Coupled Analysis of TVOC Emission and Diffusion in a Ventilated Room by CFD

Shuzo Murakami[1], Shinsuke Kato[2], Kazuhide Ito[3]

Institute of Industrial Science, University of Tokyo
7-22-1, Roppongi, Minato-ku, Tokyo 106-8558, Japan
[1] murakami@iis.u-tokyo.ac.jp, [2] kato@iis.u-tokyo.ac.jp, [3] kazuhide@cc.iis.u-tokyo.ac.jp

ABSTRACT

This paper presents an analysis of the emission of chemical compounds and their diffusion in a room by the technique of computational fluid dynamics. A polypropylene styrene-butadiene rubber (SBR) plate was chosen as the TVOC emission source. The emission rate and room-averaged concentration are analyzed under various conditions of ventilation rate and temperature. Further, the concentration distribution of TVOC within a room is also examined and evaluated from the viewpoint of ventilation efficiency.

KEYWORDS

CFD, TVOC, Emission, Diffusion, Ventilation, Airing

INTRODUCTION

A method for predicting the distribution of chemical pollutants in a room in which they are generated is investigated. Indoor air quality is greatly affected by the emission of chemical compounds from building materials. In this paper, the emission of such compounds and their diffusion in a room are analyzed by a computational fluid dynamics (CFD) technique. Here, TVOC (total volatile organic compounds) emission from a floor covered with polypropylene styrene-butadiene rubber plate is examined.

Many factors affect the concentration of chemical pollutants within a room, as shown in Fig. 1. These include chemical reactions within the source material and the room air, adsorption and desorption, temperature, ventilation rate, etc., [1]. The final goal of this study was to predict the concentration of chemical pollutants in air inhaled by the occupants of a room, taking into account the pollutant generation processes. In this paper, a CFD technique is applied for this purpose.

The modeling methods for describing TVOC emission may be classified into two groups, experimental and physical. Experimental methods are based on curve-fitting of experimental data obtained from small-scale chamber tests, etc., [2]. The latter, physical methods, take into account the elemental mass transfer processes of source materials, both internally and at their surfaces [3]. Physical methods are generally superior to experimental ones from the viewpoint of accuracy and generality

