

Applications of a Coupled Multizone and CFD Model to Calculate Airflow and Contaminant Dispersion in Built Environment for Emergency Management

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ABSTRACT

Current simulation tools of airflow and contaminant dispersion in built environment cannot provide detailed information with little computing effort, which is critical for emergency management. Multizone airflow network models are fast but cannot provide detailed flow and contaminant transport information in an indoor space. Computational Fluid Dynamics (CFD), on the other hand, gives very detailed information whereas needs hours or days of computing time on a PC. A coupled multizone-CFD model can offer detailed information of contaminant dispersion while reduce the computing time. The study presented in this paper applied the coupled model to calculate airflow and contaminant dispersion in a three-story, naturally ventilated building with a large atrium, assuming that a contaminant was released in the atrium. This investigation studied the effectiveness using emergency ventilation to protect the building occupants. It was demonstrated that the coupled model can provide important information of contaminant distributions with a reasonable computing time. The information is useful for evaluation of placement of contaminant sensors and determination of evacuation strategies for the emergency management.

Key words: Multizone, CFD, Coupled model, Contaminant Dispersion, Emergency

INTRODUCTION

The attacks on September 11, 2001 in the World Trade Center and the following anthrax cases spawned serious concerns about various possible terrorist attacks in built environment, including releases of Chemical, Biological, Radiological Warfare Agents (CBRWA) in buildings and subways (Stenner et al. 2001). The anthrax attacks through letters in Florida, New York City, and Washington, DC caused 5 deaths and affected over 20 other people in 2001 (Ko 2003). In March of 1995, the Japanese cult Aum Shinrikyo used Sarin to attack the Tokyo subway system that caused 12 deaths and hundreds hospitalized. Once entering a building, CBRWA could disperse quickly in the whole building through the HVAC system. Therefore, to design a built environment that can protect its occupants from these threats, it is crucial to know how a CBRWA is dispersed after its release.

A popular tool to predict CBRWA dispersion is multizone network model, e.g. CONTAM (Walton and Dols 2003) and COMIS (Feustel 1999). Kowalski et al. (2003) used CONTAM to evaluate the performance of air cleaning and disinfection systems against CBRWAs for a 40-story office building. Their results indicated that the office building could be protected by using affordable air filters combined with ultraviolet germicidal irradiation. A multizone airflow simulation helped Li et al. (2005) to find that natural ventilation may have helped circulate SARS viruses at a building complex in Hong Kong. Multizone models use simple flow mass balance equations so they need little computing time but assume well-mixed contaminant in a zone (or a room).

However, Schaelin et al. (1994) and Upham (1997) noticed that the results of a multizone model may not be accurate enough when the well-mixing assumption was used for cases with non-uniform distributions of contaminant concentrations. Wang and Chen (2007b) studied the non-uniform distribution of a contaminant in a four-zone building and found that the well-mixing assumption could cause significant inaccuracy in the calculation of contaminant distribution. The problem is especially severe in large spaces with contaminant dispersion at transient state. Since the flow resistance to define a subzone for a large space is unknown, a multizone model has to simulate a large space as a single zone, which causes apparent errors for building ventilation designs as found by Jayaraman et al. (2004), and Wang and Chen (2007b). To provide more detailed contaminant information in a zone, especially for large space simulation, more sophisticated models, such as Computational Fluid Dynamics (CFD), are used.

CFD can provide very detailed information of contaminant transport in a zone. Boris (2002) used CFD to simulate atmospheric contaminant dispersion in downtown Portland, Oregon and provided superb spatial resolution of contaminant concentrations. Zhai et al. (2003) applied CFD

to predict CBRWA dispersion in buildings and determined the best locations of CBRWA sensors. However, compared to multizone models, CFD calculations normally use hours or even days of computing time. CFD is a very slow tool for finding CBRWA dispersion during a CBRWA release (Settles 2006).

