

Coupled Analysis of Emission, Sorption and Diffusion of Chemical Pollutants in Ventilated Room by CFD

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ABSTRACT

This paper presents an analysis of emission/sorption of chemical compounds from building materials and their diffusion in a room by a technique of computational fluid dynamics. A polypropylene styrene-butadiene rubber (SBR) floor plate is chosen as the VOCs emission source. Sorptive surface is arranged at walls. The emission rate, adsorptive amount, room-averaged concentration and their distributions in the room are analyzed under various conditions, in particular ventilation rate and sorptive effect.

INTRODUCTION

A method for predicting distribution of chemical pollutants in a room in which they are emitted and adsorbed/desorbed is investigated. Indoor air quality is greatly affected by the emission/sorption of chemical compounds from building materials [1-5]. In this paper, the emission and sorption of such compounds and their distribution in a room are analyzed by a computational fluid dynamics (CFD) technique. Here, VOCs (volatile organic compounds) emission from the floor covered with polypropylene styrene-butadiene rubber (SBR) plate is examined. Sorptive surfaces are arranged at the walls. It is assumed that the composition ratio of VOCs does not change and a virtual VOC species which represents the total property of VOCs emitted into the air is used in this study. The virtual VOC is defined as representative VOC (or simply VOCs) in this paper [6].

Many factors affect the concentration of chemical pollutants within a room, as shown in Fig. 1. These include emission, sorption (adsorption/desorption), ventilation rate, chemical reactions within the source material and the room air, etc. [1-7]. The final goal of this study is to predict the concentration of chemical pollutants in the air inhaled by the occupants in a room, taking into account all the factors shown in Fig. 1. In this paper, emission under the control of internal diffusion and adsorption/desorption on the side walls are studied, using CFD technique.

MODEL OF EMISSION, DIFFUSION AND SORPTION EFFECT OF VOCs

The emission, diffusion and sorption processes of various VOCs, are virtually substituted by those processes of one representative compound. Representative VOC (hereafter simply VOCs) is defined as this virtual representative compound of various VOCs in the present study [6].

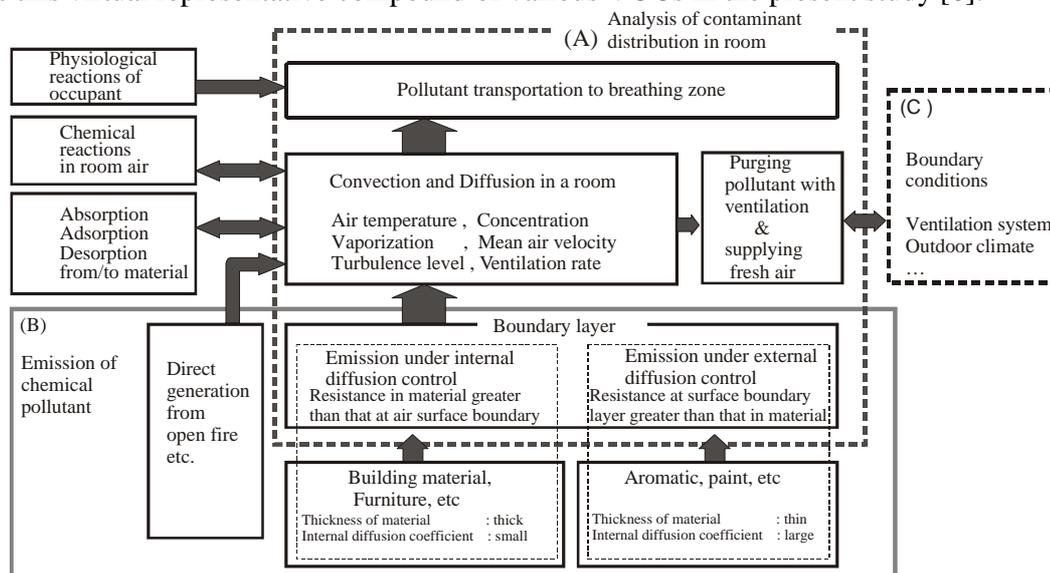


Fig. 1 Mechanism of transport, emission/sorption and diffusion of chemical pollutant within a room

