MEASUREMENTS OF MASS ACCOMMODATION COEFFICIENTS USING A FLAT PLATE TYPE TEST CHAMBER

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ABSTRACT
This paper reports the development of a flat plate type test chamber (FPT chamber) that can be used to obtain the mass accommodation coefficients (γ) of ozone depositing to different surface materials. The FPT chamber has one supply inlet and one exhaust outlet, with a channel cavity of dimensions 2,000 [mm] (channel length) × 300 [mm] (width) × 10 [mm] (height). Using this FPT chamber, ozone was introduced into the supply air at a constant concentration and the reduction in the concentration of the ozone after passing over the surface of the test materials was measured at a temperature of 293 [K]. Furthermore, in order to estimate directly the γ for ozone depositing to the surface of the building materials, a theoretical analysis incorporating an ozone deposition flux model was carried out in accordance with the experimental setup, and a chart was constructed which shows the relationship between γ and the average ozone concentration after ozone has passed over the surface of a given material.

KEY WORDS
Ozone, Flat Plate Type Test Chamber, Mass Accommodation Coefficient, Deposition Flux

INTRODUCTION
Indoor ozone has received attention because of its well-documented adverse effects on health. In addition to the harmful effects of ozone in itself, ozone can also initiate a series of reactions that generate potentially irritating oxidation products, including free radicals, hydroperoxides, aldehydes, ketones, organic acids and secondary organic aerosols [Weschler, 2000; 2004].

Sørensen and Weschler (2002) have used CFD simulations to examine the distribution of a hypothetical product resulting from the reaction of ozone with limonene. However, a major drawback to using numerical simulations is the lack of sufficient data on boundary conditions. In this study, we focus on heterogeneous reactions between ozone and the surfaces of various building materials. The purpose of this study is to develop a numerical method based on Computational Fluid Dynamics (CFD) to predict the ozone distribution in a room. More specifically, this study is designed to develop a reliable method, using a flat plate type test chamber (FPT chamber), to examine ozone deposition on building materials, and to estimate the mass accommodation coefficients of ozone, which are a fundamental parameter of the surface deposition flux model for ozone.

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MODELING THE WALL SURFACE DEPOSITION FLUX OF OZONE

The surface deposition of the local concentration close to the surface and, from molecular theory, the flux at the surface is given by [Cano-Ruiz et al., 1993]:

$$Js = -\gamma \frac{\langle v \rangle}{4} C_o \Big|_{y=\frac{2}{3}\lambda} \quad (1)$$

Here, γ [-] is the mass accommodation coefficient; $\langle v \rangle$ [m/s] is the Boltzmann velocity for ozone; and λ [m] is the mean molecular free path of ozone (6.5×10^{-8} [m]).

PREVIOUS RESEARCH TO ESTIMATE γ FOR OZONE

The γ value measured by the Tube Penetration Experiment, as reported by Altshuller et al. (1961), is on the order of $1.0\times10^{-7} – 1.0\times10^{-6}$ [-] for ozone depositing to solid surfaces such as teflon, glass, stainless steel, and polyethylene. Cohen et al. (1968) also reported a value for γ on the order of 1.0×10^{-5} [-] for silicon rubber, and on the order of $1.0\times10^{-7} – 1.0\times10^{-6}$ [-] for other solid surfaces such as glass, polyethylene, and PVC. Sabersky et al. (1973) and Simmons et al. (1990) reported a value for γ measured by the Chamber Decay Method on the order of 1.0×10^{-5} [-] for a concrete slab and red tiles, and 1.0×10^{-4} [-] for bricks.

OUTLINE OF FLAT PLATE TYPE TEST CHAMBER AND ITS CONDITIONS

Figure 1 shows a perspective layout of the FPT Chamber and a photo of its external appearance. The FPT chamber is a channel cavity measuring 2,000(x) ×300(y) ×10(z) [mm] in which a two-dimensional mean flow field is developed. The FPT chamber consists of three sections, a running-section (300(x) [mm]), a test-section (1500(x) [mm]), and a running-section (200(x) [mm]). It is equipped with 10(z) [mm] width inlet and outlet slots. The four boundaries – ceiling, floor, right, and left walls – are made of glass. The deposition of ozone onto glass is known to be comparatively small [Cano-Ruiz et al., 1993] and is neglected.

