

# CFD and Model Experiment with Chemical Reaction

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## Abstract

Recently, the results of theoretical analysis and investigations suggest that some free radicals are generated by chemical reactions. The free radicals and other products of reactions are often more irritating than their precursors. In particular, the products of ozone / terpenes reactions cause greater airway irritation in mice than would be predicted based on the known response of mice to ozone or terpenes. This paper reports the results of a room model experiment and CFD (Computational Fluid Dynamics) analysis of chemically reactive pollutants in indoor air. The analyzed room model had one supply inlet and one exhaust outlet, and its cavity was composed of 1.5m (x) : 0.3m (y) : 1.0m (z) in which a two-dimensional flow field was developed. A clear recirculating flow was observed in the room generated by the forced ventilation. In this experiment, ozone and terpenes were used as chemically reactive pollutants in the air phase. In order to discuss the order of chemical reaction, the concentration distributions of ozone and terpenes in the model room were measured in cases with and without a chemical reaction. Furthermore, to estimate the concentration of reactive products, the number of particles generated by the chemical reaction in the model room was measured with a laser particle analyzer. In addition, CFD analysis corresponding to the experimental conditions and with a built-in rate constant chemical reaction model was carried out, and it confirmed that the results are in good agreement with the results of the room model experiment.

**Keywords:** Chemical Reaction; Ozone; Terpenes; Model Experiment; CFD

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## Introduction

The concentration distribution of the chemical pollutants (e.g. VOC) in a room was analyzed and reported by modeling the diffusion within the building material and within the room air; this included the sorption on the building material surface [Murakami et al., 2001]. The results of a numerical prediction of the concentration distribution and time history of the emission rates were reported [Murakami et al., 2000]. These results were sufficiently consistent with the results from experiments in a test chamber. However, in actual measurements of VOC concentrations in a room, the measured concentration and the values estimated from the emission flux from each material in the room and the ventilation rate are not necessarily consistent with each other, and the existence of a phenomenon known as "lost TVOC" has been confirmed [Wolkoff, 1995]. One of the causes of this is

believed to be the generation and decomposition of VOC due to chemical reactions in the air. In particular, it has been confirmed that ozone [O<sub>3</sub>] in the room air actively generates various free radicals by reacting with the organic and inorganic compounds existing in the air. The free radicals and other products of reactions are often more irritating than their precursors. Against this background, simplified equations for the chemical reactions were modeled in this research, with the aim of establishing a method of estimating the concentration in the room that incorporates these phenomena. In order to verify the chemical reaction model, a room model experiment with and without a chemical reaction in the air were carried out.

## Modeling the Equations for the Chemical Reaction

Various chemical reactions are assumed to take place in room air. In particular, various free radicals exist as intermediate products from these chemical reactions; however, these free radicals are in unstable states, posing great difficulties in both qualitative and quantitative estimation. In addition, it imposes a considerable additional burden on the computational process to accurately compute the behavior of these free radicals. Therefore, the purpose of the modeling

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was to estimate the total concentrations of the final products. In this research, the Second Order Rate Constant model which is a simple model reproducing bimolecular Reaction was adopted [Charles et al., 2000].

### Uni-molecular Reaction and Reaction Modeling Using the Rate Constant

A uni-molecular reaction is a chemical reaction involving the photochemical reaction of ozone. Assuming the concentration of the reaction substance "A" at a point in space to be  $C_1$  (i,j,k) [ppb], the transportation of the reaction substance is expressed by equation (1), and the uni-molecular reaction by equation (2).

$$\frac{\partial C_1}{\partial t} + \frac{\partial U_j C_1}{\partial x_j} = \frac{\partial}{\partial x_j} D \frac{\partial C_1}{\partial x_j} + S_A \quad (1)$$

$$S_A = -k_u \cdot C_1 \quad (2)$$

Here,  $S$  is the source term;  $k_u$  is the first order rate constant [1/h]. When the activation energy is the same in the analyzed space, concentration distributions governed by Equations (1) and (2) correspond to the distribution of the reciprocal of the age of the air [Murakami, et al., 1986].