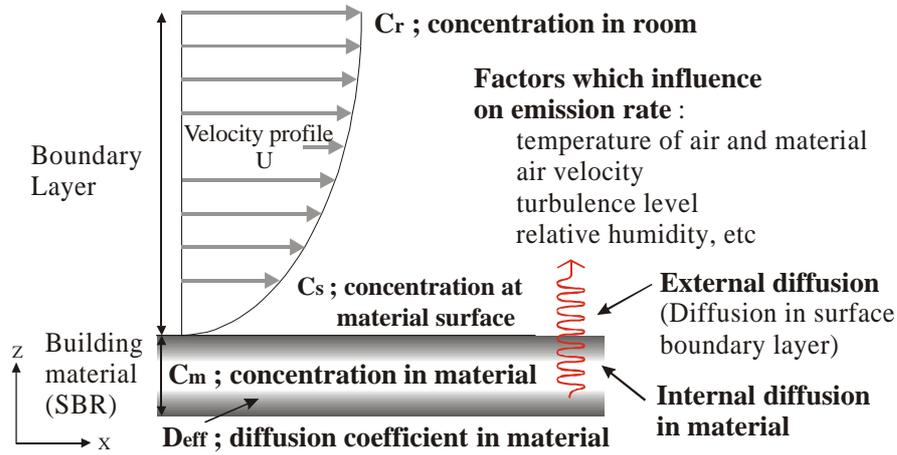


Fig. 2 Modeling of VOCs emission at material surface

Modeling for emission

[1] 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 VOCs in the emission source material (here SBR floor, cf. Fig. 3) 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 [8].

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

Here, D_{eff} is the effective diffusion coefficient of VOCs in a material [m^2/s], C is the equivalent air phase concentration of VOCs in the material [$\mu\text{g}/\text{m}^3$]. In this modeling, the adsorption/desorption by the emission source material itself is implicitly considered by introducing the equivalent air phase concentration and the effective diffusion coefficient [8, 9].

[2] Solid-air interface

The VOCs emission rate at the material 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)

$$-D_{\text{eff}} \frac{\partial C}{\partial z} \Big|_{\text{w.s.}+} = -D_a \frac{\partial C}{\partial z} \Big|_{\text{w.s.}-} \quad (2)$$

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

Modeling for sorption

In this study, the sorptive material is arranged at the side walls, as shown in. Fig. 3. It is assumed to be plane and thickless here. The internal diffusion in the sorptive material is neglected.

[1] Transportation at sorption surface

VOCs near the sorptive surface is governed by Eq. (3).

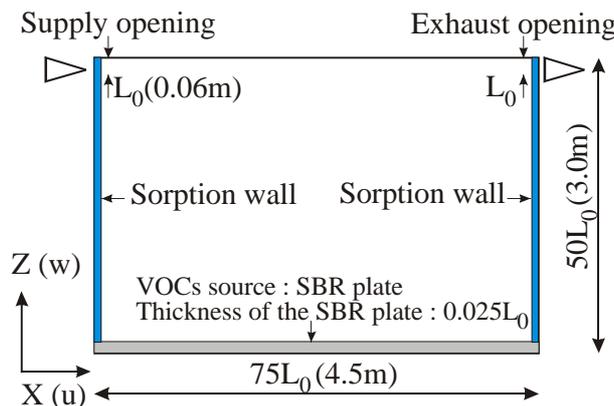


Fig. 3 Room model analyzed (2D)

$$\rho' \frac{\partial M}{\partial t} = \text{ads} \quad (3)$$

Here, M is the amount of VOCs adsorbed/desorbed by the sorptive material [$\mu\text{g}/\text{kg}$]; ads is the adsorption/desorption velocity (positive/negative values of ads means the adsorption /desorption velocities respectively) [$\mu\text{g}/\text{m}^2 \text{ s}$]; ρ' is the plane density of the sorption material [kg/m^2].

[2] Sorption isotherm model

$$M = f(C/\rho) \quad (4)$$

Here, ρ is the air density [kg/m^3]; $f(C/\rho)$ is the sorption isotherm model. In this paper, we adopt the Henry's model (linear model [10]), which is expressed by Eq. (5). This model is pretty crude and limited for use.

$$M = f(C/\rho) = k_h \cdot (C/\rho) \quad (5)$$

From Eqs. (3) and (5), Eq (6) is introduced.

$$\text{ads} = \rho' \frac{\partial M}{\partial t} = \rho' k_h \frac{\partial(C/\rho)}{\partial t} = k_h (\rho'/\rho) \frac{\partial C}{\partial t} \quad (6)$$

Here, k_h is the Henry's coefficient [-]. Adsorption/desorption is coupled with the VOCs concentration in room air as shown in Fig. 6.

