AN INTEGRATED ZONAL MODEL FOR PREDICTING TRANSIENT VOC DISTRIBUTION IN A VENTILATED ROOM

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ABSTRACT
A material VOC emission model has been integrated with a zonal model to predict the transient VOC distribution within a ventilated room. This integrated zonal model is developed based on the conservation of air mass, energy and VOC mass. In the zonal model, the room is partitioned into coarse grids and Newton Raphson global convergent method is used to solve a set of coupled mass and energy nonlinear equations. In the VOC emission model, the material is divided into fine grids and control volume finite difference method is used to solve the transient VOC diffusion equation. This integrated zonal model is applied to a ventilated room with a carpet floor. It is found that VOC concentration is not uniform in the space and is influenced by the airflow pattern. The integrated zonal model can give a good prediction of the average VOC concentration in a room. Moreover, it is found that the integrated zonal model is a practical tool for the long-term VOC distribution prediction.

Keywords: zonal model, material VOC emission model, transient VOC distribution in a room, convection and diffusion

INTRODUCTION
Building materials may release a wide variety of pollutants, especially, the volatile organic compounds (VOC), which could cause indoor air related health problems. Recently, there has been a growing interest in the development of mathematical models to predict the quality of indoor air. To describe VOC concentration in a room, there are three kinds of models: total mixing model, CFD model and zonal model. In the total mixing model, the room is treated as a mono-zone and assumed to have only one concentration. Except in the mass boundary layer, air movement effect is not considered. The total mixing model can provide general information about VOC concentration in a room. However, it cannot give detailed VOC concentration distribution within a room. Actually, VOC concentration varies in the space and is influenced by the characteristics of a room, such as ventilation system pattern, temperature distribution, etc. A detailed knowledge of VOC distribution is important for local pollutant control. CFD model can provide the detailed knowledge of air flow pattern, temperature and contaminant distributions within a room, but it is too complicated to be used as a daily design tool to predict VOC distribution in a room. On the other hand, CFD is too time consuming and expensive. Actually, users are not usually interested in excessively detailed results obtained from CFD models. Zonal model is an intermediate model between CFD model and mono-zone model. Compared to mono-zone model, zonal model can provide users with an estimated view of airflow, temperature and contaminant distribution within a room. Zonal model has advantages over CFD model in their simple use, time saving and satisfactory precision characteristics (Haghighat et al., 2002).

Zonal models are always integrated with convection, conduction and radiation heat transfer models to predict the temperature distribution within a room (Wutz et al., 1999; Musy et al., 2001; Haghighat et al., 2002) While, zonal models integrated with mass transfer models to simulate the contamination distribution within a room are seldom available. Recently, Molina et al. (2000) proposed a model which considered the air movement effect using a zonal model and the sorption effect using a sorption mass transfer model. Simple theoretical results were presented in this research by assuming that the contaminant concentration in the room was constant. Although great efforts have been made in the development of the zonal models, a zonal model which integrated with material emission model for predicting VOC distribution in a room is not yet available.

This paper describes the development of an integrated zonal model for predicting the transient VOC distribution within a ventilated room. The integrated zonal model includes a three-dimensional zonal model and a three-dimensional material emission model.

INTEGRATED ZONAL MODEL DEVELOPMENT

Zonal Model

Different zonal models distinguish themselves in terms of modeling the airflow and the driving forces. The zonal model applied in here follows what has become the common practice in this field (Wutz et al., 1999; Haghighat et al., 2002).

The physical system considered here is a room with typical walls, floor, ceiling and mechanical ventilation system. The room is in a non-isothermal condition. It is subdivided into a number of three-dimensional small cells. The room configuration and partition are shown in Figure 1.

