CFD Analysis of Pollutant Distribution in a Room with Adsorptive Walls

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Abstract

The distribution of an air pollutant which is emitted from the building materials in a room can be quantitatively predicted by the CFD (Computational Fluid Dynamics) technique. The authors develop a CFD analysis incorporating a pollutant sorption model which allows the detailed analysis of the effect of reducing the concentration of the indoor air pollutant through the sorption on walls and other interior surfaces.

In order to demonstrate the usefulness of the CFD analysis incorporating the sorption model, we conduct an analysis of concentration distribution for an indoor air pollutant in a closed heated room. We examine the effect of reducing the concentration of the indoor air pollutant by installing an adsorber in the walls and ceiling, assuming that the pollutant was emitted from the floor of the room. The sorption model incorporated is very simple and assumes zero concentration at the adsorbing surfaces. The CFD analysis shows the significant effect of reducing the concentration of the indoor air pollutant by the absorbing surfaces.

Keywords: CFD; adsorption; concentration distribution

Introduction

The concentration of indoor air pollutants, such as VOCs, is usually not uniformly and varies significantly distributed in an indoor space. The distribution of the pollutant concentration is significantly dependent on the location of the pollutant source as well as the profile of the indoor airflow. It is also significantly influenced by the pollutant sorption effect of the interior surfaces and furnishings (Haghighat et al., 1998; Meininghaus. et al., 1998; Chang, J.C.S. et al., 1992; Christianson J, Yu, J.- W. et al., 1993 Bluysen, P.M., et al., 1995). Predicting these profiles requires a detailed analysis of the distribution of the indoor airflow and the sorption properties of the interior walls.

The CFD (Computational Fluid Dynamics) technique allows a detailed analysis of indoor airflow distributions and pollutant concentration distribution. With incorporating the sorption model the CFD allows an analysis of the effect of reducing the concentration of indoor air pollutant by the sorption of the pollutant on the walls and ceilings. The final object of this study is to develop the physical models of emission and sorption of pollutants, in both building materials and room air (Murakami et al., 2001). In the first step of this study, the simple sorption model is developed and its usefulness is examined in the paper.

We conducted an analysis of the concentration distribution of the indoor air pollutant in a closed heated room with natural ventilation through the crack of the floor and the ceiling, as an example of the CFD analysis incorporating the sorption model. In the analysis, we assumed ideal adsorbing surfaces and used a simple sorption model that allows the zero value of the concentration at the adsorbing surfaces. Fresh air inflows from the outside through the baseboard around the perimeter of the room and the room air is exhausted through the ceiling around the perimeter. We assumed that the pollutant would be emitted from the floor surface. Adsorbing surfaces are attached to the walls and ceiling. We studied the effect of reducing the concentration of pollutant by the adsorbing surfaces by comparison between cases with and without those surfaces.

Physical Models of Pollutant Transfer
Transportation in room air

Air pollutants, such as VOCs, emitted from building materials are transported by the convection of the room air and dispersed by molecular diffusion ($\lambda_a/\rho_{air}$ [m$^2$/s]) and turbulent diffusion ($\nu$ [m$^2$/s]). The vapor phase concentration C [kg/kg] of pollutants in the room air can be described by the mass conservation equation given in Eq. (1).
Here, C [kg/kg] is the vapor phase concentration in the air, ρ_{\text{air}} [kg/m^3] is the air density, \( \lambda_a \) [kg/(ms.(kg/kg))] is the molecular mass conductivity, \( \nu_t \) [m^2/s] is the turbulence eddy viscosity, and \( \sigma \) is the turbulent Prandtl number (=1.0). Velocity \( u_j \) [m/s] and \( \nu_t \) are given by solving for the flow field with CFD technique such as a standard k-ε turbulence model. Thus, Eq. (1) is closed.

Simple transportation model in absorptive material

In general, the diffusion and adsorption process in a material can be described using the effective diffusion coefficient \( D_c \) [m^2/s], which implicitly includes the effect of adsorption. The pollutant concentration used here in the material is the equivalent vapor phase concentration. Pollutant transfer in the materials is governed by Eq. (2).

\[
\rho_{\text{air}} \frac{\partial C}{\partial t} + \rho_{\text{air}} \frac{\partial (u_j C)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \lambda_a + \frac{\rho_{\text{air}} \nu_t}{\sigma} \frac{\partial C}{\partial x_j} \right)
\]  

(1)

Boundary conditions at the air-material interface

Since the transportation of C in the material and in the room air is solved simultaneously, a boundary condition should be set at the air-material interface. The pollutant transfer rate at the air-material interface should be the same as the transportation rate of internal diffusion from the inside shown in Fig. 1. This condition is expressed as the conservation law at the surface of the material, as shown in Eq. (3).

\[
-\rho_{\text{air}} D_c \frac{\partial C}{\partial x} \bigg|_{B^+} = \left( \lambda_a + \frac{\rho_{\text{air}} \nu_t}{\sigma} \right) \frac{\partial C}{\partial x} \bigg|_{B^-}
\]  

(3)

Here, \( B^+ \) is the air-material surface in the material-side region, and \( B^- \) is the air-material surface in the air-side region. Eq. (3) is used as the boundary condition at the air-material interface when the transportation in the material and the room air is solved simultaneously.