[3] Sorption-air interface

The sorption rate (velocity) controls the diffusion processes at the air interface. The molecular diffusion at the surface is set at the same with the sorption rate.

$$-\text{ads} = -D_a \frac{\partial C}{\partial x} \Big|_{\text{w.s.}} \quad (7)$$

Here, w.s.- is the wall surface in the air-side region.

Transportation in room air

Emitted VOCs is transported by the room air convection, diffused by molecular diffusivity (D_a) and turbulent diffusivity (v_t/σ), and then expelled through an exhaust opening, as shown in Eq. (8) (cf. Fig. 3).

$$\frac{\partial C}{\partial t} + \frac{\partial(u_i C)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(D_a + \frac{v_t}{\sigma} \right) \frac{\partial C}{\partial x_j} \right) \quad (8)$$

Here, v_t is the turbulence eddy viscosity; σ is the plandtl number of VOCs (=1.0). Velocity u_i is given by solving Navier-Stokes equation.

FLUSHING

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

ROOM MODEL AND VOCs SOURCE ANALYSIS

The room model (2D) shown in Fig. 3 is used for analyzing the emission/sorption, diffusion and flushing of VOCs. The room model has dimensions of $(x) \times (z) = 75 L_0 \times 50 L_0$ ($= 4.5\text{m} \times 3.0\text{m}$; $L_0 = 0.06\text{m}$ = width of supply inlet). As the VOCs source, a polypropylene styrene-butadiene rubber (SBR) plate ($0.025L_0$ thick) was adopted at the floor. 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. In this paper, the initial VOCs concentration distribution in SBR is assumed to be uniform, $C_0 = 1.92 \times 10^8 \mu\text{g}/\text{m}^3$, and the effective diffusion coefficient D_{eff} to be $1.1 \times 10^{-14} \text{ m}^2/\text{s}$ (at 23 °C), following Yang, X., Chen, Q., and Bluysen, P. M. [9]. The sorption varies greatly with various adsorptive materials. In this study, sorption factor $\{k_h \cdot (\rho'/\rho)\}$ defined by Eq. (6) are adopted as follows; 6.0×10^{-8} , 6.0×10^{-7} and 6.0×10^{-6} [m]. [note 1]

NUMERICAL METHODS AND BOUNDARY CONDITIONS

Table 1 shows the numerical conditions. Flow fields were analyzed with a low Reynolds number $k-\epsilon$ model (MKC model [11]) with an inflow velocity of $0.1 U_0$ ($= 0.1 \text{ m/s}$; air change rate = 1.6 h^{-1}) under ordinary conditions (with no flushing) and U_0 ($= 1.0 \text{ m/s}$; air change rate = 16

Table 1 Numerical Conditions

Number of grid points (2D)	Air region : 68(x)×64(z) Material region : 68(x)×41(z)
Reynolds number	$U_0 L_0 / \nu = 4.2 \times 10^3$
Normalized molecular diffusivity of VOCS in air	$D_a / U_0 L_0 = 9.8 \times 10^{-5}$ (23)
Normalized diffusion coefficient of VOCS in the material	$D_{\text{eff}} \cdot T_0 / L_0^2 = 1.8 \times 10^{-13}$ (23)

Table 2 Cases Analyzed

Case NO.	Flushing (hours)	Sorption Factor (m)	Temperature ()
Case1	-	$\{k_h (\rho'/\rho)\}=0.0$	23
Case2	8 / 24		
Case3	-	$\{k_h (\rho'/\rho)\}=6.0 \times 10^{-8}$	
Case4	-	$\{k_h (\rho'/\rho)\}=6.0 \times 10^{-7}$	
Case5	-	$\{k_h (\rho'/\rho)\}=6.0 \times 10^{-6}$	

$U_{\text{in}} = 0.1 U_0$ (= 0.1 m/s, no flushing), $U_{\text{in}} = U_0$ (= 1.0 m/s, flushing), k_h = Henry's coefficient

h^{-1}) on flushing. A centered difference scheme is used for the convection term. Using the results of flow field simulations, the emission/sorption and diffusion fields were analyzed. In the emission and diffusion analysis, time-dependent Eqs. (1) and (8) were solved by coupling Eq.(2). In the sorption analysis, Eqs. (6) and (8) were solved by coupling Eq.(7). The emission, sorption and diffusion processes were solved simultaneously. Table 2 shows the cases analyzed. Five cases were examined in total, under different conditions of inflow velocity (flushing) and sorption factor $\{k_h \cdot (\rho'/\rho)\}$. The time history of room air concentration was obtained over a duration of $8.6 \times 10^6 T_0$ (6 days, T_0 ; representative time scale defined by L_0/U_0).