In addition, assuming the concentration of the hypothetical products (all products) by reaction to be  $C_{prod}$  [ppb], the amount of change over time is expressed by equations (3) and (4).

$$\frac{\partial C_{prod}}{\partial t} + \frac{\partial U_j C_{prod}}{\partial x_j} = \frac{\partial}{\partial x_j} D \frac{\partial C_{prod}}{\partial x_j} + S_{prod} \quad (3)$$

$$S_P = k_{prod} \cdot C_{prod} = k_u \cdot C_1 \quad (4)$$

Here,  $k_{prod}$  is the first order rate constant [1/h] of the hypothetical reaction product  $C_{prod}$ .

### Bi-molecular Reaction and Reaction Modeling Using the Rate Constant

A bi-molecular reaction is a chemical reaction involving multiple substances, and in order to numerically analyze this, it is necessary to solve multiple scalar equations corresponding to the number of reaction substances and products. The generation of unstable substances in a room during a bi-molecular reaction with highly reactive ozone and terpenes has been drawing attention.

The simplest chemical reaction modeling uses the rate constant [Nazaroff et al., 1986]. Assuming the concentration of the reaction substances "A" and "B" at a point in space to be  $C_1$  (i,j,k) [ppb] and  $C_2$  (i,j,k) [ppb] respectively, the transportation of the reaction substances are expressed by equations (1) and (5), and the bi-molecular reaction by equation (6).

$$\frac{\partial C_2}{\partial t} + \frac{\partial U_j C_2}{\partial x_j} = \frac{\partial}{\partial x_j} D \frac{\partial C_2}{\partial x_j} + S_B \quad (5)$$

Table 1. Second Order Rate Constant

Ozone	d-Limonene	0.0184	[1/ppb·h]
Ozone	$\alpha$ -Pinene	0.00756	[1/ppb·h]
Ozone	$\alpha$ -terpinene	0.756	[1/ppb·h]

(Atkinson et al, 23°C)

$$S_A = S_B = -k_b \cdot C_1 \cdot C_2 \quad (6)$$

Here,  $S$  is the source term;  $k_b$  is the second order rate constant [1/ppb·h]. From equation (6), changes over time in the concentration of substances "A" and "B" due to the bi-molecular reaction are computed. In addition, assuming the concentration of the hypothetical products (all products) by reaction to be  $C_{prod}$  [ppb], the amount of change over time is expressed by equations (3) and (7).

$$S_{prod} = k_{prod} \cdot C_{prod} = k_b \cdot C_1 \cdot C_2 \quad (7)$$

Here,  $k_{prod}$  is the first order rate constant [1/h] of the hypothetical reaction product  $C_{prod}$ .

### Existing Research on Rate Constants

A lot of second order rate constants have been measured in research by Atkinson et al. [Atkinson et al., 1990]. Data on the second order rate constants for ozone at 296K (23°C) and terpenes have been collected for reactions that are believed to exist in room air. Some of the results of measurements made by Atkinson et al., are shown in Table 1. In this research, the data shown in Table 1 were used to estimate the chemical reactions and concentration distribution in the room air.

### Wall Surface Deposition Flux Modeling of Ozone

This research accounted for ozone as one of the reaction substances in the room. In accounting for the phenomena of the transportation of ozone in a room, it is necessary to consider not only its transportation with ventilation, and chemical reaction, but also the phenomena of sorption by the solid walls.

We proposed simple adsorption/desorption models for a sorptive material surface using the adsorption isotherms described in the previous report [Murakami et al., 2001]. Seinfeld J. H. et al proposed a model of deposition using the deposition velocity  $v_d$  [m/s], taking into account the deposition of ozone on the solid wall surfaces [Seinfeld, 1985]. The deposition flux against a solid surface using the deposition velocity  $v_d$  is expressed by the following equation:

$$J_s = v_d (C_s - 0) \quad (8)$$

Here,  $J_s$  is the deposition flux.  $C_s$  is a reference concentration. The deposition velocity  $v_d$  corresponds to the convective mass transfer coefficient where the surface concentration is assumed to be zero. According to Nazaroff et al., ozone deposition rates in general building materials are estimated to be from

$2.5 \times 10^{-4}$  to  $7.5 \times 10^{-4}$  [m/s] [Nazaroff et al., 1986].