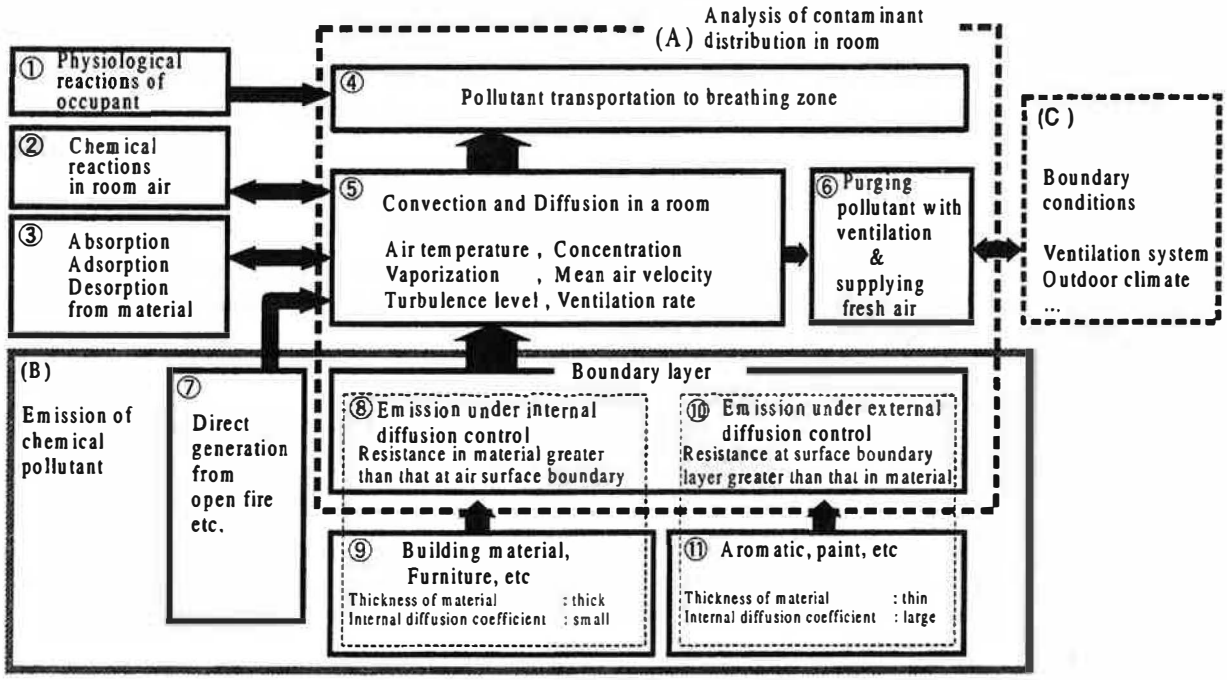


Fig. 1 Mechanism of transport and diffusion of chemical pollutant within a room

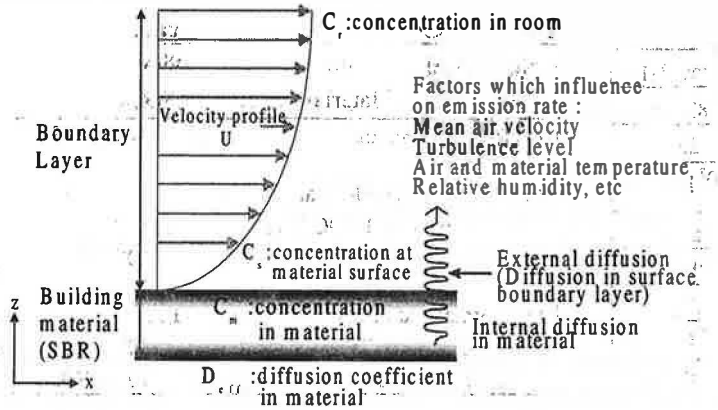


Fig. 2 Modeling of TVOC emission at material surface

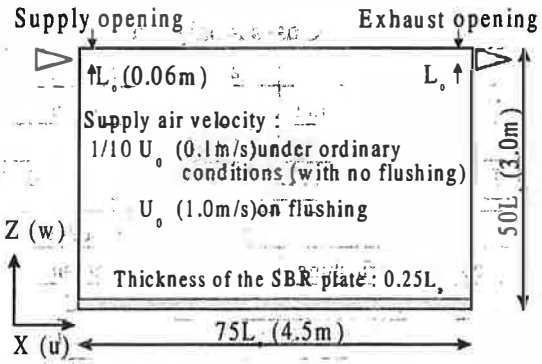


Fig. 3 Room model analyzed (2D)

as regards adaptation to various conditions. Here, we use physical methods [4,5]. In applying physical methods, TVOC emission from source materials is classified into two types, one being emission under the control of internal diffusion, the other being that under the control of external diffusion (at a surface boundary) as shown in Fig. 1. In this paper, emission under the control of internal diffusion is studied.

MODEL OF TVOC EMISSION AND DIFFUSION

TVOC emission and diffusion processes, i.e., the emission and diffusion of various chemical compounds, are virtually substituted by the process of applying them to one representative compound. TVOC was selected as this virtual representative compound in the present case [4-7].

Internal diffusion in materials

The mechanism of the diffusion process is modeled as shown in Fig. 2. It is assumed that the internal diffusion of TVOC in the solid material is governed by a one-dimensional diffusion equation, as shown in Eq. (1). Here, the equivalent air phase concentration (C) is used to express the source phase (solid phase) concentration and the diffusion process[4,5]. The TVOC effective diffusion coefficient (D_{eff}) and initial concentration distribution ($C_0(z)$) in materials are estimated from experimental data obtained by small-scale chamber tests (cf. Appendix A).

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial z}\left(D_{eff}\frac{\partial C}{\partial z}\right) \tag{1}$$

Here, D_{eff} is the effective diffusion coefficient of TVOC in a material [m^2/s], and C is the equivalent air phase concentration of TVOC in the material [$\mu g/m^3$].

Solid-air interface

The TVOC emission rate at the mate ial surface is set at the same value as the transportation rate by internal diffusion. This condition is expressed as the conservation law at the surface, as shown in Eq. (2)

$$-D_{eff}\frac{\partial C}{\partial z}\Big|_{w.s.+}=-Da\frac{\partial C}{\partial z}\Big|_{w.s.-} \tag{2}$$

Here, w.s.+ is the wall surface in the material region, and w.s.- is that in the air region; D_a is the molecular diffusion coefficient in air [m^2/s]; C is the equivalent air phase concentration of TVOC on the material side and also that on the air side [$\mu g/m^3$].

