Experimental and CFD Analyses Examining Ozone Distribution in Model Rooms with Laminar and Turbulent Flow Fields

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Abstract
The principle goal of this work was to better understand ozone distribution within rooms. Towards this end, the paper has two parts. The first describes the development of a flat plate test chamber (FPT chamber) that can be used to obtain mass accommodation coefficients ($\gamma$) for ozone that deposits on the surface of different materials. The second consists of model room experiments coupled with Computational Fluid Dynamics (CFD) analysis of the experimental scenarios to obtain ozone distribution in turbulent flow fields.

Keywords: ozone; flat plate test chamber; mass accommodation coefficient; surface removal; CFD

1. Introduction
Indoor ozone has received attention because of its well-documented adverse effects on health. In addition to the inherently harmful effects of ozone, it 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, Wolkoff, 1999].

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 have focused on heterogeneous reactions between ozone and the surfaces of various building materials. The purpose of this study was to develop a numerical method based on CFD to predict the ozone distribution in a room. To achieve this, two different sets of experiments were conducted. First, this study developed a reliable method using a flat plate test chamber (FPT chamber), to examine ozone deposition onto building materials and estimate the corresponding mass accommodation coefficients. The latter are a fundamental parameter in the surface deposition flux model for ozone. This study then isolated the surface reactions and measured the distribution of ozone within a model room. The results were subsequently used to validate a CFD model, corresponding to the experimental set-up, which includes the removal of ozone via surface deposition.

2. Theory
2.1 Modeling the wall surface deposition flux
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):

$$J_S = -\frac{\gamma}{4} \frac{\langle v \rangle}{\lambda} C_n$$

(1)

Here, $\gamma$ is the mass accommodation coefficient; $\langle v \rangle$ (m/s) is the Boltzmann velocity for ozone; and $\lambda$ (m) is the mean molecular free path of ozone (6.5$\times$10$^{-8}$ m). However, the grid scale (on the order of 10$^{-8}$ m) is very small compared to the length scales necessary to resolve the flow field and concentration field within the CFD model. In this paper, to enable an increased length scale at the surface, the following flux model is adopted (Sørensen and Weschler, 2002):

$$J_S = \frac{\gamma}{4} \frac{\langle v \rangle}{\Delta y} C_n$$

(2)

Here, $\Delta y_i$ is the distance to the center of the first computational cell ($\Delta y_i < \langle y \rangle$).

2.2 Equation for ozone transport in indoor air
Assuming the concentration of ozone at a point in space to be $C_n$ (ppm), the transport of ozone is expressed by Equation (3):

$$\frac{\partial \bar{C}_n}{\partial t} + \bar{U}_j \frac{\partial \bar{C}_n}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_n + \frac{\nu_j}{\sigma_j} \right) \frac{\partial \bar{C}_n}{\partial x_j}$$

(3)

Here, the overbar ($\bar{}$) denotes the ensemble-mean value. $D_n$ (m$^2$/s) is the molecular diffusion coefficient of ozone in the gas phase, $\bar{U}_j$ (m/s) is the ensemble-mean velocity, $\nu_j$ (m/s) is the turbulent eddy viscosity, and $\sigma_j$ is the turbulent Schmidt number.

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(Received March 26, 2007; accepted July 10, 2007)
2.3 Previous research of \( \gamma \) for ozone

The \( \gamma \) value measured by the tube penetration experiment, as reported by Altshuller et al. (1961), is in the order of \( 1.0 \times 10^{-7} \text{ to } 1.0 \times 10^{-6} \) for ozone depositing to solid surfaces such as teflon, glass, stainless steel, and polyethylene. Cohen et al. (1968) also reported a value for \( \gamma \) in the order of \( 1.0 \times 10^{-5} \) for silicon rubber, and in the range of \( 1.0 \times 10^{-7} \text{ to } 1.0 \times 10^{-6} \) for other solid surfaces such as glass, polyethylene, and PVC. Sabersky et al. (1973) and Simmons et al. (1990) reported a value for \( \gamma \) measured by the Chamber Decay Method of \( \approx 1.0 \times 10^{-4} \) for a concrete slab and red tiles, and \( \approx 1.0 \times 10^{-4} \) for bricks.