In this paper, a model of deposition from molecular theory was adopted, taking into account the deposition of ozone on the solid wall surfaces. According to this theory, the surface flux is written as follows [Sorensen et al., 2002];

$$J_s = \frac{-\gamma \langle v \rangle / 4}{1 + (\gamma \langle v \rangle / 4 / Dm) \Delta z_1} C(\Delta z_1) \quad (9)$$

Here,  $\gamma$  is the mass accommodation coefficient;  $\langle v \rangle$  is the Boltzmann velocity for the chemical species;  $\Delta z_1$  is the distance to the center of the first computational cell.

### Outline of the Room Model Experiment

In order to measure the amount of the chemical reaction in the indoor air quantitatively, a room model experiment was carried out. The room model shown in Figure 1 was used for analyzing the chemical reaction. The model is a cavity composed of 1.5m (x) : 0.3m (y) : 1.0m (z) in which a two-dimensional mean flow field is developed. It is equipped with 0.02m width 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 other sidewall. Four boundaries (ceiling, floor, right and left walls) consist of SUS 304 and the others are glass.

Air inlet velocity ( $U_{in}$ ) is set at 2.8 m/s. Inlet air and all the walls are controlled in isothermal conditions ( $23 \pm 1.0^\circ\text{C}$ ). The test conditions of the room model are shown in Table 2.

### Measurement Cases and Method

In this experiment, target chemical compounds were Ozone and Terpenes (d-Limonene and  $\alpha$ -Pinene). Ozone was assumed to have entered the supply air-flow by infiltration from the outdoor air. d-Limonene and  $\alpha$ -Pinene were assumed to be generated from the wood floor material. In this experiment, liquid d-Limonene and  $\alpha$ -Pinene were set up on the floor as the first approximation of emission. The emission rates of d-Limonene and  $\alpha$ -Pinene were calculated in measuring the weight change. The measurement cases in combining the three chemical compounds are shown in Table 3.

Ozone was analyzed using a UV Photometric Analyzer, and GC/MS was used for d-Limonene and  $\alpha$ -Pinene as shown in Tables 4 and 5. The Ozone concentration was calculated as a time-averaged concentration over ten minutes. The d-Limonene and  $\alpha$ -Pinene sampling conditions are shown in Tables 4 and 5.

In the chemical reaction of ozone and terpenes, the generation of particulate matters has been pointed out [Weschler et al., 2002]. In this experiment, the number of particles, which are chemical reaction products, were measured. Analysis conditions for the particles are shown in Table 6.

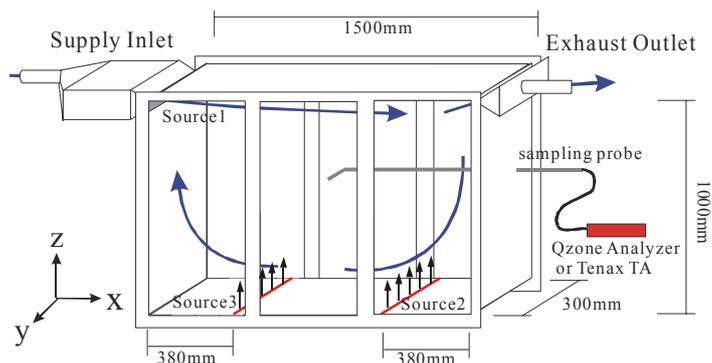


Fig. 1. Room Model

Table 2. Test Conditions

Room Model Volume	1500(x)×300(y) ×1000(z)mm
Air Inlet Velocity	$U_{in} = 2.8$ m/s
Air Change Rate	110 /h
Temperature	$23 \pm 1^\circ\text{C}$
Relative Humidity	$30 \pm 5\%$