Transportation in room air

Emitted TVOC is transported by the room air flow, diffused by molecular diffusivity (D_a) and turbulent diffusivity (ν_t/σ), and then expelled through an exhaust opening, as shown in Eq. (3) (cf. Fig. 3).

$$\frac{\partial C}{\partial t}+\frac{\partial(u_i C)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\left(Da+\frac{\nu_t}{\sigma}\right)\frac{\partial C}{\partial x_j}\right) \qquad \nu_t \text{ (turbulence eddy viscosity)},\ \sigma : 1.0. \tag{3}$$

Table 1 Cases Analyzed

	case1-1	case2-1	case3-1
Hours of air flushing	-	1h/24h	8h/24h
Temperature	23℃	23℃	23℃
D_{eff} : 1.1×10^{-14} m²/s, Da : 5.9×10^{-6} m²/s, C_0 : 1.92×10^{8} μg/m³			

	case1-2	case2-2	case3-2
Hours of air flushing	-	1h/24h	8h/24h
Temperature	30℃	30℃	30℃
D_{eff} : 4.2×10^{-14} m²/s, Da : 6.2×10^{-6} m²/s, C_0 : 1.92×10^{8} μg/m³			

Inflow velocity with no flushing : U_{in}=1/10 U_0=0.1m/s
Inflow velocity at Flushing : $U_{in}=U_0$=1.0m/s

Table 2 Conditions for numerical analysis

Number of grid points	Air region	: 68(x)×64(z)
	Material region	: 68(x)×7(z)
(1) Reynolds number		: $U_0L_0/\nu = 4.2\times10^3$
(2) Normalized molecular diffusivity of TVOC in air		: D_a/U_0L_0 = 9.8×10^{-5} (23℃) 1.0×10^{-4} (30℃)
(3) Normalized diffusion coefficient of TVOC in the material :		: $D_{eff}\cdot T_0/L_0^2$ = 1.8×10^{-13} (23℃) 7.0×10^{-13} (30℃)

FLUSHING

Contaminated oom air can be flushed by airing or by ventilation at a greater air change rate. In this study, the effect of regular flushing (increase in ventilation rate once a day) is investigated. The daily pattern of this intermittent increase in ventilation rate is called 'flushing' in this paper.

ROOM MODEL AND TVOC SOURCE ANALYSIS

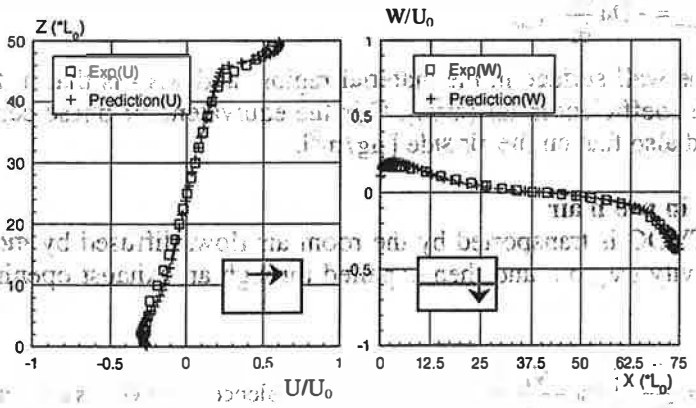
The room model shown in Fig. 3 is used for analyzing the emission, diffusion and flushing of TVOC. The room model has dimensions of (x) × (z) = 75 L_0 × 50 L_0 (= 4.5m × 3.0m; L_0 = 0.06m = width of supply inlet). As the TVOC source, a polypropylene styrene-butadiene rubber (SBR) plate ($0.25L_0$ hick) was adopted. The emission rate is strongly related to both the initial concentration distribution ($C_0(z)$) and the effective diffusion coefficient (D_{eff}) within the SBR. Thus, it is very impo tant to evaluate accurately the set of $C_0(z)$ and D_{eff} in the source material. In this paper, the initial TVOC concentration distribution in SBR is assumed to be uniform, $C_0 = 1.92\times10^8$ μg/m³, and the effective diffusion coefficient D_{eff} to be 1.1×10^{-14} m²/s (at 23℃) and 4.2×10^{-14} m²/s (at 30℃), in accordance with Yang et al. [5] (cf. Appendix A).