A better approach would integrate a multizone model with a CFD model. The CFD model is only applied to zones where the well-mixing assumption of multizone methods fails. The coupled multizone-CFD model can thus reduce the computing time if compared with a CFD-alone simulation of a whole building; and can provide more accurate results than a multizone-alone simulation. Jayaraman et al. (2004) showed that the calculated personal exposure to contaminants by a coupled multizone-CFD model is more reasonable than that of a multizone model, especially for buildings with large spaces. Wang and Chen (2007b) demonstrated that a coupled multizone-CFD model can predict better contaminant distributions than a multizone model in an experimental chamber with four rooms. However, most of the previous studies are limited to simple two-dimensional cases and/or idealized conditions at steady state. Since airflow and contaminant dispersion in built environment under a CBRWA attack are transient and three-dimensional, it is necessary to examine further the capability of a coupled multizone-CFD model to such scenarios.

This study is to demonstrate a coupled multizone-CFD model, which used a stable integration method (Wang and Chen 2007a), for simulating airflow and contaminant dispersion in a complex three-story building under a CBRWA attack. The simulations are for both steady and transient states to show the problems of the well-mixing assumption for a large space, to evaluate the effectiveness of emergency ventilation, to determine the optimal placement of sensors, and to determine evacuation routes for building occupants.

METHODS

This section briefly explains the fundamentals of the coupled multizone-CFD model. A multizone model, such as CONTAM, calculates airflow and contaminant distributions between the zones of a building and between the building and its outdoors. If airflow path ij connects zone i and zone j and F_{ij} is the airflow rate through path ij , we define the default positive direction of F_{ij} to be from zone i to zone j . F_{ij} is often calculated by a multizone model with a power-law function of the pressure drop, ΔP_{ij} , across path ij ,

$$F_{ij} = \alpha_{ij} c_{ij} |\Delta P_{ij}|^{n_{ij}} \quad (1)$$

where, c_{ij} is the flow coefficient, n_{ij} is the flow exponent of path ij , $\alpha_{ij} = (P_i - P_j)/|P_i - P_j|$, P_i and P_j is the total pressure at either zone i or j side of path ij , respectively. For each zone, a multizone model solves air mass balance equations under steady state condition for zone j as

$$\sum_i F_{ij} + F_j = \sum_i \alpha_{ij} c_{ij} |\Delta P_{ij}|^{n_{ij}} + F_j = 0 \quad (2)$$

where, F_j is the air mass sources in zone j .

Similarly, contaminant/species mass balance at steady state condition in zone j is,

$$\sum_i F_{ij} C_{ij} + S_j = 0 \quad (3)$$

where, $C_{ij} = C_i$ when the airflow is from zone i to zone j ($F_{ij} > 0$) and $C_{ij} = C_j$ when the airflow from zone j to zone i ($F_{ij} = -F_{ji} < 0$); C_i and C_j are the contaminant concentrations in zone i and zone j , respectively; F_{ij} is the airflow rate from zone i to zone j ; and S_j is the contaminant sources inside zone j . The multizone model assumes the air and contaminant in each zone is well mixed so that there is one unknown zone pressure and contaminant concentration for each zone. With Eqs. (2) and (3) applied for each zone, N zones will have N unknown zone pressures and contaminant concentrations and a series of air and contaminant mass conservations are obtained. The model further assumes that the transport of contaminants along each flow path or within a zone is temporally instantaneous. Clearly, the applicability of these assumptions can be limited in some zones, such as atria, lobbies, conference rooms, long corridors, etc.

A CFD model calculates detailed spatial distribution of air pressure, air temperature, and contaminant concentration that can be used to remedy the problems created by the mixing assumption in a multizone model. The most popular CFD models for calculating airflow and contaminant transport in buildings are the Reynolds Averaged Navier-Stokes (RANS) equations with turbulence models (Emmerich 1997). A RANS model, such as CFD0 (Srebric et al. 1999), solves a set of partial differential governing equations for mass, momentum, energy, and species conservation. The equations can be written in a general form (Patankar 1980):

$$\sum a_{\phi, nb} \phi_{nb} - a_{\phi, P} \phi_P + b_{\phi} = 0 \quad (4)$$

When the ϕ stands for pressure (P), Eq. (4) becomes the mass continuity equation; for air velocity component (U , V , and W), it becomes the momentum equations; for temperature (T), it

becomes the energy conservation equation; and for species concentration (C), it becomes the species conservation equation.

