An integrated zonal model for predicting airflow and VOC concentration distributions in a room

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ABSTRACT
An Integrated Zonal Model was developed to predict the three-dimensional airflow and contaminant concentration distributions in a room. This model integrated a zonal model with material emission/sink models. This Integrated Zonal Model was applied to a mechanically ventilated room to simulate airflow pattern and VOC concentration distributions. Results were compared with prediction made by a CFD model. It was found that the Integrated Zonal Model could provide sufficiently reliable results and some global information regarding airflow pattern and VOC distributions within a room.

INDEX ITERMS
Zonal model, Material VOC emission/sink, VOC distribution, Mechanical Ventilation.

INTRODUCTION
Building materials play a major role in determining the indoor air quality due to their lager surface areas and permanent exposure to indoor air: they release a wide variety of pollutants, especially, the volatile organic compounds (VOC). Three kinds of models could be used to predict room air VOC concentration and they are total mixing model, CFD model and zonal model. Zonal model is an intermediate model between CFD model and mono-zone total mixing model. Compared to total mixing model, zonal model can provide users with an estimated view of airflow, temperature and contaminant distributions within a room. Zonal model has advantages over CFD model in its simple use, time saving and satisfactory precision characteristics (Haghighat et al., 2001). This paper describes the development of an Integrated Zonal Model for predicting the transient VOC distribution within a ventilated room. The model integrates a three-dimensional zonal model with air jet and material emission/sink models.

ZONAL MODEL
The physical system considered is a room with typical building materials and mechanical ventilation system. In the zonal model, the room is subdivided into a number of three-dimensional small cells. Within each cell, it is assumed that pressure at the middle of each cell obeys the perfect gas law and pressure in each cell varies hydrostatically:

$$P_{m,i} = \rho_i R T_i \tag{1}$$

$$P_{i,h} = P_{ref.i} - \rho_i g h \tag{2}$$

Where, $P_{m,i}$ is the pressure at the middle of cell i (Pa), ρ_i is the air density of cell i (kg/m^3), R is the gas constant of air (287.055 J/kg.K), T_i is the temperature of cell i (K), $P_{ref,i}$ is the reference pressure, which is located at the bottom level of cell i (Pa), h is the height from the bottom of cell i (m), $P_{i,h}$ is the pressure at the height of h in cell i (Pa) and g is the gravitational acceleration (m^2/s).

Adjacent cells exchange mass through cell interfaces. In each cell, for a steady-state condition, the general air mass balance can be written as:

$$0 = \sum_{j=1}^{6} m_{a,ij} + m_{a,source} + m_{a,\sin k} \tag{3}$$

Where, $m_{a,ij}$ is the airflow across cell i and cell j interface (kg/s), m_{source} is the air source (air supply flow rate) in cell i (kg/s) and m_{sink} is air sink (air exhaust flow rate) in cell i (kg/s).

Power law is applied to calculate airflow rate across the cell interface.

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

Where, $\dot{q}_{a,ij}$ is the airflow rate across cell i and cell j interface (kg/m^2s), ΔP_{ij} is the pressure difference between cell i and cell j (Pa), C_d is the coefficient of power law ($m/(sPa^n)$), usually taken as 0.83(Haghighat et al., 2001) and n is the flow exponent, 0.5 for turbulent airflow and 1 for laminar airflow.

Pressure at the cell bottom level is assumed to be uniform. For horizontal cell interfaces, the air flow rate can be expressed as:

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

Where, $\dot{q}_{a,hor}$ is the air flow rate across horizontal cell interface (kg/m^2s), $P_{ref,top}$ is the reference pressure of the top cell (Pa), $P_{ref,bottom}$ is the reference pressure of the bottom cell (Pa), H is the height of the bottom cell (m) and ρ_{bottom} is the air density of the bottom cell (kg/m^3).

For vertical cell interface, there is a neutral plane (Z_n) which the pressure difference between the left side and the right side of the interface is zero. The total airflow rate across the vertical cell interface becomes:

$$\dot{q}_{a,ver} = C_d \rho (\Delta \rho g)^n \frac{(Z_n)^{n+1}}{n+1} + C_d \rho (\Delta \rho g)^n \frac{(H - Z_n)^{n+1}}{n+1} \tag{6}$$

Where, $\dot{q}_{a,ver}$ is the air flow rate across vertical cell interface (kg/m^2s), $\Delta\rho$ is the density difference between the left cell and the right cell (kg/m^3) and Z_n is the neutral plane (m).