2.4 Overview of the numerical analysis for the model room

Flow fields were analyzed using the low Reynolds number type k-\( \varepsilon \) model (Murakami and Kato et al., 1996). The QUICK scheme is used for the convection term, and a SIMPLE algorithm is used. To analyze the flow field in the boundary layer, the center of the computational cells closest to the wall surface should be at a non-dimensional distance (Wall Unit) of \( y^+ \approx 1 \), where \( y^+ = u^* y_1 / \nu \), where \( u^* \) is the friction velocity, \( \nu \) is the kinematic viscosity, and \( y_1 \) is the distance normal to the wall surface, \( \nu \) is the friction velocity. Here, \( \rho \) is the air density and \( \tau_w \) is the wall shear stress. The number of meshes was set to \( 220 (x) \times 110 (z) \), and an unequal interval mesh is used for this analysis. In this analysis, the height of the cells closest to the ceiling wall surface is \( 6.0 \times 10^{-6} \text{ m} \).

When the ozone concentration in the model room is \( C \) (ppm), the transport of ozone in the air inside the room is described by Equation (3). This study is based on an analysis using the RANS model and uses the ensemble-averaged equation. Equation (2) describes the deposition flux of ozone onto wall surfaces.

2.5 Modeling ozone concentrations in the model room

In the model, ozone was added to the air supply at the supply inlet at a constant concentration (\( C_w = 1.000 \) ppm), as was done in the corresponding experiments. Table 1. shows the boundary and analysis conditions.

In the numerical analysis of the model room, only the ozone deposition at the wall surfaces of the model room was incorporated in the simulations. The mass accommodation coefficients (for the various building materials) used in the analysis were the estimated \( \gamma \) values obtained in the FPT chamber experiments as shown in Tables 2. and 3.

2.6 Different cases analyzed for the model room

Table 3. summarizes the different cases that were numerically analyzed for the model room. Besides simulating different airflow conditions, that is, air inlet velocities of \( U_w = 3.0 \text{ m/s} \), the building materials installed on the ceiling, floor, and both right and left walls in the model room were varied at each airflow to give a further set of analysis cases. In addition to the analysis cases based on the building materials used in the model room experiments (Cases a1 to a7), stepwise changes were also made in the value of the mass accommodation coefficient (\( \gamma \)) (Cases a8 to a13). The \( \gamma \) value in Case a13 is 1.0, indicating ideal conditions for adsorption to the material surface and guaranteeing a constant "zero-concentration" at the surface of the building material.

3. Methods

3.1 FPT chamber and its operating conditions

Fig. 2. shows a perspective layout of the FPT Chamber. The FPT chamber is a channel cavity measuring \( 2.0 (x) \times 0.3 (y) \times 0.010 (z) \text{ m} \) in which a two-dimensional mean flow field is developed. The FPT chamber consists of three sections, a lead-in-section (0.3 m (x)), a test-section (1.5 m (x)), and a
Table 1. Information Related to Numerical Analysis

| Turbulence Model | Mesh | Scheme | Inflow Boundary | Outflow Boundary |
|------------------|------|--------|-----------------|------------------|
| Low Re Type $k$-$\varepsilon$ model (MKC model, 2-Dimensional Cal.) | 220 (x) × 110(z) | Convection Term: QUICK | $U_i = \frac{3.0 m/s}{k_w = \frac{32x}{(U_i \times 0.015)^2}}$, $\tau_w = C_c \times \frac{k_w^{1/2}}{U_i}$, $C_c = 0.09$, $L_w = L_i$ (Slot Width: 0.02) × 1/7 |

Table 2. Materials Investigated, Ozone Concentrations (ppm) at Positions 1 and 4, and Estimated Mass Accommodation Coefficients ($\gamma$) for the FPT Chamber Experiments

| Exp. Case | Building Material | $C_z$ (ppm) [Sampling Position (1)] | Concentration at Sampling Position (4) | $\gamma$ [-] |
|-----------|-------------------|------------------------------------|--------------------------------------|-------------|
| (1) 1-sided deposition |
| Case (fb) | Glass | 1.00 [ppm] | 0.999 | < 1.1 × 10^{-6} |
| Case (11) | SUS 304 | 0.954 | 3.4 × 10^{-6} |
| Case (12) | Water-based paint | 0.934 | 4.9 × 10^{-6} |
| Case (13) | Oil-based paint | 0.921 | 6.1 × 10^{-6} |
| Case (14) | Wallpaper | 0.966 | 2.3 × 10^{-6} |
| Case (15) | Plywood | 0.894 | 8.7 × 10^{-6} |
| Case (16) | SBR rubber | 0.930 | 6.2 × 10^{-6} |
| Case (17) | Cedar | 0.932 | 5.2 × 10^{-6} |