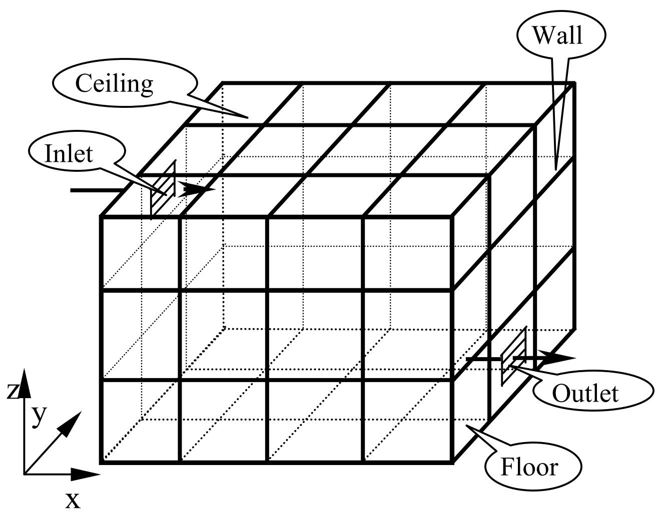

Figure1 Physical configuration and partition of a room

- *Air mass conservation equation:*

Within each cell, it is assumed that pressure in each cell varies hydrostatically and pressure at the middle of each cell obeys the perfect gas law:

$$P_{m,i} = \rho_i R T_i \quad (1)$$

$$P_{i,h} = P_{ref.i} - \rho_i g h \quad (2)$$

Where,

$P_{m,i}$: pressure at the middle of cell i, Pa

ρ_i: air density of cell i, kg/m^3

R: gas constant of air, 287.055 J/kg.K

T_i: temperature of cell i, K

$P_{ref,i}$: reference pressure at the bottom of the cell i, Pa

h: height from the bottom of cell i, m

$P_{i,h}$: pressure at the height of h in cell i, Pa

g: gravitational acceleration, m^2/s

Adjacent cells exchange mass through the cell interfaces. In each cell, the general air mass balance can be written as:

$$0 = \sum_{j=1}^{6} m_{a,ij} + m_{a,source} + m_{a,sink} \quad (3)$$

Where,

$m_{a,ij}$: air mass flow across cell i and cell j interface, kg/s

m_{source}: air mass source in cell i, kg/s

m_{sink}: air mass sink in cell i, kg/s

Power low is applied to calculate the air mass flow rate across the cell interface.

$$\dot{q}_{a,ij} = C_d \rho \Delta P_{ij}^{n} \quad (4)$$

Where,

$\dot{q}_{a,ij}$: air mass flow rate across cell i and cell j interface, kg/m^{2}s

ΔP_{ij} : pressure difference between cell i and cell j, Pa

C_d: coefficient of power law, m/sPa^n, usually taken as 0.83(Wutz et al., 1999; Haghighat et al., 2002).

n: flow exponent, 0.5 for turbulent air flow and 1 for laminar air flow (Wutz et al., 1999; Haghighat et al., 2002).

The pressure at cell bottom level is assumed to be uniform. For the horizontal cell interface, the air mass flow rate can be expressed as(Wutz et al., 1999; Haghighat et al., 2002):

$$\dot{q}_{a,hor} = C_d \rho (P_{ref,top} - P_{ref,bottom} + \rho_{bottom} g H)^n \quad (5)$$

Where,

$\dot{q}_{a,hor}$: air mass flow rate across the horizontal cell interface, kg/m^{2}s

$P_{ref,top}$: reference pressure at the bottom of the top cell, Pa

$P_{ref,bottom}$: reference pressure at the bottom of the bottom cell, Pa
H: height of the bottom cell, m
ρ_{bottom}: air density of the bottom cell, kg/m^3

For the vertical cell interface, there is a neutral plane (Zn) which the pressure difference between the left side and the right side of the interface is zero, therefore:

$$0 = \Delta P_{ref,LR} - \Delta \rho g Z_n \quad (6)$$

$$Z_n = \frac{\Delta P_{ref,LR}}{\Delta \rho g} \quad (7)$$

Where,
$\Delta P_{ref,LR}$: reference pressure difference between the left cell and the right cell, pa
$\Delta\rho$: density difference between the left cell and the right cell, kg/m^3
Z_n : neutral plane, m