RESULTS AND DISCUSSION

All results are shown as dimensionless values, dividing by the representative values C_0 , L_0 , and U_0 . C_0 represents the initial VOCs concentration in the material ($1.92 \times 10^8 \mu\text{g}/\text{m}^3$), 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).

For the flow field of the objective room (cf. Fig. 3), we have conducted precise model experiment under identical Reynolds number condition. Details of the model experiment are reported in [11]. The velocity distribution given from the prediction with the low Reynolds number k - ϵ model and the results obtained in the model experiment are in very good agreement [12, 13].

VOCS concentration in room air

As shown in Fig. 4(1), the maximum value for room-averaged VOCs concentration (C_{max}/C_0) reaches 1.0×10^{-6} just after the start of numerical experiment in case1 (no flushing). Such pattern of time history can be regarded to be similar to the one which is observed in a room just after furnishing newly produced materials with VOCs emission. Here, C_0 distribution in SBR is assumed to be uniform as described previously. The computation was started with an initial condition of zero concentration within the room. The room-averaged VOCs concentration decays gradually over a duration of 8.6×10^6 (6 days). Case 2 (8 hour flushing for 24 hours) shows that room-averaged VOCs concentration decreases to 1/10 of case 1 (no flushing) only during the flushing time. As shown in Fig. 4(2), the time history of room-averaged concentration in case 3 (sorption coupled, sorption factor $\{k_h (\rho'/\rho)\}$ is 6.0×10^{-8}) is almost the same with case1. The larger values of the sorption factor lead to the faster decay of the room averaged concentration as shown in Fig. 4(2). [note 1]

The concentration distributions within the room are shown in Figs. 5(1) - 5(4). The distributions are not uniform. They are highly non-uniform near the floor. The VOCs concentrations near the SBR floor are about six times higher than those of room-average for each case, as shown in Fig. 5(1). This means that an infant, a child, or a person sleeping on the floor, are likely to be exposed to a higher VOCs concentration. The averaged VOCs concentration in the breathing zone of standing people (C_{ave}/C_0 , $z < 25L_0 = 1.5\text{m}$) is about 1.0×10^{-7} , whereas that for sleeping people (C_{ave}/C_0 , $z < 8.3L_0 = 0.5\text{m}$) is about 1.2×10^{-7} in case 1. For case 5 ($\{k_h (\rho'/\rho)\}$ is 6.0×10^{-6}), the concentration of VOCS is about 25% smaller than that of case 1 ($\{k_h (\rho'/\rho)\}$ is zero).

