposure. Additional research is warranted to further explore and understanding the association between humidity and reaction probability. Besides, the estimation of dynamic indoor ozone concentration with an indoor ozone source need further field measurements to validate.

5 CONCLUSIONS

This paper develops a mass balance model tool to estimate indoor ozone concentration levels considering indoor ozone sources, which both steady state and dynamic ozone concentration can be predicted. Values of γ of totally 54 common indoor materials are compiled from literatures. Field measurements are conducted to validate the estimation model in steady state and dynamic conditions. The estimated results are consistent with the measured data, which means it is useful for predicting indoor ozone concentration levels and then taking strategies to control ozone exposure.

6 ACKNOWLEDGEMENT

The research was supported financially by the national key project of the Ministry of Science and Technology, China on “Green Buildings and Building Industrialization” through Grant No. 2016YFC0700500.

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