Table 3. Cases Analyzed

Case	Source 1 [ Ozone ]	Source 2 [d-Limonene ]	Source 3 [ $\alpha$ -Pinene]
Case 1	0.87ppm	-	-
Case 2	-	0.23 mg/s	-
Case 3	-	-	0.23 mg/s
Case 4	-	0.23 mg/s	-
Case 5	0.87ppm	-	0.23 mg/s
Case 6	-	0.23 mg/s	0.23 mg/s

[Inlet Con.]                      [on the floor]

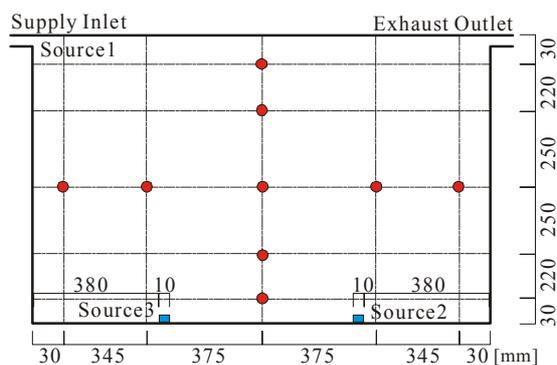


Fig. 2. Contaminant Source & Sampling Position

In order to prevent photochemical reaction of the ozone, the model experiments were carried out in dark room.

### Results of the Model Experiment

Concentration distributions in the model room for each experimental case are shown in Figure 3. In this paper, only case 1, case 2 and case 3 are shown; other cases are omitted.

In case 1 where ozone is generated in the supply

Table 4. Analysis Conditions for Ozone

Ozone Analyzer	UV Photometric Analyzer (SOZ-3300, Seki Electrons)
Meas. Range	0 - 9,999 ppm
Min. Range	0.001 ppm
Sample Flow	1.5 L/min

Table 5. Analysis Conditions for Terpenes

GC/MS	HP6890
TDS	Gestel TDS
Column	HP5 (0.25mm $\phi$ ×60m×1 $\mu$ m)
Oven Temp.	40°C(3min)→10°C/min →220°C(10min)
Detector	HP5973MSD
Sampler	Tenax TA (60/80 mesh) Sampling rate; 50mL/min, total 1L

Table 6. Analysis Conditions for Particles

Analyzer	Micro Laser Particle Counter (LPC-110, Particle Meas. Sys. Inc.)
Meas. Range	0.1, 0.2, 0.3, 0.5, 1.0, 3.0, 5.0 $\mu$ m

Table 7. Results of Particle Measurement

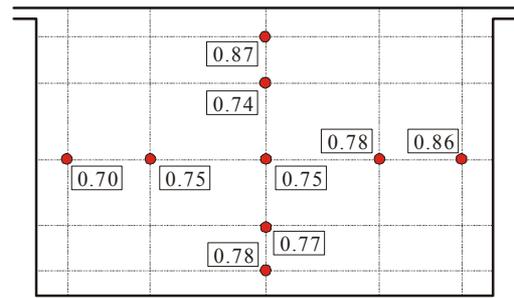
Case 1	0.1 $\mu$ m	111
	0.2 $\mu$ m	77
	0.3 $\mu$ m	19
	0.5 $\mu$ m	1
	1.0 $\mu$ m	0
Case 2	0.1 $\mu$ m	-
	0.2 $\mu$ m	-
	0.3 $\mu$ m	-
	0.5 $\mu$ m	-
	1.0 $\mu$ m	-
Case 4	0.1 $\mu$ m	375
	0.2 $\mu$ m	279
	0.3 $\mu$ m	2370
	0.5 $\mu$ m	7371
	1.0 $\mu$ m	458

(Values used to subtract background particles, [ /ft<sup>3</sup>])