\( (\lambda_a + \rho_{\text{air}} \nu_t/\sigma) \times (\rho_{\text{air}} D_c) \) in Eq. (3) corresponds to the convective mass transfer coefficient. Generally, when a convective heat transfer coefficient is known, the convective mass transfer coefficient can be obtained using the Lewis correlation. \( (\lambda_a + \rho_{\text{air}} \nu_t/\sigma) \times (\rho_{\text{air}} D_c) \) in Eq. (3) also expresses the permeability of pollutant from the surface to the inside of the material. Introducing the convective mass transfer coefficient \( \alpha_m \), which represents \( (\lambda_a + \rho_{\text{air}} \nu_t/\sigma) \times (\rho_{\text{air}} D_c) \), and the permeability of pollutant in the material \( t_m \), which represents \( (\rho_{\text{air}} D_c) \times (\rho_{\text{air}} D_c) \), the Eq. (3) is expressed as Eq. (4).

\[
t_m (C_x - C_S) = \alpha_m (C_S - C_i)
\] 

(4)

Here, \( C \) is the representative concentration in the material, \( C_i \) is the surface concentration, and \( C_x \) is the concentration in the room air which is the value just outside of the surface boundary layer of the concentration distribution shown in Fig. 1.

From the Eq. (4), the surface concentration of \( C_s \) is expressed as Eq. (5).

\[
C_S = \left( C_x + \frac{(\alpha_m / t_m) \times C_i}{1 + \alpha_m / t_m} \right)
\]  

(5)

When \( t_m \) is sufficiently larger than \( \alpha_m \), \( C_S \) becomes the same with \( C \). If the adsorption capacity of the building material and the permeability of the material, \( t_m \) can be assumed to be as large as enough, the surface concentration of \( C_s \) can be assumed to be of zero and the same with \( C \).

Convective mass transfer coefficient \( \alpha_m \) and permeability of material \( t_m \)

It is generally assumed that the convective heat transfer coefficient \( a_c \) in a usual room ranges about 2 to 7 [W/(m^2·ºC)]. The corresponding convective mass transfer coefficient \( a_m \) ranges about 1.7×10^{-3} to 5.8×10^{-3} m/s when the density of the air in 1.2 kg/m^3, the specific heat of the air in 1.0 [kJ/(m^2·ºC)] and Lewis number is 1.0. Thereby the absorptive materials of which permeabilities are larger than about 10 times of 1.7×10^{-3} to 5.8×10^{-3} m/s will suit the assumption of zero value at the surface.

A granulated activated carbon, a gypsum board and so on are the examples which have high adsorption capacity and high permeability. In case of the materials which have low adsorption capacity and low permeability, the assumption of zero value at the surface could not be applied. The further study of adsorption-desorption model would be needed.
In order to demonstrate the effect of adsorption on the air pollutant concentration, the concentration distribution is analyzed with CFD for a model room with adsorptive walls.

**Model room for simulation**

Fig. 2 shows the room model analyzed. The conditions of the analysis assume the winter condition of the typical Japanese detached house with the recommended thermal insulation and ventilation rate. The details of the model room are given in Table 1. The room is heated with a fan convector. Infiltration air flows into the room from the floor corner and out from the ceiling corner. Outdoor temperature is 3.5°C. The heat transmittance through the floor, ceiling and walls is considered. The average room air temperature is set at the target temperature of 22°C and the heating input is controlled to obtain the targeted average room air temperature.

**CFD Analysis of Pollutant Distribution**

In order to demonstrate the effect of adsorption on the air pollutant concentration, the concentration distribution is analyzed with CFD for a model room with adsorptive walls.