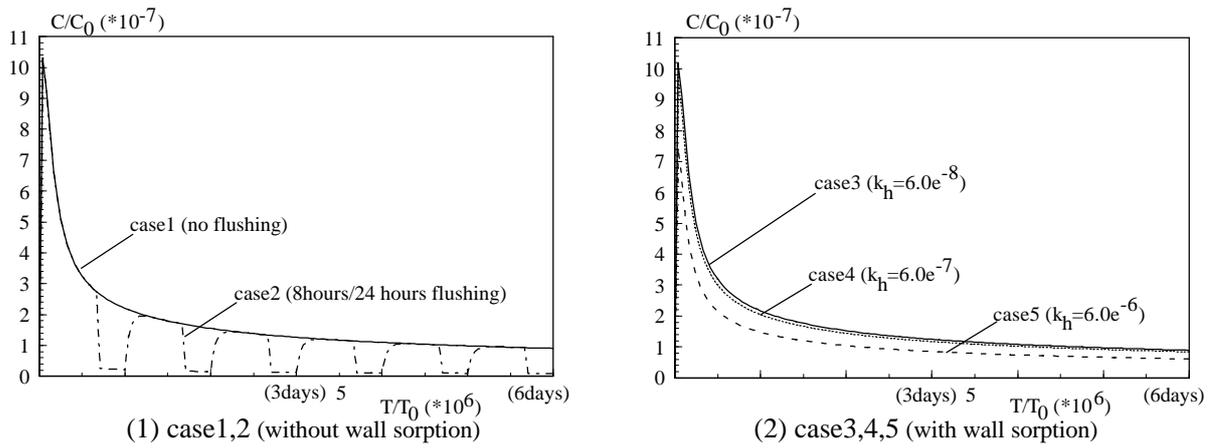


Fig. 4 Time history of room-averaged concentrations

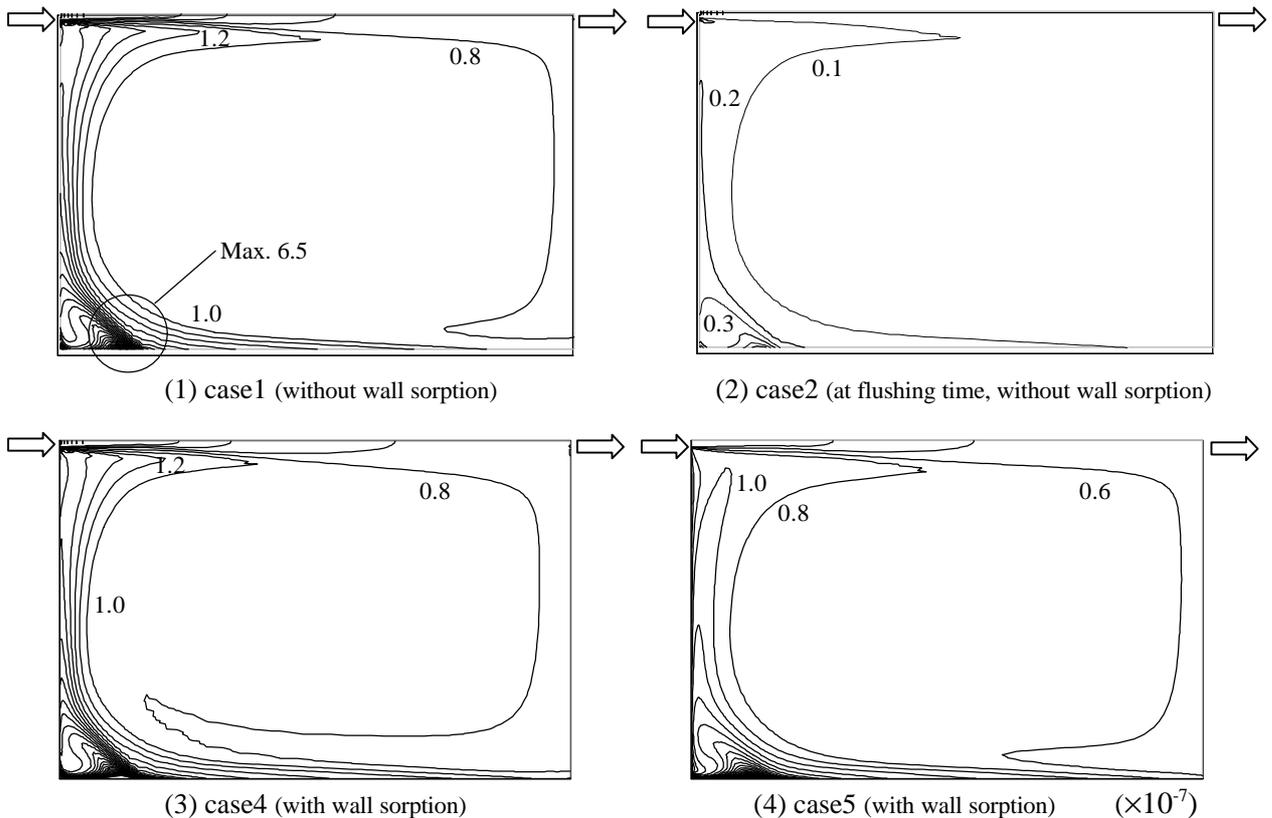


Fig. 5 Concentration distribution of VOCs C/C_0 (at $T/T_0=7.2 \times 10^6$ (5 days))

VOCs emission rate

As shown in Fig. 6, the distribution of VOCs emission rates at the floor material are almost constant in all cases. The differences in the VOCs emission rate are only about 1- 2 % between all cases. The emission from SBR which is governed by internal diffusion control is not affected by the ventilation rate, surface velocity and room averaged concentration, etc in the conditions treated here. This is caused by the small value of D_{eff} within the material. When D_{eff} becomes much larger, emission rate is naturally influenced by the flowfield near the material.