NUMERICAL METHODS AND BOUNDARY CONDITION

Flow fields were analyzed with a low Reynolds number k- ε model (MKC model) with an inflow velocity of 1/10 U_0 (= 0.1 m/s; air change rate = 1.6 h^{-1}) under ordinary conditions (with no flushing) and U_0 (= 1.0 m/s; air change rate = 16 h^{-1}) on flushing [8]. An upwind scheme was used for the convection term, and a centered difference scheme for the diffusion term. Using the results of flow field simulations, emission and diffusion fields were analyzed. In the emission and diffusion analysis, time-dependent Eqs. (1) and (3) were solved by coupling Eq.(2). Table 1 shows the cases analyzed. Six cases were examined in total, under differ nt conditions of inflow velocity and material temperature. The p ofile of room air concentration was obtained over a duration of 2.0×10^7 T_0 (T_0 ; representative time scale defined by L_0/U_0, 14 days).

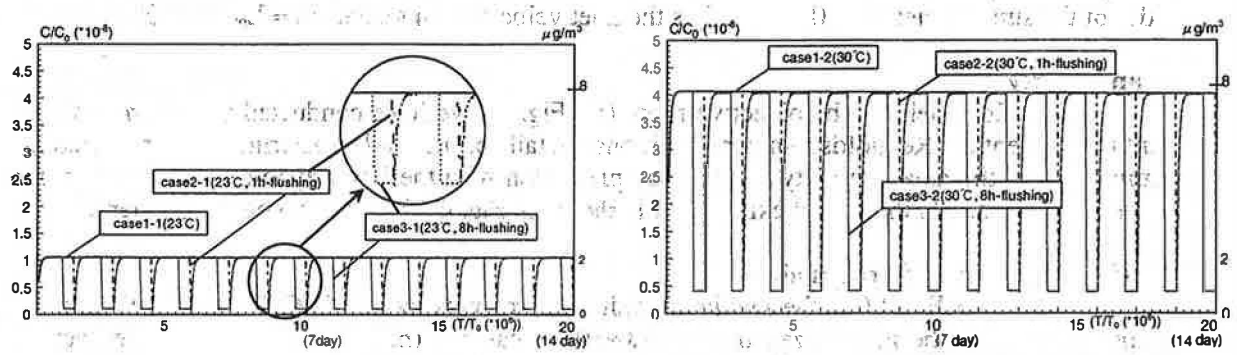
RESULTS AND DISCUSSION

All results are shown as dimensionless values, with division by the representative values C_0, L_0,



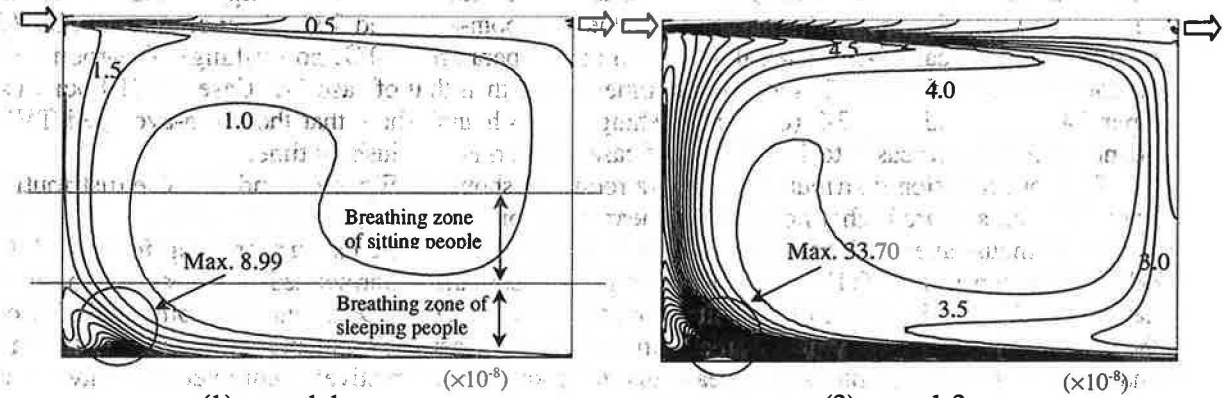
(1) Vertical profile of U/U_0 ($x=37.5L_0$ line) (2) Horizontal profile of W/U_0 W ($z=25L_0$ line)