Thus, the air mass flow rate below the neutral plane (0-Zn) and above the neutral plane (Zn-H) can be described as(Wutz et al., 1999; Haghighat et al., 2002):

$$\dot{q}_{0-Z_n} = C_d \rho (\Delta \rho g)^n \frac{(Z_n)^{n+1}}{n+1} \quad (8)$$

$$\dot{q}_{Z_n-H} = C_d \rho (\Delta \rho g)^n \frac{(H-Z_n)^{n+1}}{n+1} \quad (9)$$

Therefore, the total air mass flow rate across the vertical cell interface becomes:

$$\dot{q}_{a,ver} = \dot{q}_{0-Z_n} + \dot{q}_{Z_n-H} \quad (10)$$

- *Energy conservation equations:*

Within each cell, temperature is assumed to be uniform. In each cell, the general energy balance can be written as:

$$0 = \sum_{j=1}^{6} Q_{T,ij} + Q_{T,source} + Q_{T,sink} \quad (11)$$

Where,

$Q_{T,ij}$: heat flow rate cross cell i and cell j interface , w

$Q_{T,source}$: heat energy source in cell i, w
$Q_{T,sink}$: heat energy sink in cell i, w

Heat transfer between cells is mainly through convection and the heat transfer along wall surfaces is modeled by the Newton cooing law, thus,

$$Q_{T,ij} = m_{a,ij} C_p T \quad (12)$$

$$\Rightarrow \begin{cases} \text{if } m_{a,ij} > 0,\ Q_{T,ij} = m_{a,ij} C_p T_j \\ \text{if } m_{a,ij} < 0,\ Q_{T,ij} = m_{a,ij} C_p T_i \end{cases}$$

$$Q_{T,i-wall} = h_T A \Delta T_{i-wall} \quad (13)$$

Where,
T: temperature of the air entering or leaving cell i, K
T_i: temperature of cell i, K
T_j: temperature of cell j, K
C_p: specific heat of air, J/kg.K
h_T: convective heat transfer coefficient, w/m^2 K
$\Delta T_{,i-wall}$: temperature difference between cell i and wall, K
A: cell I and wall interface area, m^2

Where the convective heat transfer coefficient, h_T, is a function of the surface to air temperature difference (Wutz et al., 1999).

Integrating Material Emission Model into Zonal Model

- *Material emission model:*

The physical system considered here is a dry building material (carpet, vinyl flooring, particleboard, etc.), where one surface is exposed to air. When VOC concentration in the material is higher than VOC concentration in the room air, VOC diffuses through material to reach material surface. At material/ air interface, VOC changes from material phase to gas phase. At atmospheric pressure, for low VOC concentration and isothermal conditions, the equilibrium relationship between VOC concentration in the air phase and VOC concentration in the material phase can be described by a linear isotherm. Finally, VOC passes through its overlying concentration boundary layer and transports to the room air by diffusion and convection. Thus the governing equations and the initial and boundary conditions in the emission model become:
Governing equations:

$$\frac{\partial C_m}{\partial t} = D_m \left(\frac{\partial^2 C_m}{\partial x^2} + \frac{\partial^2 C_m}{\partial y^2} + \frac{\partial^2 C_m}{\partial z^2} \right) \quad (14)$$

$$C_m \big|_{z=b} = k C_{s,i} \quad (15)$$

$$R = h_m \left(C_{s,i} - C_{a,i} \right) \quad (16)$$

Initial and boundary conditions:

$$C_m\big|_{t=0} = C_{m0} \quad (17)$$

$$-D_m \frac{\partial C_m}{\partial z}\bigg|_{z=b} = h_m\left(\frac{C_m\big|_{z=b}}{k} - C_{a,i}\right) \quad (18)$$

$$\frac{\partial C_m}{\partial z}\bigg|_{z=0} = 0 \quad (19)$$

Where,
C_m : VOC concentration in the material, μg/m^3
D_m : VOC diffusion coefficient of the material, m^2/s
C_{m0}: VOC initial concentration in the material, μg/m^3
k: material/air partition coefficient.
$C_{s,i}$: VOC concentration in the near material surface air in cell i, μg/m^3
$C_{a,i}$: VOC concentration in the air in cell i, μg/m^3
h_m: Convective mass transfer coefficient, m/s
b: material thickness, m
t: time, s