Our coupled multizone-CFD model integrates CONTAM and CFD0 by applying CFD0 to the zones where the well-mixing assumption fails and CONTAM to the remaining zones. The solving procedure is realized through a mode of “CONTAM – CFD0 – CONTAM” so that the output of one program becomes the input of the other. When both inputs and outputs stabilize (their values do not change), the solution of the coupling is considered convergent (Wang and Chen 2007a). However, the coupling can be unstable if the boundary conditions are incorrectly exchanged (Negrao 1998; Bartak et al. 2002). The best coupling method is to assemble a matrix equation by linearizing and combining Eqs. (2) and (4) for pressure:

$$CP + F = B \quad (5)$$

where C is the airflow coefficient matrix; P is the pressure vector of zones and cells; F is the flow rate vector of paths and cells at multizone and CFD zone interfaces; and B is the vector of air mass sources.

A stable and convergent solution of Eq. (5) can be achieved when CONTAM gives pressure boundary conditions to CFD0 and CFD0 returns pressure boundary conditions to CONTAM, i.e. “the pressure-pressure coupling method” (Wang and Chen 2007a). The coupled CONTAM-CFD0 model will apply CFD equations to the zone, where CFD0 is needed, and obtain a local pressure to be used as boundary condition for CONTAM. Then the CFD zone is removed from CONTAM equations and a CONTAM simulation is performed to provide pressure boundary condition for the next run of CFD0. When the inputs and outputs of CONTAM and CFD0 stabilize, the coupled simulation is considered convergent. The coupled program has also been validated by using experimental data obtained in a four-zone facility (Wang and Chen 2007b). The calculated results by the coupled model generally agree well with the experimental data for non-uniform distributions of airflows and contaminant concentrations in built environment. The coupled CONTAM-CFD0 model is therefore used here for studying airflow and contaminant dispersion in a three-story building.

CASE SETUP

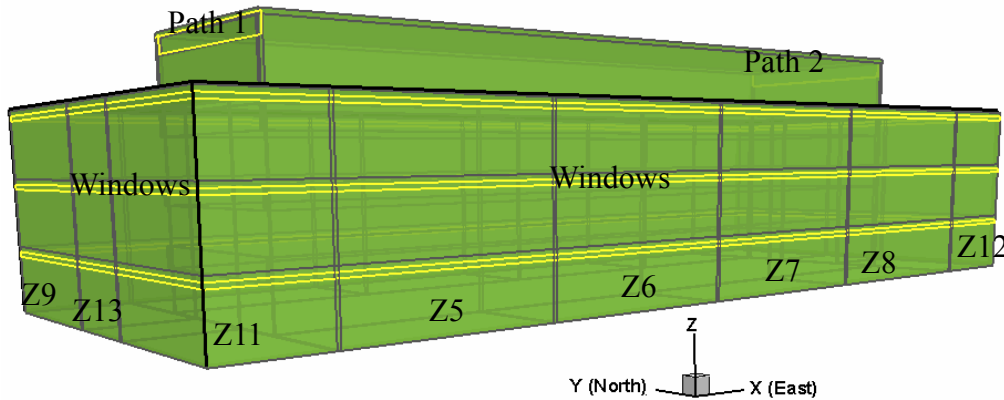
To demonstrate how the coupled CONTAM-CFD0 model, this study used a three-story building as shown in Figure 1. The building had a large atrium in the center and used natural ventilation. Natural ventilation does not have a pre-defined pattern of airflow distribution, so it is more challenging to calculate contaminant dispersion in the building. The building was very large with the room dimension as follows:

- Zones 1-8: 12 m×6 m×2.7 m
- Zones 9-12: 6 m×9 m×2.7 m
- Zones 13-14: 6 m×5 m×2.7 m
- Atrium: 48 m ×11 m×10.8 m

The flow paths on the building external walls were open windows with a height of 0.2 m and the same width as the rooms. The remaining flow paths in Figure 1 were sized as follows (height × width):

- Path 63 - 66 and Path 78 - 81 : 0.9 m × 12 m
- Path 69, 70, 75, and 76: 0.9 m × 3 m
- Path 73 and 74: 0.9 m × 5 m
- Path 1 and 2: 0.7 m × 11 m

Figure 1(c) shows the building model for the first story in CONTAM, which was the same for the other two stories. Note that Figure 1(c) was not the building in real scale but only the modeled building in CONTAM. The symbol “◇” in CONTAM represents an airflow path. The flow paths at the corner zones of the building were simulated as a single leakage path to simplify the simulation, for example, the two external windows of Z11 were combined as Path 77 in Figure 1(c).