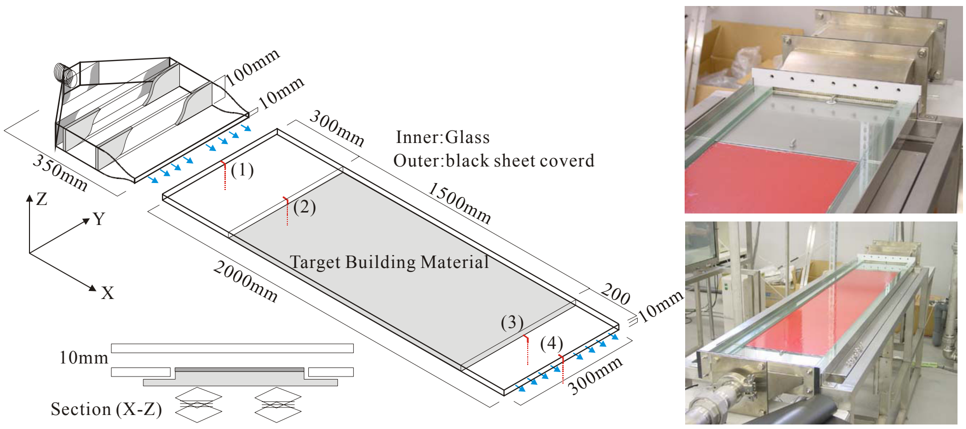


Figure 1 Perspective layout and photo of FPT Chamber

The air inlet velocity (U_{in}) was set at 1.0 [m/s] (air change rate: 2400 [times/h]). The inlet air and all the walls were maintained at isothermal conditions (293 ± 1.0 [K]). The supply air was passed through activated carbon and HEPA filters to keep the concentration of background contaminants low. In order to prevent photochemical reactions involving ozone, the FPT chamber experiments were carried out in a darkroom. The points of measurement in the FPT chamber are shown in Figure 1 (Positions (1) – (4)). The height of the floor of the FPT chamber is adjustable in proportion to the thickness of the target building materials to accurately maintain the 10 [mm] height in the z direction.

MEASUREMENT DATA AND METHOD

In this experiment, the target chemical compound was ozone. Ozone was introduced into the supply airflow at a constant concentration of 1.000 [ppm]. Ozone was analyzed using a UV Photometric Analyzer at a wavelength of 254 [nm]; its concentration range was 0 - 9.999 [ppm], and its precision was 0.001 [ppm]. The sampling flow rate of the UV Photometric Analyzer was 1.5 [L/min] and the ozone concentration was calculated as a time-averaged concentration over ten minutes. GC/MS and HPLC were used for the background volatile organic compounds (VOCs) and aldehydes. A digital dust concentration analyzer (light scattering method) was used to monitor background Suspended Particulate Matter (SPM).
This experiments focused on the heterogeneous reactions between ozone and various building materials, which are assumed to occur at the wall surfaces set at the floor level in the FPT chamber. Seven building materials; stainless steel (SUS 304), water- and oil-based paints, wallpaper, plywood, SBR rubber, and cedar were selected as test materials. Water- and oil-based paints were applied to the SUS 304 board with a coverage of 300 ± 15 [g/m^2] and allowed to dry. The experimental cases are shown in Table 1.

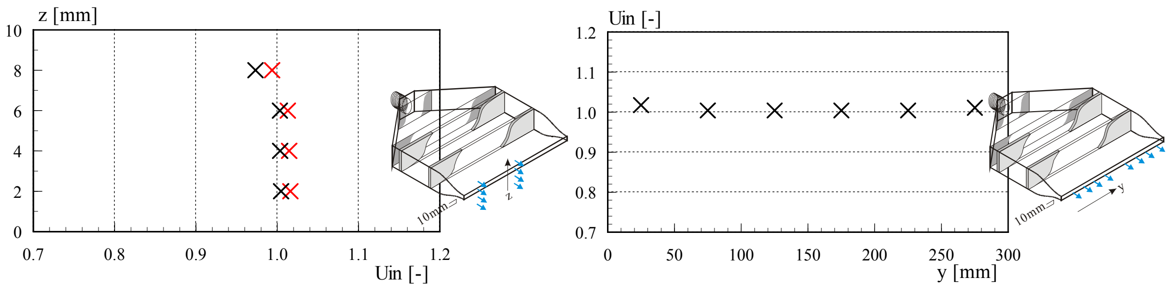
Table 1 Experimental cases

Exp. Case	Building Material	C_{in} [Ozone]	U_{in} (= $\bar{u}$)
Case (eb)	Glass		
Case (e1)	SUS 304		
Case (e2)	Water-based paint		
Case (e3)	Oil-based paint	1.000 ppm	1.0 m/s
Case (e4)	Wallpaper		
Case (e5)	Plywood		
Case (e6)	SBR rubber		
Case (e7)	Cedar		

RESULTS OF EXPERIMENT

Mean Velocity

The Reynolds number at the supply inlet position is Re=700 (U_{in}=1.0 [m/s], L_{in}=10 [mm]=channel height (z)) and hence a laminar flow field is generated in the FPT chamber. Figure 2 shows the vertical and horizontal profiles of U_{in} as measured by a thermistor anemometer. Constant flow distributions are formed at the supply inlet position.