VOCs adsorption/ desorption rate

As shown in Fig. 7, the time history of the amount of VOCs adsorbed at the sorption walls (M defined by Eq. (3)) is almost zero in case 3 ($\{k_h \cdot (\rho'/\rho)\}$ is 6.0×10^{-8}). The larger value of the sorption factor $\{k_h \cdot (\rho'/\rho)\}$ lead to the larger amount of VOCs adsorbed at the sorptive walls. For case 4 (6.0×10^{-7}) and case5 (6.0×10^{-6}), the amount of VOCs adsorbed at the sorptive walls (M) are decreased in accordance with the decay of the room averaged concentration. The amount of adsorption/desorption is naturally coupled with the room air concentration of VOCs.

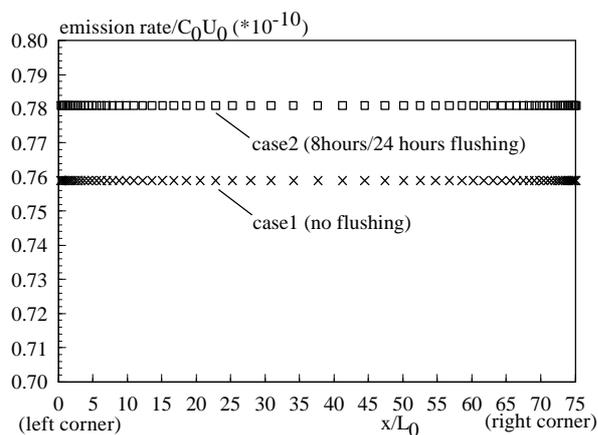


Fig. 6 VOCs emission rate from SBR floor
(at $T/T_0=7.2 \times 10^6$ (5 days))

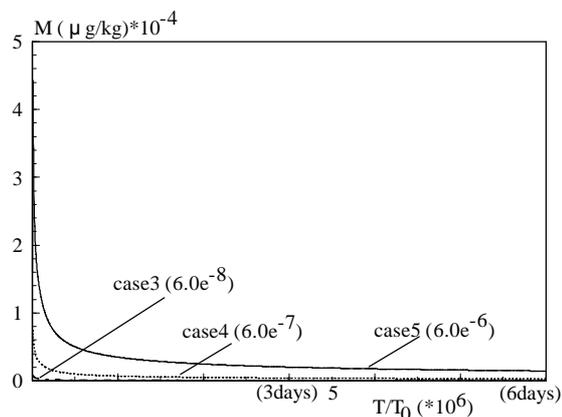


Fig. 7 Time history of the amount of VOCs adsorbed at sorption plate

CONCLUDING REMARKS

- (1) The room-averaged VOCs concentration decays gradually during the duration of simulation ($8.6 \times 10^6 T_0$, 6 days).
- (2) The concentration of VOCs near the SBR floor, from which the VOCs are emitted, is about six times larger than the room-averaged value.
- (3) The VOCs emission from SBR which is governed by internal diffusion control with small value of D_{eff} is not affected by ventilation rate and room averaged concentration.
- (4) For the sorption effect, the larger value of the sorption factor $\{k_h \cdot (\rho'/\rho)\}$ leads to the faster decay of the room averaged concentration.

Note 1

The amount of sorption material at side walls is expressed here as ρ' [kg/m^2], i.e. the weight of sorptive material per square meter. We would like to evaluate this amount used here when activated carbon is selected as sorptive material. Henry's coefficient (k_h) of activated carbon is roughly given as 1×10^3 (adsorbate; toluene, adsorptive; activated carbon, at $C=100$ [$\mu\text{g}/\text{kg}$], $M=1.0 \times 10^8$ [$\mu\text{g}/\text{kg}$] [7]). The air density (ρ) is about 1.2 [kg/m^3]. The sorption factor $\{k_h \cdot (\rho'/\rho)\}$ used in this study are 6.0×10^{-8} , 6.0×10^{-7} , 6.0×10^{-6} [m]. Thereby the values of ρ' [kg/m^2] i.e. the amounts of sorptive material per unit area are 7.2×10^{-11} , 7.2×10^{-10} , 7.2×10^{-9} [kg/m^2] respectively. The amount of activated carbon set at side walls in this study is very small as shown here. It is plausible to arrange much larger amount of activated carbon in real situation. In such case, we can expect much large value of sorption than the result predicted here.

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