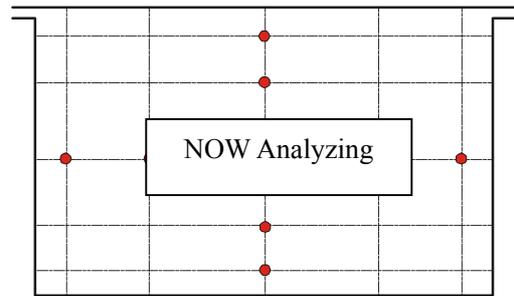
inlet (source 1), ozone is uniformly distributed in the model room if there are no decomposition and deposition on the wall surface. As shown in Figure 3 (1), ozone is not uniformly distributed and about 10% is uneven to the room averaged concentration in this experiment

In case 2 and 4, because data is being analyzed, figure is omitted now.

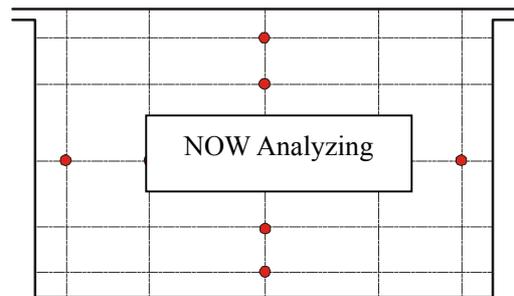
Table 7 shows the results of particle measurement in case 1 and 4.



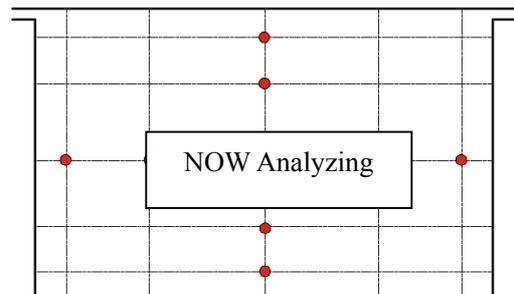
(1) Case 1 (Ozone)



(2) Case 2 (d-Limonene)



(3) Case 4 (Ozone)



(4) Case 4 (d-Limonene)

Fig. 3. Concentration Distribution by Experiment [Units: ppm]

### Outline of the Numerical Analysis

Flow fields and diffusion fields were analyzed, targeting the room model. An outline of the space analyzed is shown in Figure 1. When the air supply slot width is the representative length ( $L_0=20\text{mm}$ ), the space is a 2-dimensional room of  $75 L_0 (x) \times 50 L_0 (z)$  ( $=1500\text{mm} \times 1000\text{mm}$ ). Flow fields were analyzed using the low Reynolds type k- $\epsilon$  model [Murakami et al., 1996]. Numerical conditions are shown in Table 8. The bi-molecular reactions in the room were analyzed. In this analysis, the generation rate of ozone from

Table 8. Numerical Conditions

Turbulence Model	Low Re Type k-ε model (MKC model, 2D Cal.)
Mesh	96(x) × 70(z)
Scheme	Convection Term; QUICK
Inflow Boundary	$U_{in} = 3.0\text{m/s}$ , $k_{in} = 3/2 \times (U_{in} \times 0.015)^2$ , $\epsilon_{in} = C_{\mu} \times k_{in}^{3/2} / l_{in}$ , $C_{\mu} = 0.09$ , $l_{in} = (\text{Slot Width}; 0.02) \times 1/7$ $C_{in} (\text{ozone}) = 1.0 \text{ ppm}$
Outflow Boundary	$U_{out} = \text{free slip}$ $k_{out} = \text{free slip}$ , $\epsilon_{out} = \text{free slip}$
Wall Treatment	Velocity; No-slip $k _{wall} : \text{free slip}$ , $\epsilon _{wall} = 2\nu(\partial\sqrt{k}/\partial y)^2$ $\gamma = 20 \times 10^{-6}$ , $\langle v \rangle = 360 \text{ m/s}$
Rate Constant	Ozone; $k_u = [1/\text{h}]$ Ozone/d-Limonene; $k_b = 0.0184 [1/\text{ppb h}]$ Ozone/α-Pinene; $k_b = 0.00756 [1/\text{ppb h}]$