(1) Vertical Profile of U_{in} (2) Horizontal Profile of U_{in}

Figure 2 Flow field at supply inlet

Figure 3 shows the vertical flow patterns along the x direction (downstream direction) based on a laminar flow analysis. The analysis, in which a constant flow distribution is given as a boundary condition at the supply inlet position, establishes that fully-developed and constant laminar flow profiles are generated at the test section (x>300 [mm]).

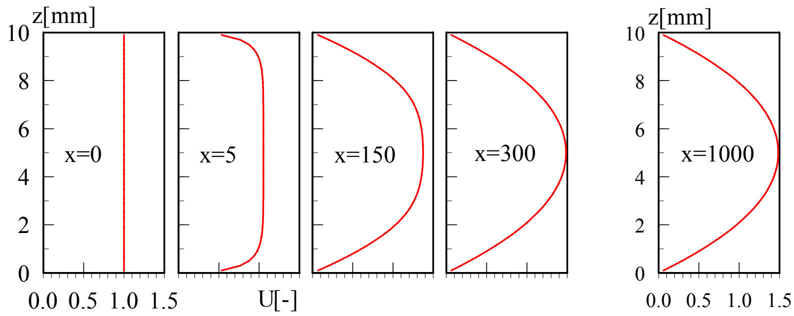


Figure 3 Vertical flow patterns along the *x* direction (downstream direction)

Background Concentration

The background concentration of the sum of the airborne organic compounds was confirmed to be below 30 [μg/m^3], while the Suspended Particulate Matter (SPM) in the supply air was 0.01 [mg/m^3] (total concentration of particles of diameter 10μm or less). Hence, uni- and bi-molecular chemical reactions of ozone in the air phase were negligible in the FPT chamber experiment.

Ozone Concentration

Table 2 shows averages for the measured ozone concentrations at sampling position (4). Ozone concentration measurements were conducted in triplicate for each target building material. In these experiments, target building materials were set up on the floor (1-sided deposition) in the FPT chamber. Ozone concentrations at sampling position (4) are normalized to the supply inlet concentration of ozone (C_{in}). In Case (eb), which estimates the background deposition onto the glass surface in the FPT chamber, the ozone concentration reduction at position (4) after passing over the target building material was less than 1 %. Hence, it was confirmed that the background ozone deposition in the FPT chamber was negligible. Among the evaluated building materials, plywood produced the maximum reduction in ozone concentration.

Table 2 Ozone concentration and estimated mass accommodation coefficient (γ) (1-sided deposition)

Exp. Case	C_{in} (Sampling Position (1))	Concentration at Sampling Position (4)	γ [-]
Case (eb)	1.000 [ppm]	0.999	< 1.1×10^{-7}
Case (e1)		0.954	3.4×10^{-6}
Case (e2)		0.934	4.9×10^{-6}
Case (e3)		0.921	6.1×10^{-6}
Case (e4)		0.968	2.3×10^{-6}
Case (e5)		0.894	8.7×10^{-6}
Case (e6)		0.920	6.2×10^{-6}
Case (e7)		0.932	5.2×10^{-6}

Table 3 Ozone concentration and estimated mass accommodation coefficient (γ) (2-sided deposition)

Exp. Case	C_{in} (Sampling Position (1))	Concentration at Sampling Position (4)	γ [-]
Case (eb)	1.000	0.999	< 1.1×10^{-7}
Case (e1)*		0.903	3.7×10^{-6}

Table 3 shows the average measured ozone concentrations at sampling position (4) in the case of 2-sided deposition (target building materials are set up both on the ceiling and the floor). When SUS 304 (Case (e1)*) was evaluated, the ozone concentration was significantly reduced compared with Case (e1) for 1-sided deposition.

ESTIMATION OF γ

The equations governing ozone transport are shown in Table 4 under the conditions of a fully-developed two-dimensional laminar flow field with diffusive streamwise transport neglected.