Fig. 4 Flow field comparison between prediction and experiment



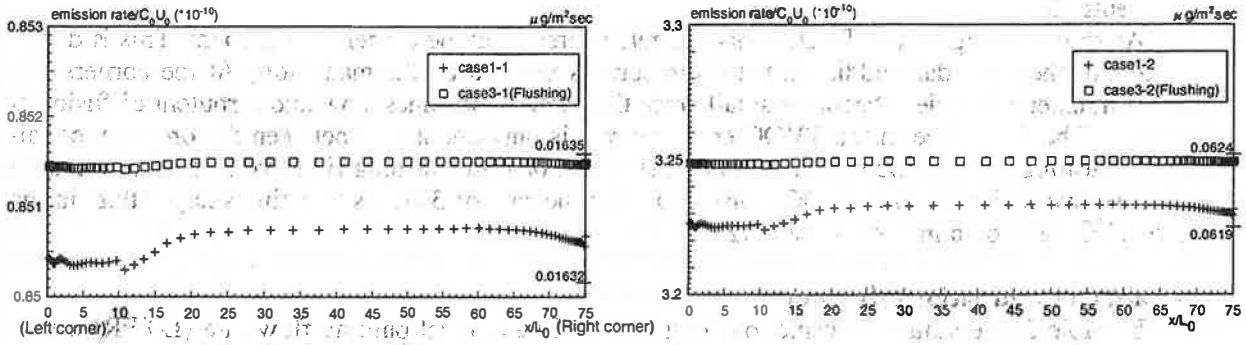
(1) cases of 23℃ (2) cases of 30℃

Fig. 5 Time profile of room-averaged concentrations



(1) case1-1 (2) case1-2

Fig. 6 TVOC concentration C/C_0 (at $T/T_0=7.2\times10^6$(5 days))



(1) cases of 23℃ (2) cases of 30℃

Fig. 7 TVOC emission rate from SBR floor (at $T/T_0=7.2\times10^6$ (5 days))

(Horizontal axis indicates position of the floor, cf. Fig. 3)

Table 3 Analysis of ventilation efficiency (at $T/T_0=7.2\times10^6$ (5 day))

case1-1	Averaged concentration	Visitation frequency	Local purging flow rate
Breathing zone of Sitting people ($8.3\,L_0$ (0.5m)<z< $25L_0$ (1.5m))	1.1×10^{-8}	8.1	0.63
Breathing zone of sleeping people (z<$8.3\,L_0$ (0.5m))	1.2×10^{-8}	3.6	0.56

(Averaged concentration is normalized by C_0, L-PFR is normalized by inflow rate of ventilation)

and U_0. C_0 represents the initial TVOC concentration in the material ($1.92\times10^8\,\mu g/m^3$), L_0 is the width of the supply inlet slot (0.06m), U_0 is the inlet velocity (1m/s), and $T_0 = L_0/U_0$ (0.06sec).

Mean velocity

For the flow field of the objective room (cf. Fig. 3), we have conducted precise model experiment under identical Reynolds number conditions. Details of the model experiment are reported in [9]. Comparison of the mean velocity obtained by prediction with the low Reynolds number k- ε model and results obtained in the model experiment is shown in Fig. 4. They are in good agreement.

TVOC concentration in room air

As shown in Fig. 5(1), the maximum value for room-averaged TVOC concentration (C_{max}/C_0) reaches 1.1×10^{-8} at the normalized time of 1.0×10^6 in case1-1 (material and room air temperature : 23℃, no flushing). The computation was started with an initial condition of zero concentration within the room. The room-averaged TVOC concentration is almost constant over a duration of 2.0×10^7 (14 days). Case 2-1 (1-hour flushing per 24 hours) and case 3-1 (8-hours flushing per 24 hours) show that room-averaged TVOC concentrations decrease to 1/10 of case 1-1 (no flushing) during the flushing time. As shown in Fig. 5(2), the maximum value for room-averaged TVOC concentration (C_{max}/C_0) reached 4.1×10^{-8} in case 1-2 (material and room air temperature : 30℃, no flushing). The room averaged concentration of case 1-2 is about four times larger than that of case 1-1. Case 2-2 (1-hour flushing per 24 hours) and case 3-2 (8-hours flushing per 24 hours) show that the room-averaged TVOC concentration also decreases to 1/10 of that of case 1-2 during the flushing time.