| (2) 2-sided deposition |
| Case (fb) | Glass | 1.00 [ppm] | 0.999 | < 1.1 × 10^{-6} |
| Case (11)* | SUS 304 | 0.903 | 3.7 × 10^{-6} |

lead-out-section (0.2 m (x)). It is equipped with 0.010 m (z) wide inlet and outlet slots. The four boundaries for air passing through the chamber – ceiling, floor, right, and left walls – are made of glass.

The air inlet velocity ($U_i$) was set at 1.0 m/s (air change rate: 2400 h^{-1}). The inlet air and all the walls were maintained at isothermal conditions (293 ± 1.0 K). The air supply was passed through activated carbon and ULPA 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 dark room. The points of measurement in the FPT chamber are shown in Fig.2. [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 0.010 m height (z direction).

3.2 FPT chamber experiments: measurements and materials

In the FPT chamber experiments, ozone was introduced into the air supply at a constant concentration of 1.00 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 to measure 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).

These experiments focused on the heterogeneous reactions between ozone and various building materials; these are assumed to occur at the surface of the materials, which are positioned at the floor level in the FPT chamber. Seven building materials, including stainless steel (SUS 304), water- and oil-based paints, wallpaper, plywood, SBR rubber, and cedar, were selected for evaluation. Water and oil-based paints were applied to the SUS 304 plate with a coverage of 300 ± 15 g/m^2 and allowed to dry. The experimental cases are presented in Table 2.

3.3 Overview of the model room experiments

The model room is shown in Fig.1a; it is a box measuring 1.5 m (x) × 3.0 m (y) × 1.0 m (z) in which a two-dimensional mean flow field is developed. It is equipped with 0.02 m wide inlet and outlet slots. The supply inlet slot is positioned along the ceiling, and the exhaust outlet slot is set along the ceiling on the opposite sidewall. The four boundaries for air flowing through the room – ceiling, floor, right, and left walls – were made of SUS 304 stainless steel and the ends were glass. These experiments assumed that ozone entered the room from outdoors with the ventilation air and measured the resulting distribution of ozone concentrations in the model room. The air inlet velocity was controlled at 3.0 m/s (144 air changes/hour; the turbulent intensity of the supply inlet flow was 0.015). The inlet air and walls were controlled to maintain isothermal conditions (293 ± 1.0 K). The relative humidity of the supplied air was maintained at 30 ± 5%. Contaminants in the air supply (i.e., VOCs and suspended particulate matter) were removed by an active carbon filter and a HEPA filter. In order to prevent photochemical reactions, the model room experiments were carried out in the dark. The central section in the Y direction is taken as the measurement plane (x – z plane in Fig.1a). Points of measurement in the model room are shown in Fig.1b.
3.4 Flow field in the model room

We conducted detailed measurements of the flow fields in the model room using Laser Doppler Velocimetry (LDV); as a consequence numerous statistical data related to the turbulent flow as well as the average air velocity are available. Details of the modeling experiment for flow fields were reported in Ito et al. (Ito, 2000 and Kato, 2003). In the model room, a large circulating flow was formed along the wall surface in the room, and a secondary vortex against the major flow was observed in the floor corner as shown in Fig.1a.

3.5 Experimental conditions in model room experiments

The experimental cases are shown in Table 3. The target building materials were installed on all four sides - ceiling, floor, right and left wall in the model room as shown in Fig.1a. The air inlet velocity was set at 3.0 m/s. In all the experimental cases, the measurements were focused on the convection and diffusion of ozone contained in the air supply and its deposition on the wall surfaces.

The outdoor air was assumed to be the source of the ozone, which was thoroughly mixed into the air transported through the supply inlet. The ozone was produced by a UV ozone generator and the ozone concentration in the supply air, \( C_{in} \), was maintained at a constant 1.00 ppm. At the air supply slot position, the ozone concentration was measured in the \( y \) and \( z \) directions to confirm that uniformity was maintained. The ozone concentration was always monitored in the center of the air supply slot and fluctuation with time was also checked. It was confirmed that \( C_{in} \) was within a 2% range of the target concentration over the period of the experiments. The wall surfaces of the model room and the air temperature were controlled to a constant 293 ± 0.1 K. In these experiments measurements of ozone concentrations at the different sampling points were conducted for approximately one hour after introducing ozone to the room in order to confirm that ozone concentrations had reached a steady state.