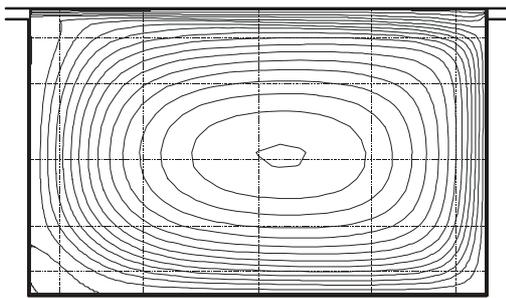


Fig. 4. Mean Streamlines (Prediction)

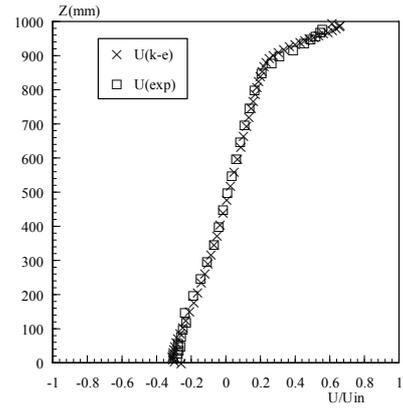
source 1, d-Limonene from source 2 and α-Pinene from source 3 were under the same conditions as in the experiment.

In this analysis, the wall surface deposition of ozone was analyzed in all analytical cases. The room temperature was assumed to be a constant 23 °C. Analysis cases are shown in Table 3. The amount of chemical pollutants generated from the contamination sources and the supply opening velocity were assumed to be representative scales, and the results of the analyses were all non-dimensional.

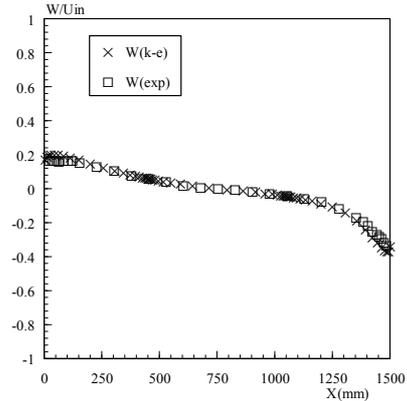
### Results of the Numerical Analysis

In this analysis, the first grid point from the wall  $\Delta z_1$  is much smaller than  $z^+ = 1$ . Here,  $z^+$  is a wall unit.

Stream lines predicted by CFD are shown in Figure 4. 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. A comparison between the CFD analysis and the experiment are shown in Figure 5. The experimental results were very consistent with the results for the



(1) Vertical profile of  $U/U_0$  ( $x=37.5L_0$  line)



(2) Horizontal profile of  $W/U_0$  ( $z=25L_0$  line)

Fig. 5. Comparison between Prediction and Experiment

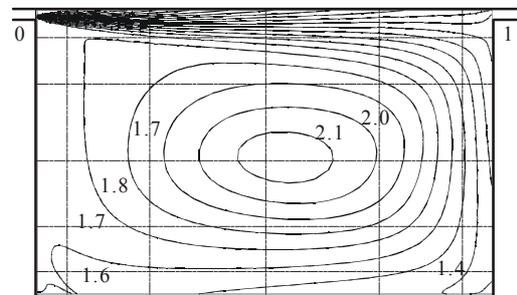


Fig. 6. Distribution of Age of Air (SVE3)

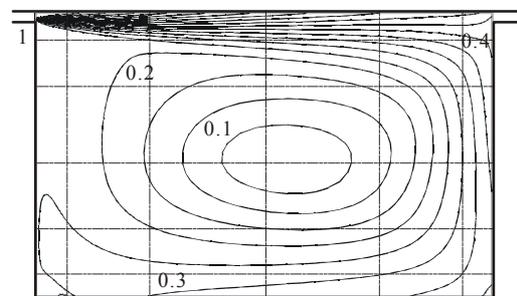


Fig. 7. Reciprocal Distribution of Age of Air (Supply Inlet; 1.0, Max Age of Air; 0.0)