The concentration distributions within a room are shown in Fig. 6 (1) and (2). The distributions are not uniform, and are highly non-uniform near the floor.

The exhaust-averaged concentration of TVOC (C_{ex}/C_0) at the exhaust opening for case 1-1 is 0.7×10^{-8} as shown in Fig. 6(1). The room-averaged concentration normalized for concentration at the exhaust (SVE1, [10]) is 1.5 for the condition used here, in which TVOC is emitted from the SBR floor. If the room air were perfectly mixed, the room-averaged concentration would necessarily be the same as that at the exhaust. A value of 1.5 means that the room is not effectively ventilated compared to the case in which the air is perfectly mixed.

TVOC emission rate

As shown in Fig. 7, the TVOC emission rate decreases at the corners of the room. This is due to the effect of the secondary eddies at the room corners induced by the main flow. At the corners, the material transfer coefficient becomes small since the velocity becomes slow and turbulent diffusion is not active. The difference in the TVOC emission rate is only about 1 % between the ordinary condition (no flushing, inlet velocity; $1/10U_0$) and the condition with flushing (inlet velocity; U_0) for each case, as shown in Fig. 7. The TVOC emission rate in the case of 30℃ is four times larger than in the case of 23℃, as shown in Fig. 7(1) and (2).

Evaluation of ventilation efficiency

In Table 3, the values of visitation frequency (VF) and local purging flow rate (L-PFR) are illustrated. These are the new scales for ventilation performance (cf. Appendix B). VF represents the number of times a contaminant passes through the local domain in question [12]. It indicates how effectively the exhaust opening eliminates pollutants. A higher value of VF means that elimination of a pollutant is not effective, and that the emitted pollutant revisits the local domain in question many times. L-PFR is an index of ventilation efficiency in a local domain. It was originally defined as the effective airflow rate necessary for the removal / purging of contaminants from the local domain [13]. Here, the breathing zones are defined as the local domains. The breathing zones in which VF and L-PFR are evaluated in this study are shown in Fig. 6.

The TVOC generated from the SBR floor return 8.1 times to the breathing zone of sitting people, and 3.6 times to the breathing zone of sleeping people in case 1-1, as shown in Table 3. For the ideal case involving the most efficient ventilation, the value of VF would be 1. In this context, the combination of the position of the exhaust outlet and the room airflow here is not efficient in eliminating the TVOC emitted from the floor. The effective airflow rate necessary to remove / purge the TVOC is 63% of the air flow rate of ventilation in the breathing zone of sitting people and 56% of that in the breathing zone of sleeping people. The present low L-PFR means that the air supplied into the room does not efficiently dilute the TVOC emitted from the floor in either zone. The remaining 37% or 44% of the air supplied does not contribute to dilution of the TVOC and by-passes the zone in question in this room air flow situation. There should be a more efficient way (e.g., positioning of the exhaust outlet) of diluting and exhausting the TVOC emitted from the floor region in this room configuration.

Discussion

Compared with the normalized characteristics time for internal diffusion (= $\{(0.25)^2 L_0/D_{eff}\}/T_0$, 0.25 : normalized SBR thickness; $T_0=L_0/U_0$), the analyzed duration and the flushing time are too short. The normalized characteristics time for internal diffusion is in the order of 3.5×10^{11} (680 years) whereas the analyzed duration is in the order of 2.0×10^{7} (14 days) and the flushing time is in the order of 6.0×10^{4}(1h) and 4.8×10^{5}(8h). This large value for the time scale (680 years) is obtained from the small value of D_{eff} estimated [5] and the relatively large value for thickness of SBR (0.015m) used here. If the thickness of SBR becomes 1/10, the time scale becomes 1/100 (6.8 years). If the D_{eff} becomes 1/1,000 (cf. Appendix A), the time scale becomes 1/1,000 (0.68 years). Here, the normalized characteristics time for internal diffusion is defined using the length scale of width of SBR ($0.25L_0$). Flushing well decreases the averaged concentration of TVOC in the room only during the flushing time. However this is only very short, and thus it does not effectively affect the emission rate or room-averaged concentration of TVOC during and after flushing. On the other hand, the TVOC emission rate strongly depends on the material temperature.