3.6 Sampling and analysis in model room

Ozone was sampled through Teflon tubes inserted into the model room, and its concentration was measured using a UV Photometric Analyzer. The ozone concentration for each measurement point is reported as the average of triplicate measurements, each time-averaged over a ten-minute interval. The conditions for the operation of the ozone analyzer are the same as in the FPT chamber experiments.

Prior to measuring ozone concentrations, the model room was cleaned with neutral detergent and pure water. In each case the ozone concentration was measured at 11 points, including the supply inlet and exhaust outlet positions as shown in Fig.1b.

3.7 Numerical conditions in model room

The analysis was carried out in two dimensions for the central plane (the \( x-z \) plane in Fig.1a) of the model room in the \( y \) direction. When the air supply slot width is the representative length (\( L_o = 0.02 \) m), the analytical space is a two-dimensional room measuring \( 75 \times 50 \times (x \times z) \) (equal to 1.5 m x 1.0 m). The air inlet velocity was set to two different values, \( U_{in} = 3.0 \) m/s, which are the same inlet velocities that were used in the experiments. The turbulence intensity was set to 1.5% based on the experimental results. Numerical cases in the model room are shown in Table 4.

4. Results

4.1 FPT chamber experiments: mean velocities

The Reynolds number (\( Re \)) at the supply inlet position is \( 700 \) \( [U_{in} = 1.0 \) m/s, \( L_o = 0.010 \) m = channel height (\( z \)], indicating a laminar flow field in the FPT chamber. The vertical and horizontal profiles of \( U_{in} \) are measured by a thermistor anemometer. A relatively uniform flow distribution is formed at the supply inlet position.

The vertical flow patterns along the \( x \)-axis (downstream direction) were confirmed 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).

4.2 FPT chamber experiments: background VOC and particle concentrations

The background concentration of the sum of the airborne organic compounds was confirmed to be below 30 µg/m³, while the Suspended Particulate Matter (SPM) in the air supply was 0.01 mg/m³ (total concentration of particles < 10 µm diameter). Hence, gas phase reactions of ozone, as well as reactions on particle surfaces, were negligible in the FPT chamber.

Table 3. Experimental Cases (Model Room)

| Exp. Case | Building Material       | \( C_{in} \) [Ozone] | \( U_{in} \) |
|-----------|------------------------|----------------------|-------------|
| Case (e1) | SUS 304                | 3.4×10^-6            | 1.00 ppm    |
| Case (e2) | Water-based Paint       | 4.9×10^-6            | 3.0 m/s     |
| Case (e3) | Oil-based Paint         | 6.1×10^-6            |             |
| Case (e4) | Wallpaper               | 2.5×10^-6            |             |
| Case (e5) | Plywood                | 8.7×10^-6            |             |
| Case (e6) | SBR Rubber             | 6.2×10^-6            |             |
| Case (e7) | Cedar                | 5.2×10^-6            |             |

Table 4. Numerical Cases (Model Room)

| Anal. Case | Building Material | \( \gamma \) | \( C_{in} \) | \( U_{in} \) |
|-----------|-------------------|-------------|-------------|-------------|
| Case (a1) | SUS 304           | 1.0×10^-6   | 1.00 ppm    | 3.0 m/s     |
| Case (a2) | Water-based Paint | 1.0×10^-4   |             |             |
| Case (a3) | Oil-based Paint   | 1.0×10^-4   |             |             |
| Case (a4) | Wallpaper         | 1.0×10^-4   |             |             |
| Case (a5) | Plywood           | 1.0×10^-4   |             |             |
| Case (a6) | SBR Rubber        | 1.0×10^-4   |             |             |
| Case (a7) | Cedar             | 1.0×10^-4   |             |             |
4.3 FPT chamber experiments: ozone concentrations

Table 2. shows averages for the measured ozone concentrations at sampling position (4) (see Fig.2.). Ozone concentration measurements were conducted in triplicate for each target building material. In these experiments, target-building materials were placed 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 (fb), 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 background ozone deposition in the FPT chamber was negligible. Among the evaluated building materials, plywood produced the maximum reduction in ozone concentration of (11%).