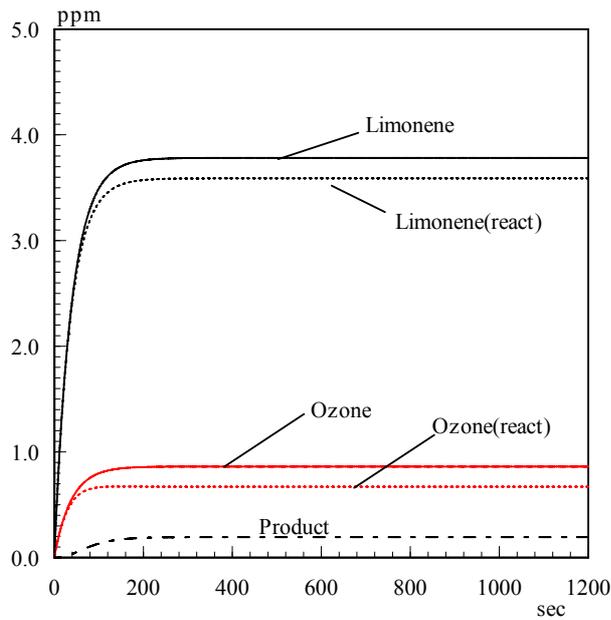


Fig. 8. Time History of the Average Concentration in Room (Prediction)

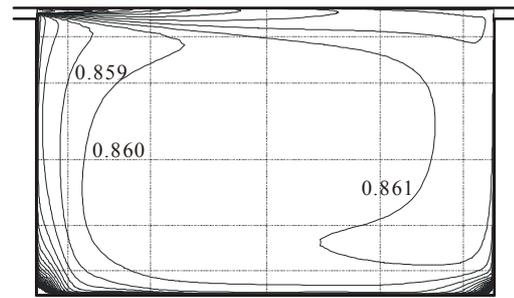
low Reynolds number-type  $k-\epsilon$  model, and it was confirmed that they analyze the flow fields with sufficient accuracy [Ito et al., 2000].

The age distribution of the air and its reciprocal distribution are shown in Figures 6 and 7 respectively. Staying time of air from the supply inlet was long in the center of the model room.

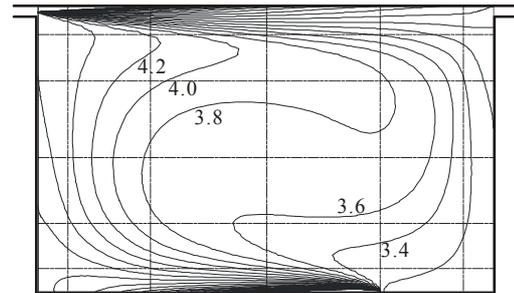
Results of the time history of the average concentration in the room in each case are shown in Figure 8. Results for cases 1 and 2, in which only contaminants sources were present, and disregarding chemical reactions, are shown together in the figure for comparison with case 4. When equations (3), (6), and (7) were assumed to apply in each case, both chemical substances ( $C_1$  and  $C_2$ ) always decreased when chemical reactions were generated in the room. Also, since  $C_{prod}$  was proportional to the second-order rate constant  $k_b$  [1/ppb·h],  $C_{prod}$  always increased when chemical reactions were generated in the room. In case 4 in particular, the room averaged concentration of ozone and d-Limonene are decreased by about 20%, and  $C_{prod}$ , which is the same amount of reduction, generates by the chemical reaction. The chemical reactions were an important factor in constituting the room VOC concentration.

The VOC concentration distributions in the room are shown in Figure 9. This report shows case 1, case 2, and case 4, and omits the remaining cases. The concentration distributions were plotted up to 1200 seconds after computations began.