INTEGRATING JET MODEL WITH ZONAL MODEL

A jet cell contains two sub cells, one containing air belonging to the jet itself and one containing air from surrounding neighbors. The airflow crossing the interface perpendicular to the trajectory of the jet (m_p) includes the airflow from the jet (m_{jet}), and the airflow from the neighbors ($m_{neighbor}$).

$$m_p = m_{jet} + m_{neighbor} \tag{7}$$

The airflow rate provided by an air jet is modeled by the jet characteristics equations (ASHRAE, Fundamentals, 2001). The angle of divergence of the jet boundary is usually taken as 22^0 for large open space and 18^0 for small open space. The airflow from the jet can be modeled as:

$$m_{jet} = \iint V\rho d\left(S_{jet}\right) \tag{8}$$

$$\text{Where, } V = \begin{cases} V_X = V_0 & X \le 4D_0 \\ V_X = V_0 \times \sqrt{\dfrac{1.13KH_0}{X}} & 4D_0 < X \le 25D_0 \\ V_X = 10^{-\left(\frac{1}{3.3}\right)\left(\frac{r}{r_{0.5V}}\right)^2} & X > 25D_0 \end{cases} \tag{9}$$

V is the actual velocity at point being considered (m/s), S_{jet} is the jet airflow passing area, (m^2), V_x is the centerline velocity at distance X from outlet (m/s), D_0 is the effective or equivalent diameter of stream at discharge for an open-end duct or at contracted section (m), V_0 is the average velocity at discharge from outlet (m/s), X is the distance from outlet to measurement of centerline velocity (m), H_0 is the width of jet at outlet (m), K is the centerline velocity constant depending on the outlet type and discharge pattern, r is the radial distance of point under consideration from centerline of jet (m) and $r_{0.5V}$ is the radial distance in same cross-sectional plane from axis to point where velocity is one-half centerline velocity (m).

The airflow from surrounding neighbors can be modeled as:

$$m_{neighbor} = \frac{S - S_{jet}}{S} \dot{q}_a S = \dot{q}_a \left(S - S_{jet}\right) \tag{10}$$

where, S is the total area of the interface (m^2) and $\dot{q}_a$ is the airflow rate from surrounding neighbors crossing the interface (kg/m^2s).

The airflow crossing the interface parallel to the trajectory of the jet can be modeled as the airflow crossing the standard interface.

INTEGRATING MATERIAL EMISSION/SINK MODEL WITH ZONAL MODEL

VOC emissions from building materials are through three processes (Huang and Haghighat 2002): VOC diffusion within the material (Eq.11); VOC phase change at material/air interface (Eq.12); and VOC convection and diffusion in the bulk air (Eq.13). Since the VOC internal diffusion and sorption are usually considered as fully reversible phenomena and the mass fluxes depend on the direction of the concentration gradient, the sink behavior of the building materials can be modeled by setting the initial VOC concentration lower then the room air VOC concentration. Therefore, the material emission/sink model becomes:

$$\frac{\partial C_m}{\partial t} = D_m \left(\frac{\partial^2 C_m}{\partial x^2} + \frac{\partial^2 C_m}{\partial y^2} + \frac{\partial^2 C_m}{\partial z^2} \right) \tag{11}$$

$$C_m\big|_{z=b} = kC_{s,i} \tag{12}$$

$$R_i = h_m\left(C_{s,i} - C_{a,i}\right) \tag{13}$$

Initial and boundary conditions are:

$$C_m(x,y,z,0) = C_{m0}(x,y,z) \tag{14}$$

$$-D_m \left.\frac{\partial C_m}{\partial z}\right|_{z=b} = h_m\left(\frac{C_m|_{z=b}}{k} - C_{a,i}\right) \tag{15}$$

$$\left.\frac{\partial C_m}{\partial z}\right|_{z=0} = 0 \tag{16}$$

Where, C_m is VOC concentration in the material (μg/m^3), D_m is VOC diffusion coefficient of the material (m^2/s), C_{m0} is VOC initial concentration in the material (μg/m^3), k is material/air partition coefficient, $C_{s,i}$ is the VOC concentration in the near material surface air in cell i (μg/m^3), $C_{a,i}$ is the VOC concentration in the air in cell i (μg/m^3), h_m is the convective mass transfer coefficient (m/s), R_i is the material VOC emission rate in cell i (μg/m^{2}s), b is the material thickness (m) and t is time (s),