Table 2. also shows the average measured ozone concentrations at sampling position (4) in the case of 2-sided deposition (target building materials positioned both on the ceiling and the floor). When SUS 304 (Case (f1)*) was evaluated, the ozone concentration was significantly reduced compared with Case (f1) for 1-sided deposition.

4.4 FPT chamber experiments: estimation of mass accommodation coefficients ($\gamma$)

Table 5. presents the equations governing ozone transport under the conditions of a fully developed two-dimensional laminar flow field with diffusive stream-wise transport neglected. The governing equations in Table 5. 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 ($\gamma$); the results are shown in Fig.4. The calculations were carried out for both 1-sided and 2-sided deposition. Using the data for the average concentration of ozone as a function of the mass accommodation coefficient ($\gamma$), values of $\gamma$ were estimated directly from the experimental results, and are shown in Table 2.

The $\gamma$ value was estimated to be below 1.1×10^{-7} [-] for Case (fb), which used glass as the target deposition material. The $\gamma$ values become larger in proportion to the reduction in the ozone concentration. The $\gamma$ values for the seven building materials were estimated to be between 8.7×10^{-6} (Case (f5) for plywood) and 2.3×10^{-6} (Case (f4) for wallpaper).

4.5 Model room experiments: measured ozone concentrations

Before the experiment, GC/MS and HPLC were used to measure the background volatile organic compounds (VOCs) and aldehydes. The TVOC concentration was confirmed to be 30 µg/m^3 or less.

In these experiments, ozone was introduced with the supply air at a constant concentration of 1.00 ppm. The measured ozone concentrations at the various sampling points within the model room are shown in Fig.5.; each measurement was made at least three times to insure reproducibility. Ozone deposition on
the glass surfaces in the model room was negligible. In addition, the level of TVOC in the air supply was quite low. Therefore, the dominant cause for the reduction in ozone concentration in the model room was deposition onto the surfaces of the building materials installed on the wall surfaces. In terms of ozone concentrations at the exhaust outlet position, Case e5 (plywood) shows the largest reduction in ozone concentration and Case e4 (wallpaper) and Case e1 (SUS 304) resulted in much lower reductions, although the results varied to some extent depending on the air inlet velocity. The reductions in the ozone concentrations obtained in these experiments are approximately consistent with the mass accommodation coefficients obtained in the FPT Chamber experiments (see values of $\gamma$ in Table 2.).

4.6 Results of numerical analyses of the model room

Fig.3b. shows the analysis results for the flow field using the Low-Re Type k- $\varepsilon$ model, and Figs. 3c and 3d show comparisons between the experimental results and the theoretical results. These comparisons confirm that the results for the flow field based on CFD analysis accurately reproduce the flow field measured inside the model room. Fig.6. show the results for numerical analyses of the ozone concentration distributions. In all of the cases, ozone would have been uniformly distributed inside the room if there were no deposition flux, expressed by Equation (2). In all cases, a reduction in concentration increased or decreased as would be anticipated from the value of $\gamma$.

Fig.7. presents comparisons between the measured and predicted ozone concentrations along the centerline of the model room ($x = 750$ mm, $z = 0$ to 1000 mm). Compared with the experimental results, the modeled results tended to overestimate the ozone concentration by 5% to 10%. The difference between measured and predicted was particularly large for Case a5 (plywood) and Case a7 (cedar).

Based on results from the numerical analysis, Table 6. shows the average ozone concentration in the room as well as at a point in the exhaust outlet; it also presents the relative amount of ozone removed by ventilation and by deposition onto the wall surfaces. Under the
outlined analysis conditions, in the case where an SUS 304 plate was installed, the relative amount removed by ventilation was 97.6% while that removed by deposition onto the SUS 304 wall was 2.4%. In Case a13 (γ = 1.0) in which an ideal deposition surface was hypothesized, the relative amount removed by ventilation was 46.0% and that removed by deposition onto the wall surface was 54.0%. Case a13 represents the largest possible fraction of ozone removal by deposition, as opposed to ventilation, for the conditions used in this analysis.