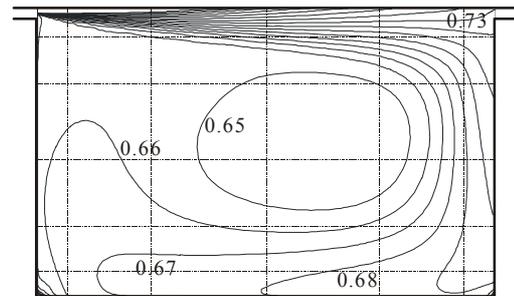
In case 1 as shown in Figure 9 (1), since the reductions in the ozone concentration in the room were approximately 2% in cases that considered the effects of ozone deposition on the solid walls, there was almost no change in the room concentration dis-



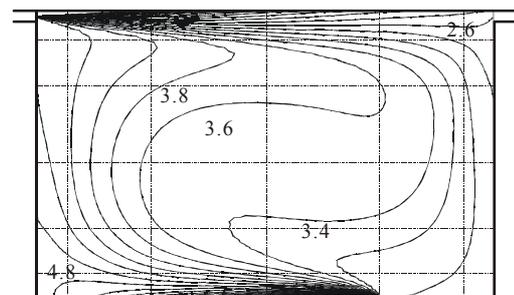
(1) Case 1 (Ozone)



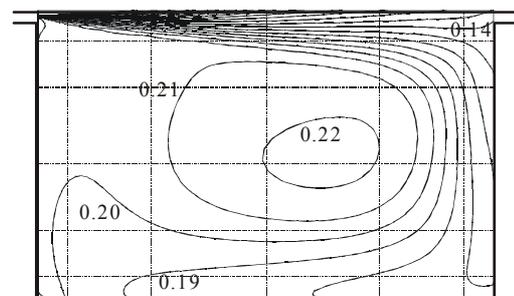
(2) Case 2 (d-Limonene)



(3) Case 4 (Ozone)



(4) Case 4 (d-Limonene)



(5) Case 4 ( $C_{prod}$ )

Fig. 9. Concentration Distribution Predicted by CFD [Units: ppm]

tribution compared to cases that did not consider the effects of deposition. Conceptually, ozone is uniformly distributed in the model room if there are no decomposition and deposition on the wall surface.

In case 2 as shown in Figure 9 (2), since a large clockwise circulating flow was formed in the room, contaminants generated from the contamination sources 2 were transported along the floor and left wall forming a concentration distribution in the room.

In case 4, which incorporated chemical reactions with ozone and d-Limonene, the room concentration of ozone and d-Limonene decreased. Also, the reaction product  $C_{prod}$  became highly concentrated near source 2 on the floor and the center of the room where both ozone and d-Limonene became highly concentrated.

### Considerations

The chemical reaction models used in the analyses were based on the rate constants. In these models, the concentration of the reaction product  $C_{prod}$  was simply proportional to the second-order rate constant  $k_b$  and also to the concentrations of contaminants  $C_1$  and  $C_2$ . In other words, these analyses were targeted exclusively under conditions where rate constants apply, and the range of application of the model needs further consideration.

### Concluding Remarks

- (1) In order to discuss the order of chemical reaction, the concentration distributions of ozone and terpenes in the model room were measured in cases with and without a chemical reaction.
- (2) In the experimental case, which incorporated chemical reactions with ozone and d-Limonene, the room concentration of ozone and d-Limonene decreased and particle generation was confirmed.
- (3) Chemical reaction equations were modeled in a simple manner by using rate constants, and were coupled with CFD analysis.
- (4) As a result of estimating the amount of chemical reaction and VOC concentration distribution in the room, using ozone and terpenes, under conditions in which rate constants apply, it was estimated that the room averaged concentration of ozone and d-Limonene are decreased by about 20% in this analytical condition.
- (5) As a result of conducting analyses coupled with models for ozone deposition onto solid wall surfaces using the deposition velocity, it became clear that the effects of reductions in the room concentration were relatively small compared to the amount of chemical reaction and elimination by ventilation.

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