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

$$\frac{M_{a,i}}{\rho_i}\frac{dC_{a,i}}{dt} = \sum_{j=1}^{6} m_{VOC,ij} + m_{VOC,sorce} + m_{VOC,\sin k} \tag{17}$$

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

APPLICATION

The Integrated Zonal Model was applied to simulate a room with a three-dimensional compact jet and an outlet on the ceiling. The dimension of the room was 3.0×3.0×2.7m^3. The inlet airflow rate was 0.08kg/s. It was assumed that the room is at an isothermal condition with a temperature of 20 °C. The geometries of the room are shown in Figures 1.

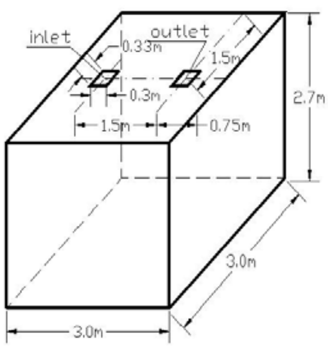
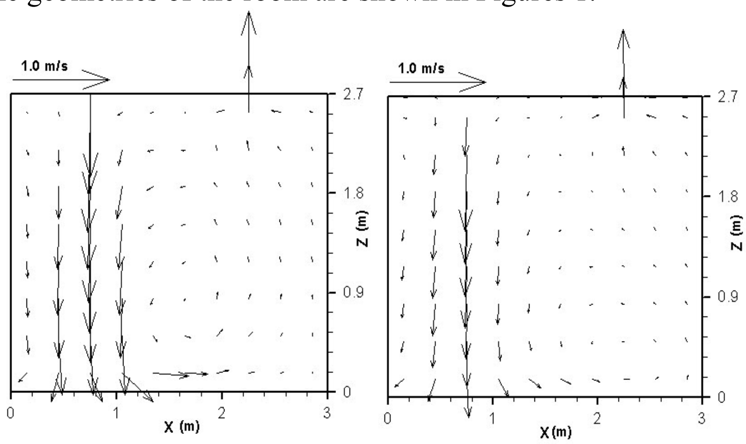


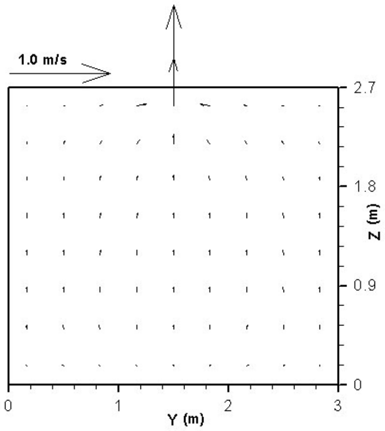
Figure 1:
Geometry of the room

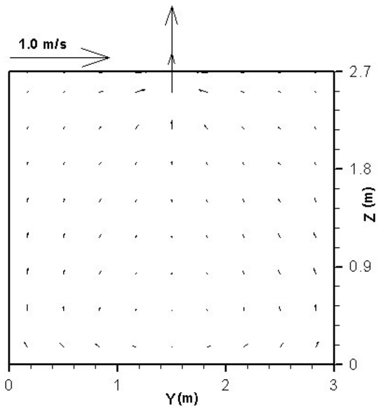


Integrated Zonal Model FLOVENT (Jiang, 2002)
Figure 2: Comparison of airflow pattern (Y=1.5m)

The walls of this room were decorated with plywood and the floor was covered with Vinyl floor tile. The Integrated Zonal Model was used to simulate the airflow pattern within the room and the results were compared with that of FLOVENT (Jiang, 2002). A 10×9×8-simulation grid was used for both models.