In all cases analyzed, the TVOC concentrations near the SBR floor are eight times higher than the room-averaged TVOC concentrations, as shown in Fig. 6. This means that an infant, a child, or a person sleeping on the floor, is exposed to a higher TVOC concentration. The averaged TVOC concentration in the breathing zone of standing people (C_{ave}/C_0, $z=25L_0$) is about 1.1×10^{-8}, whereas that for sleeping people is about 8.0×10^{-8} in case 1-1.

CONCLUDING REMARKS

(1) In this analysis, the room-averaged TVOC concentration is almost constant during the duration of simulation (14 days). This is because the duration of the simulation is very short compared to the characteristic time of internal diffusion, which is in the order of 3.5×10^{11} (680 years).

(2) Since the flushing time (in the order of hours) is much shorter than the characteristic time for internal diffusion (in the order of years), flushing is effective only during the flushing time.

(3) The TVOC emission rate in the case of 30℃ is four times larger than that in the case of 23℃.

(4) The concentration of TVOC near the SBR floor, from which the TVOC are emitted, is eight times larger than the room-averaged value.

(5) In this analysis, the TVOC generated by the SBR floor are returned 8.1 times to the breathing zone of people sitting in the room before they are eliminated.

Nomenclature

L_0 : width of supply opening, 0.06m
U_0 : supply velocity, 1m/s
T_0 : representative time = L_0/U_0
D_{eff} : TVOC effective diffusion coefficient in material [m^2/s]
D_a : TVOC diffusion coefficient in air [m^2/s]
C : TVOC concentration in air phase and in equivalent air phase concentration in material [$\mu g/m^3$]
$C_0(z)$: initial TVOC concentration in SBR floor [$\mu g/m^3$] (defined as equivalent air phase concentration)
C_0 : estimated value of $C_0(z)$ uniformly as 1.92×10^{8} $\mu g/m^3$ (cf. [5])
C_{max} : maximum value of room-averaged concentration [$\mu g/m^3$]
C_{ext} : averaged concentration at exhaust opening
C_{ave} : averaged concentration in objective local domain
J_p : amount of pollutant visiting (returning to) the local domain (p) per unit time [$\mu g/s$]
M_p : amount of pollutant generated in the local domain [$\mu g/s$]
Δq_p : rate of inflow of pollutant into the local domain (p) per unit time [$\mu g^3/s$]
q_p : pollutant generation rate per unit time [$\mu g/s$]
L-PFR : local purging flow rate [m^3/s]
V_{domain} : volume of objective local domain [m^3]
VF : visitation frequency of pollutant [-]
T_p : average staying time of pollutant in the local domain (p) [sec /one stay]
q_p : pollutant generation rate per unit time [$\mu g/s$]
C_{domain} : average concentration in the domain in question [$\mu g/m^3$]

Appendix A

In this paper, the initial TVOC concentration ($C_0(z)$) in the material and the effective diffusion coefficient (D_{eff}) in the material are given in accordance with the estimate of Yang et al [5]. These

authors carried out a numerical simulation of the TVOC emission process within a small test chamber, and then tuned $C_0(z)$ and D_{eff} to obtain the same decay curve of pollutant concentration as in the experiment. The diffusion coefficient (D_{eff}) is estimated under the condition in which the initial concentration ($C_o(z)$) in the material is almost uniform (3 days after produced ; according to Yang et al).

Since the emission rate is expressed as the product of concentration gradient ($\partial C_0(z)/\partial z$ in the material) and the diffusion coefficient, there is a possibility that various sets of D_{eff} and $\partial C_0(z)/\partial z$ can be fitted to the experimental results of emission rate. Fig. 8 illustrates an example which shows that we can obtain another set of $C_0(z)$ and D_{eff} different to those given by Yang et al. This new set of D_{eff} and $C_0(z)$ gives the same emission rate as that given by Yang et al. Here, the diffusion coefficient (D_{eff}) is 1,000 times larger than that estimated by Yang et al., and the initial concentration distribution ($C_o(z)$) is not uniform, as shown in Fig. 8. Fig. 9 shows the time profile of the concentration at the exhaust opening simulated using the room model of this study (Fig. 3). Both sets of D_{eff} and $C_0(z)$ give the same profile of exhaust concentration, i.e., the same history of emission rate, as shown here. In this study, since we have no further experimental data or knowledge concerning these values, we used those estimated by Yang et al. We believe that it is essential to develop a technique to obtain a proper combination of the diffusion coefficient (D_{eff}) and the initial concentration ($C_o(z)$) from experimental data for the emission rate.