The convective mass transfer coefficient, h_m, depends on the airflow pattern along the material surface. It can be estimated based on the correlation among the Sherwood number (Sh), Reynolds number (Re) and Schmidt number (Sc) (Huang and Haghighat 2002)

- *VOC mass conservation in the air*

Within each cell, VOC concentration is assumed to be uniform. In each cell, the general VOC mass balance can be written as:

$$\frac{M_{a,i}}{\rho_i}\frac{dC_{a,i}}{dt} = \sum_{j=1}^{6} m_{VOC,ij} + m_{VOC,sorce} + m_{VOC,sink} \quad (20)$$

Where:
$C_{a,i}$: VOC concentration in the air in cell i, μg/m^3
$m_{voc,ij}$: VOC mass flow cross cell i and cell j interface, μg/s
$m_{voc,source}$: VOC mass source in cell i, μg/s
$m_{voc,\ sink}$: VOC mass sink in cell i, μg/s
$M_{a,i}$: air mass in cell i, kg

VOC mass transfer between cells is mainly through convection, therefore,

$$m_{VOC,ij} = \frac{m_{a,ij}}{\rho} C_a \quad (21)$$

$$\Rightarrow \begin{cases} \text{if } m_{a,ij} > 0,\ m_{voc,ij} = \dfrac{m_{a,ij}}{\rho_j} C_{a,j} \\ \text{if } m_{a,ij} < 0,\ m_{voc,ij} = \dfrac{m_{a,ij}}{\rho_i} C_{a,i} \end{cases}$$

Where,
$m_{a,ji}$: air mass flow between cell i and cell j, kg/s
C_a, VOC concentration leaving or entering the cell i, μg/m^3
$C_{a,i}$, VOC concentration in cell i, μg/m^3
$C_{a,j}$, VOC concentration in cell j, μg/m^3

VOC mass transfer along material (Wall) surface is modeled by using the convective mass transfer coefficient .

$$m_{VOC,i-material} = h_m A \Delta C_{i\text{-material}} \quad (22)$$

Where,
$\Delta C_{i\text{-material}}$: VOC concentration difference between cell i and material surface air, μg/m^3
h_m: Convective mass transfer coefficient, m/s

Solution Techniques
The Newton-Raphson global convergence technique is applied to solve the set of coupled nonlinear air mass balance and energy balance equations to get the air mass flow crossing each cell interface. The convergence results are directly used in VOC mass balance equations as input. A combination of direct method (TriDiagonal-Matrix Algorithm) and the Gauss-Seidel method (Patankar, 1980) are applied to solve the set of VOC mass balance equations to get VOC distribution in the room and material.

APPLICATION
The integrated zonal model is applied to a ventilated room; its floor is covered with carpet. The dimension of the room is 3.0×3.0×2.5 m^3 with one air inlet at the top of the west side wall and one air outlet at the east side wall. The air exchange rate is 1.0 h^{-1}. The temperature at the west wall is 0 ^{o}C and at the other walls, ceiling and floor is kept at 21 ^{o}C. The inlet air temperate is 31 ^{o}C. The convective heat transfer coefficients, h_T, of 4.1, 1.0 and 5.7 w/m^{2}k at the walls, floor and ceiling respectively (Wurtz, et al., 1999). Nonane is chosen as the compound of interest, since it is commonly found in the carpet. The nonane diffusion coefficients and partition coefficient in the carpet are taken from literature (Bodalal, 1999). The initial nonane concentrations in carpet is assumed to be

1.0×10^7 ($\mu g/m^3$). All the input parameters of carpet are shown in Table 1. In order to compare the ventilation system efficiency, simulations are carried out for two different ventilation patterns: the air outlet at the top of the east wall and the air outlet at the bottom of the east wall. Both simulation results are compared with the predictions of a total mixing model, which was validated with experimental results (Huang and Haghighat, 2002). The periods of the simulations are for both short term (1 hour) and long term (10 days).