Table 4 Equations governing ozone transport in the FPT chamber (1-sided deposition)

$$\frac{3}{2}\bar{u}\left[\left(\frac{z}{h}\right)^2 - 1\right]\frac{\partial C}{\partial x} = D_o\frac{\partial^2 C}{\partial z^2},\ -h \le z \le h,\ 0 \le x \le x_L \quad (1)$$

$$J = D_o\frac{\partial C}{\partial z} = \gamma\frac{\langle v\rangle}{4}C \quad \text{at} \quad z = -h \quad (2)$$

$$\frac{\partial C}{\partial z} = 0 \quad \text{at} \quad z = h \quad (3)$$

$$C = C_{in} \quad \text{at} \quad x = 0 \quad (4)$$

x_L : length of test section (=1500mm)
h : half width of channel height (=5 mm)
C_{in} : supply inlet concentration of ozone (=1.000 ppm)
$\bar{u}$: supply inlet velocity (=1.0 m/s)
D_o : molecular diffusion coefficient of ozone (=1.81×10^{-5} m^2/s)
<v> : Boltzmann velocity (= 360 m/s)

The governing equations in Table 4 were used to calculate the average concentration of ozone at the outlet of the test section (i.e. the concentration after passing over the surface material) as a function of the mass accommodation coefficient (γ); the results are shown in Figure 4. The calculations were carried out for both 1-sided deposition and 2-sided deposition. Using the data for the average concentration of ozone as a function of the mass accommodation coefficient (γ), values of γ were estimated directly from the experimental results, and are shown in Tables 2 and 3.

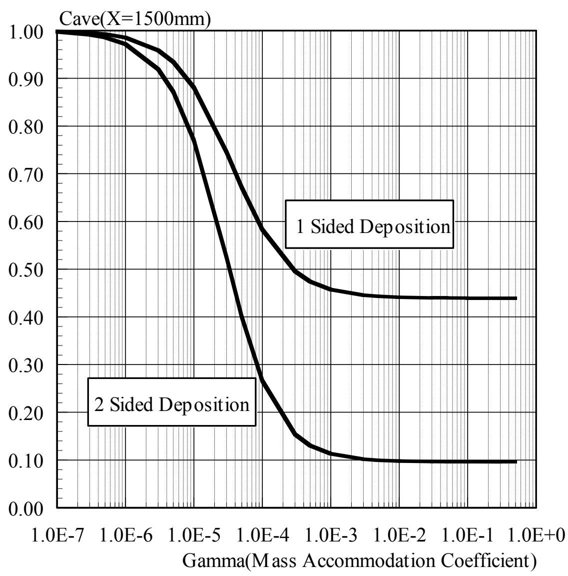


Figure 4 Average concentrations at the outlet of the test section (C_{ave}) for various γ values

The γ value was estimated to be below 1.1×10^{-7} [-] for Case (eb), which used glass as the target deposition material. The γ values become larger in proportion to the reduction in the ozone concentration. The γ values for the seven building materials were estimated to be between 8.7×10^{-6} [-] (Case (e5) for plywood) and 2.3×10^{-6} [-] (Case (e4) for wallpaper).

DISCUSSION

For 2-sided deposition, the reduction in the ozone concentration is larger than that for 1-sided deposition for the same building material. Hence, the uncertainty of the concentration measurement for 2-sided deposition is much smaller than for 1-sided deposition. The estimated γ value for SUS 304 for 1-sided deposition (Case (e1)) was 3.4×10^{-6} [-] and for SUS 304 for 2-sided deposition (Case (e1)*) was 3.7×10^{-6} [-] as shown in Tables 2 and 3. In this experimental setup, the estimation error between 1-sided and 2-sided deposition is about 8%, and it was confirmed that the measurement and estimation were sufficiently accurate.

Other studies (Cano-Ruiz et al., 1993; Morrison and Nazaroff, 2002) indicate that, for some materials, the γ value is likely to become smaller as the material is exposed to ozone for longer periods of time. This topic will be the subject of future experiments.

CONCLUSIONS AND IMPLICATIONS

(1) Figure 4 was constructed by carrying out a numerical analysis based on laminar flow with the same boundary conditions as those in the experimental setup using the FPT chamber. Direct estimation of γ for various building materials is possible using this chart.

(2) It was confirmed that nearly identical values of γ were obtained for 1-sided and 2-sided deposition.

(3) The γ value for glass was estimated to be below 1.1×10^{-7} [-], and the γ values for the seven building materials were estimated to be between 8.7×10^{-6} [-] (plywood) and 2.3×10^{-6} [-] (wallpaper).

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