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**Table 1. Conditions for Calculations and Grid System**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fan Convector</strong></td>
<td></td>
</tr>
<tr>
<td>Velocity and Airflow Rate</td>
<td>1.0 m/s, 84.6 m³/h (= 3.8 h⁻¹)</td>
</tr>
<tr>
<td>Temperature</td>
<td>43.5°C (Result for average room temperature of 22°C)</td>
</tr>
<tr>
<td>Turbulence Energy and Energy Dissipation Rate</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$k_{in} = 3/2 \times (U_{in} \times l_{in})^2$, $e_{in} = C_p \times k_{in}^{1/2}/l_{in}$, $l_{in} = \text{width of the opening}$</td>
</tr>
<tr>
<td><strong>Infiltration Air</strong></td>
<td></td>
</tr>
<tr>
<td>Velocity and Airflow Rate</td>
<td>0.05 m/s, 22.0 m³/h (= 1.0 h⁻¹)</td>
</tr>
<tr>
<td>Temperature</td>
<td>3.5°C</td>
</tr>
<tr>
<td>Turbulence Energy and Energy Dissipation Rate</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$l_{in} = 0.1, l_{in} = \text{width of the opening}$</td>
</tr>
<tr>
<td><strong>Thermal transmittance of the walls</strong></td>
<td></td>
</tr>
<tr>
<td>Ceiling</td>
<td>0.25 W/(m²·°C)</td>
</tr>
<tr>
<td>Wall</td>
<td>0.45 W/(m²·°C)</td>
</tr>
<tr>
<td>Floor</td>
<td>0.45 W/(m²·°C)</td>
</tr>
<tr>
<td>Windows, door</td>
<td>4.65 W/(m²·°C)</td>
</tr>
<tr>
<td><strong>Contaminant Source and Emission Rate</strong></td>
<td></td>
</tr>
<tr>
<td>Floor (9.2 m²), 1.0×10⁻³ mg/(m²·s)</td>
<td></td>
</tr>
<tr>
<td><strong>Convective Heat Transfer Coefficient</strong></td>
<td></td>
</tr>
<tr>
<td>4.0 W/(m²·°C)</td>
<td></td>
</tr>
<tr>
<td><strong>Convective Mass Transfer Coefficient</strong></td>
<td></td>
</tr>
<tr>
<td>3.3×10⁻³ m/s</td>
<td></td>
</tr>
<tr>
<td><strong>Mesh System for CFD</strong></td>
<td>31(x)×29(y)×26(z)</td>
</tr>
</tbody>
</table>

* Concentration in case of perfect mixing condition without sorption is 0.15 mg/m³

** No adsorption except for adsorptive walls

*** Log-law for all walls

[Symbol] $C_p = 0.09$, $U_{in}$: velocity of inflow [m/s], $k_{in}$: turbulence energy of inflow [m²/s²], $e_{in}$: turbulence energy dissipation rate [m²/s], $l_{in}$: turbulence intensity, $l_{in}$: specific length scale [m]
emitting wood based board. In order to examine the effect of pollutant removal from the air by adsorption, we analyzed the cases in which interior surfaces such as walls and ceilings are finished with the materials that have ideal sorption capacities as mentioned before. Forced flow convector does not remove the pollutant in this study.

**Conditions of CFD and cases analyzed**

The airflow in the room is simulated numerically based on the standard k-ε model of turbulence. The pollutant distribution is calculated based on the obtained flow field. Table 1 shows the boundary conditions for the CFD and pollutant distribution simulations. Three cases of pollutant distributions are being conducted shown in Table 2. Case 1 is without adsorptive materials, case 2 is with adsorptive walls, and case 3 is with an adsorptive ceiling.
Result

Velocity and temperature field

Fig. 3 shows the velocity distribution in the room. The warm air supplied from the fan convector rises up to the ceiling. Down streams are observed near the walls since they are cooled by the cold outdoor air. Fig. 4 shows the temperature field. Thermal stratification is formed in the room. About 4°C in temperature difference occurs between the top and bottom of the room, excluding the region of up-flow produced by the heater. The temperature of the region near the floor is apparently low due to the cool down-flow from the walls and air infiltration from the perimeter of the room. The temperature in the upper region is relatively uniform.

Air pollutant distribution

Fig. 5 shows the air pollutant distribution in the room. The pollutant concentration distribution is non-dimensional using the representative concentration which is defined with perfect mixing condition. Case 1 shows a high concentration near the floor surface where the pollutant is emitted. The air in the room is well mixed by the forced flow of the convector and consequently a nearly uniform concentration is achieved in the upper region of the room. The average concentration in the room is slightly lower than the concentration of the perfect mixing assumption, at 0.95. In case 2 where wall surfaces are absorptive, the concentration decreases to about 1/100 of that in case 1. In case 3 where the ceiling surface adsorbs the pollutant, the concentration is slightly higher than in case 2 due to the smaller adsorbing area. However, it is about 1/50 of that in case 1. Thus, the adsorbing material was found to be effective in reducing the concentration of the indoor air pollutant.

Percentage of pollutant removal in the room

Percentages of pollutant removal by infiltration and absorptive walls in the room are shown in Fig. 6. In case 1, which has no absorptive wall, all pollutant generated from the floor is removed by infiltration. Since almost of pollutant generated is removed by the absorptive walls in case 2, pollutant concentration in the room is very small compared to case 1. Only 0.3 % of pollutant exhausts through the infiltration airflow. In case 3, 98.9 % of pollutant is absorbed to the ceiling. Installing absorptive wall could reduce pollutant level efficiently.

Conclusion

In the paper, we analyzed the effect of the adsorbing material on the reduction of indoor air pollutant concentrations using a CFD analysis incorporating the sorption model. The analysis produced the following conclusions:

1) If the permeability of the sorptive material is larger than the convective mass transfer coefficient and sorptive capacity is large enough comparing the room air pollutant the surface concentration of the sorptive material can be assumed to be of zero.
2) Pollutant adsorption by the walls had a significant effect in decreasing the pollution level in the room.
3) The effect depends on the characteristics of the adsorptive materials in particular on the mass transfer coefficient.

References