Table 1 Properties of Nonane in the carpet

C_0 ($\mu g/m^3$)	D_a (m^2/s)	D_m (m^2/s)	k
1.0×10^7	6.23×10^{-6}	2.83×10^{-11}	6216

Nonane concentration distributions in the middle section of the room after the carpet is exposed to the air for one hour are graphically displayed in Figure 2 (outlet at the bottom) and Figure 3 (outlet at the top). The nonane concentration is not uniform in the space and is affected by the characteristics of the room. The nonane concentration around the outlet area is around 1.4 times high than that near the inlet area. The nonane concentration distribution for the outlet at the bottom is lower than that for the outlet at the top due to the influence of the airflow pattern. This integrated zonal model also can predict the temperature distribution in the room, as shown in Figure 4

The room-averaged nonane concentration and the outlet nonane concentration for 1 hour and 10 days are shown in Figure 5 and Figure 6 for the two ventilation patterns. The room-averaged concentration for the outlet at the bottom is lower than that for the outlet at the top. The outlet nonane concentrations in both ventilation patterns are higher than the room-averaged nonane concentration. Figure 5 and Figure 6 also show the predictions of the total mixing model. The prediction of average nonane concentration is little higher for the total mixing model than that for the integrated zonal model in both ventilation patterns. However, the average concentration discrepancy between the total mixing model and the integrated zonal model is not significant. This indicates that the integrated zonal model can give good prediction of the average VOC concentration in a room.

The total simulation time for 10 days VOC distribution prediction only takes a few minutes, which means that the integrated zonal model is a practical tool for long-term VOC distribution prediction.

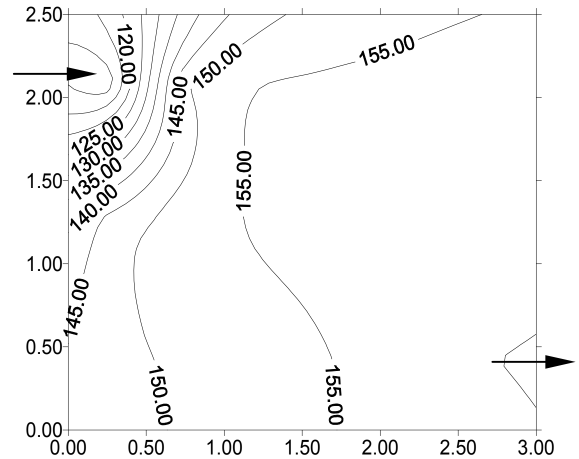

Figure 2 Nonane distribution at the middle section of the room (outlet at bottom, 1hour)

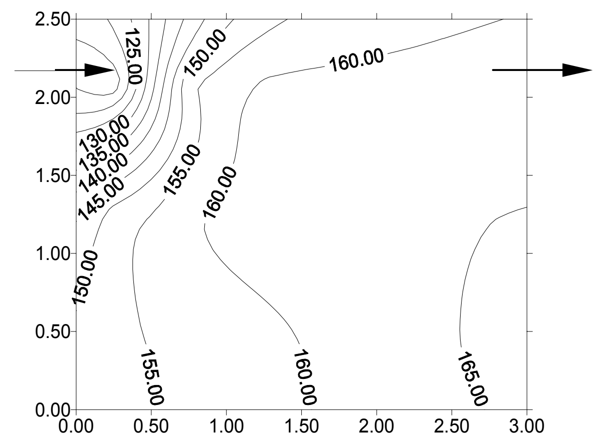

Figure 3 Nonane distribution at the middle section of the room (outlet at top, 1hour)