Figure 2 shows the airflow patterns in the middle section of the room (Y=1.5m) simulated by the Integrated Zonal Model and the CFD model. This figure shows both models detected a strong air stream located around the centerline of the jet. Both models also detected a circulation on the right side of the jet centerline: there is, however a small discrepancy. The airflow patterns at the outlet centerline section (X=2.25m) predicted by both models are illustrated in Figure 3. Even though there was a small discrepancy for the values of velocities, the airflow patterns at this section followed the same trend in both models.





Integrated Zonal Model FLOVENT (Jiang, 2002)

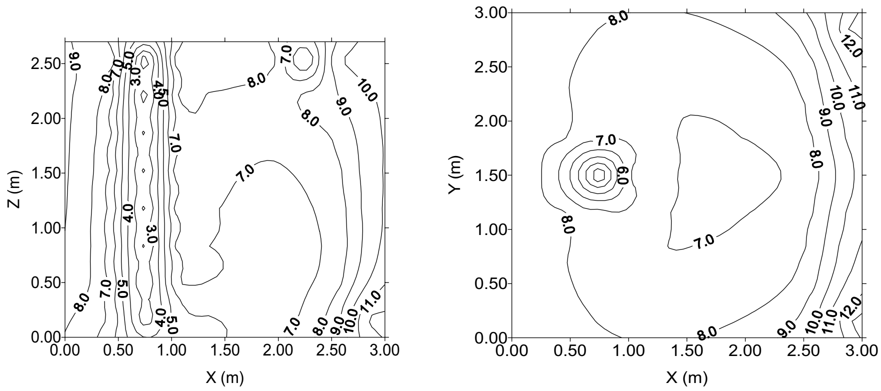
Figure 3: Comparison of airflow pattern (X=2.25m)

For VOC distribution prediction, we considered that other materials might adsorb some VOC emitted from an emitting material. VOC emitted from source materials and VOC adsorbed by sink materials affect indoor air quality synchronically. To simulate this scenario, we assumed that the vinyl floor tile as the source material and the plywood walls as the sink materials. Toluene was chosen as the compound of interest, since toluene is one of the VOC compounds in the vinyl floor tile and is not in the plywood. The properties of the toluene in vinyl floor tile and plywood were obtained from literature (Plett, et al., 2001), they are listed in Table 1.

Table 1 Properties of toluene in plywood and vinyl floor tile

Parameters	C_0	D_m	k	b
(unit)	(μg/m^3)	(m^2/s)	(—)	(m)
Plywood	1.0×10^7	1.75×10^{-10}	358	0.016
Vinyl floor tile	1.0×10^7	5.42×10^{-10}	539	0.003

Toluene concentration distributions in the middle section of the room (Y=1.5m) and at the height of a seated person (Z=1.18m) are graphically displayed in Figure 4 after room was ventilated for 12 hours. Toluene concentration around jet centerline region was much lower than the other regions due to the fresh air directly coming down from the jet. Compared with the average toluene concentration in the room air (8.3 μg/m^3 at 12h), except in the near east wall region, toluene concentration at the height of a seated person was lower than the average concentration. This indicates that this air distribution system provided good air distribution and has able to efficiently remove contaminant from the room.



Y=1.5m Z=1.18m

Figure 4: Toluene concentration distribution after 12 hours

7. CONCLUSIONS

An Integrated Zonal Model was developed to predict the three-dimensional airflow pattern and VOC concentration distribution in a ventilated room. This model integrated a zonal model with an air jet model and material VOC emission/sink model.

This Integrated Zonal Model was utilized to simulate the airflow pattern and VOC distribution in a room with a compact jet. The airflow pattern predicted by the Integrated Zonal Model was compared with that of FLOVENT. Both models detected similar airflow patter. Moreover, it was found that VOC concentration was not uniform in the space and it was affected by the air distribution system.

Overall, the Integrated Zonal Model, with quite coarse mesh, can provide sufficiently reliable results and some global information regarding airflow pattern and VOC distributions within a room. The model can be used to exam the ventilation strategy efficiency. Further, it was found that the Integrated Zonal Model is a feasible approach for building material VOC emission/sink and VOC distribution analysis from the viewpoint of engineering.

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