Table 6. also shows the analysis results for the deposition velocity, \( v_d \) (m/s), calculated using Equation (8).

\[
v_d = \frac{|\gamma|}{C_o} \left[ \frac{\gamma v}{4} \right] = \frac{C_i}{C_o} \left[ \frac{\gamma v}{4} \right] \left[ 1 + \frac{\Delta y}{\Delta y + \frac{\gamma v}{4 D_o}} \right]
\]

Here, \( C_o \) represents the concentration in the core of the room. The present analysis used the inlet concentration, \( C_i \), for this value. Using the results shown in Table 6, the relationship between the mass accommodation coefficient (\( \gamma \)) and the deposition velocity, \( v_d \), is shown in Fig.8. This plot indicates that the deposition velocity, \( v_d \), is almost constant when the mass accommodation coefficient (\( \gamma \)) is greater than 1.0 \( \times 10^{-3} \). The constant value for the deposition velocity (\( v_d \)) shown in Fig.8, corresponds to the mass transfer coefficient \( \alpha_m \) (m/s) assuming that the concentration at a solid surface is zero. This implies that, when the ozone concentration field analysis in a room is carried out for building materials whose mass accommodation coefficient (\( \gamma \)) is greater than 1.0 \( \times 10^{-3} \), a value of \( \alpha_m = 4.5 \times 10^{-3} \) to 6.5 \( \times 10^{-3} \) m/s can be applied based on the assumption that the concentration at the construction material surface is zero.

5. Discussion

The reduction in the ozone concentration for 2-sided deposition is larger than for 1-sided deposition for the same building material (e.g., for SUS 304 the respective reductions are 9.7% and 4.6%). Hence, the uncertainty of the concentration measurement for
2-sided deposition is much smaller than for 1-sided deposition. For SUS 304, the estimated γ value for 1-sided deposition (Case (f1)) was 3.4×10^-8, and for 2-sided deposition (Case (f1)) it was 3.7×10^-8 as shown in Tables 2. and 3. If we assume that the value derived from 2-sided deposition is more accurate, then the error in the value derived from 1-sided deposition is about 8%; this is a rough estimate of the uncertainty associated with γ values derived from one-sided measurements.

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. The present studies were not designed to examine such "aging" phenomena. Ozone concentration measurements were conducted for only about an hour after initiating the supply of ozone, and it was confirmed that the ozone concentrations had reached a steady state during this period.

As shown in Fig.3., the flow field analysis based on CFD matches experimental measurements reasonably well. Therefore, if there are estimation errors in the numerical analysis, the difference from the experimental results can be attributed to that part of the model that accounts for ozone loss. While the comparisons shown in Fig.7. of the ozone concentrations along the center line of the model (x = 750 mm, z = 0 to 1000 mm) indicate that the qualitative trends of the concentration distribution profiles obtained by experiment and calculation are similar, the value of the ozone concentration measured by experiment tends to be lower than that obtained by the model, particularly in the center of the room. In the center of the room there is a stagnant region inside the large circulation flow formed in the space. The reduced ozone concentration in this stagnant region suggests that ozone-consuming chemistry is occurring; such a phenomenon is consistent with the observation that the concentration is reduced in proportion to the ozone residence time. Given that the concentrations of organic compounds and suspended particles in the supply air are negligible, the reduced ozone concentrations in the center of the model room is assumed to be due to ozone reactions with unsaturated organic compounds that have diffused into the air from the various building materials installed on the walls (e.g., terpenes emitted from plywood or terpene and sesquiterpenes emitted from cedar). To more fully evaluate this conjecture, it is necessary to measure the concentrations of organic chemicals in the air when various building materials are installed into the model room.

6. Summary

This work has produced a chart which permits estimations of the mass accommodation coefficients (γ) for various building materials based on the ozone concentrations measured at the outlet of the FPT chamber. The γ value for glass was estimated to be below 1.1×10^-8; the γ values for the seven building materials were estimated to be between 8.7×10^-8 (plywood) and 2.3×10^-8 (wallpaper).

The ozone concentration distributions in the model room were measured in cases where various building materials were placed against the wall surfaces. A numerical analysis was conducted that incorporated the ozone deposition flux model for a wall surface and used the γ values measured in the FPT Chamber experiments. The errors in the numerical estimations in the center of the room were about 10% at their largest compared with measured results from the model room experiments.

Acknowledgement

The Author thanks Prof. D. N. Sørensen and Prof. C. J. Weschler for their detailed comments that have made possible an improvement of this study.

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