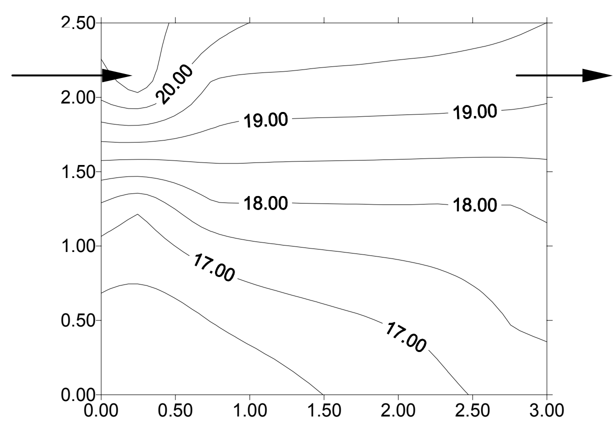

Figure 4 Temperature distribution in the middle section of the room (outlet at top)

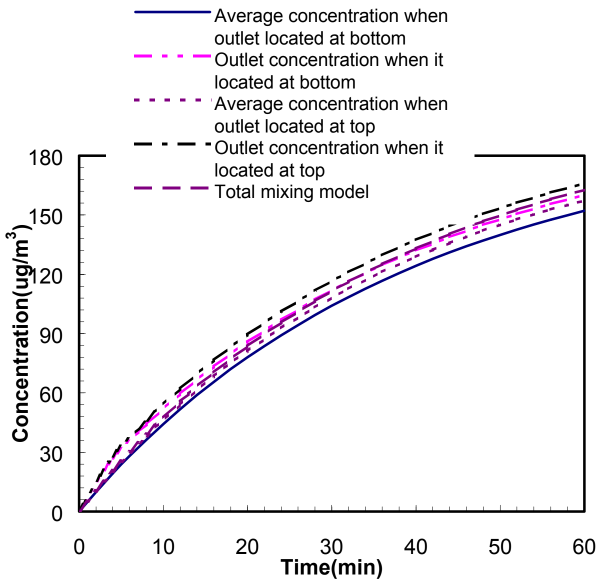

Figure 5 Comparison of nonane concentration in the room

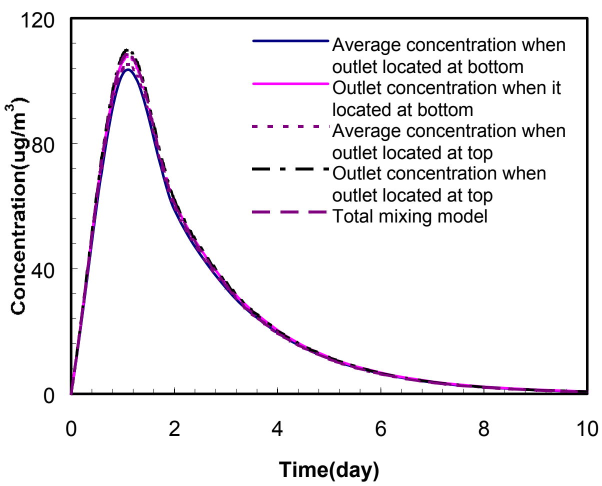

Figure 6 Comparison of nonane concentration in the room

CONCLUSIONS

An integrated zonal model has been developed to predict the three-dimensional air velocity profiles, temperature distribution and VOC concentration distribution in a ventilated room. It was found that VOC concentration is not uniform in the space and is influenced by the characteristics of the room. Moreover, the average VOC concentration predicted by the integrated zonal model was compared with that of the total mixing model, the discrepancy between them was not significant, which indicated that the integrated zonal model can give good prediction for the average VOC concentration in a room. Moreover, it is found that the integrated zonal model is a practical tool for long-term VOC distribution prediction.

The three-dimensional air velocity profiles, temperature distribution and VOC concentration distribution predicated by the integrated zonal model should be further validated with either the CFD simulation results or the experimental results.

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