Appendix B

VF (visitation frequency) represents the number of times a pollutant passes through a local domain. VF = 1 means that a pollutant stays only once in a local domain after being generated. In other words, it never returns after leaving the local domain. VF = 2 means that a pollutant stays in a local domain just after its generation, is then transported away, but returns once to the local domain in question due to the re-circulating flow. The average VF for all pollutants is an important index which indicates how efficient a ventilation system is in purging / removing pollutants from a local domain. From the viewpoint of the entire flow field in a room, a low value for average VF indicates a good ventilation design for a local domain, because fewer pollutants are returning to it. VF is calculated by Eq. (4).

$$VF = 1 + (J_p/M_p) = 1 + (\Delta q_p/q_p) \quad (4)$$

Here, J_p is the amount of pollutant visiting (returning to) the local domain (p) per unit time [μg /s]; M_p is the amount of pollutant generated in the local domain [μg /s]; Δq_p is the rate of inflow of pollutant into the local domain (p) per unit time [μg /s]; and q_p is the pollutant generation rate per unit time [μg/s].

The L-PFR (local purging flow rate) is an index of ventilation efficiency in a local domain, such as a breathing zone or a confined space in a room. It was originally defined as the effective airflow rate required to remove/ purge contaminants from a local domain. L-PFR indicates the degree of ability to purge contaminants from the domain in question. L-PFR is defined by the contaminant generation rate in the local domain and the averaged concentration within it. Consequently, the value of L-PFR can simply be calculated from the concentration simulation based on the scalar transport equation. L-PFR is calculated from Eq. (5).

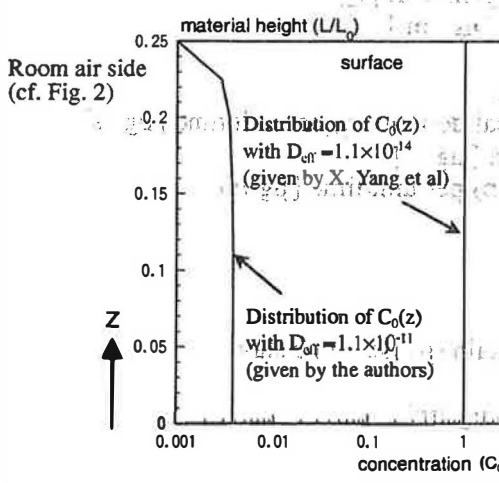


Fig. 8 Initial concentration distribution in material (C_0 : $1.92 \cdot 10^8$ μg /m^3, Both sets of D_{eff} and $C_0(z)$ give same emission rate as shown in Fig. 9.)

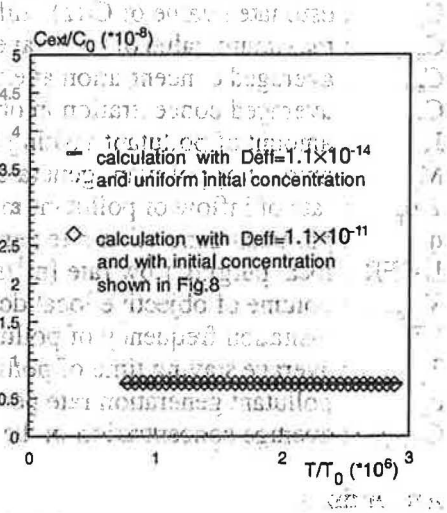


Fig. 9 Time profile of concentration at exhaust opening

$$\text{L-PFR} = V_{domain}/(VF \cdot T_p) = q_p/C_{domain} \quad (5)$$

Here, V_{domain} is the volume of the objective local domain [m^3]; T_p is the average staying time of pollutant within the local domain (p) [sec/one stay]; q_p is the pollutant generation rate per unit time [$\mu g/s$]; and C_{domain} is the average concentration [$\mu g/m^3$].

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