(a)

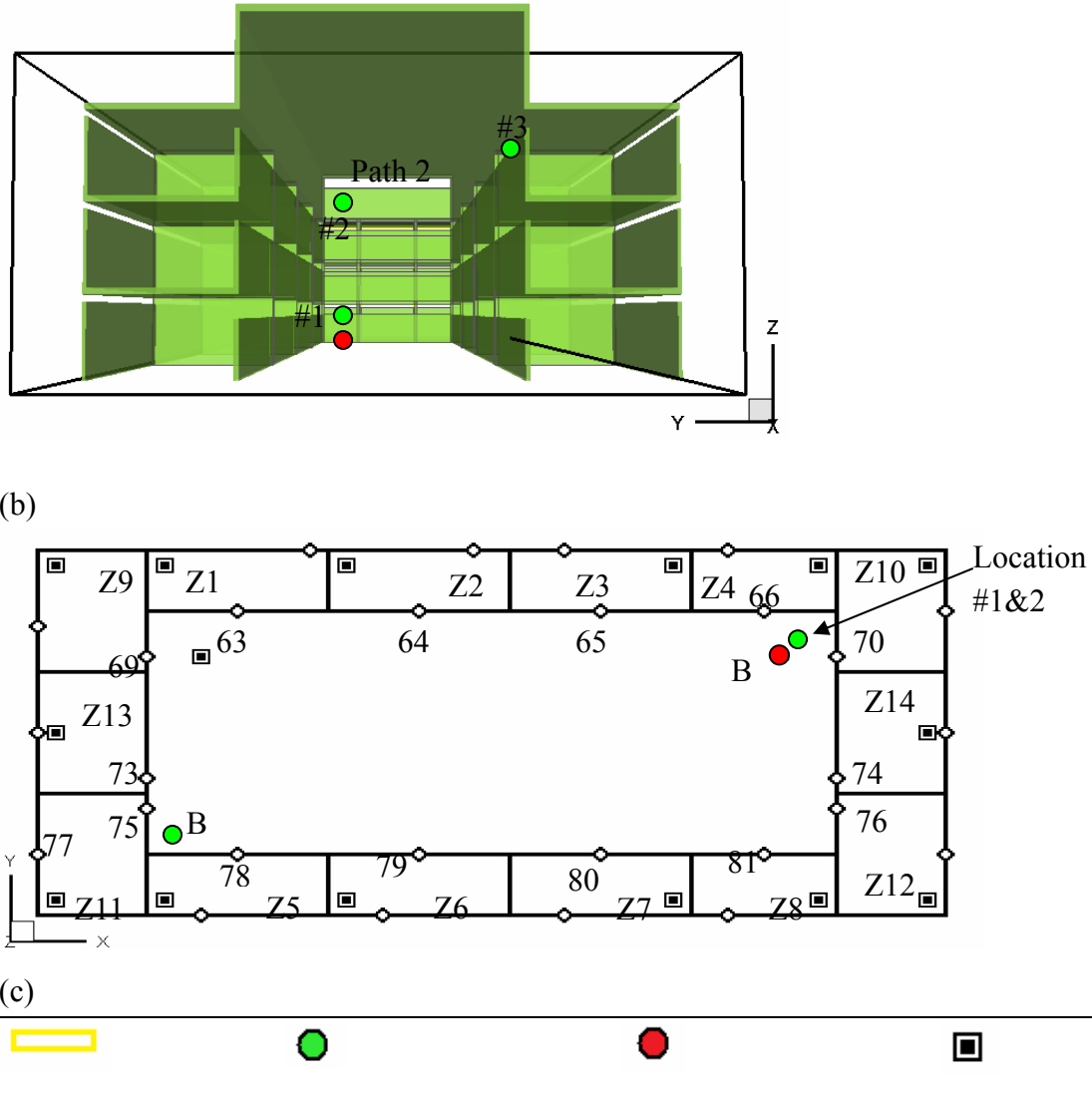


Figure 1. Views of the three-story building with natural ventilation (a) Outside perspective view; (b) Inside perspective view; and (c) Building model in CONTAM with a contaminant source of C1.

The cooling load was set to 40 W/m^2 for the occupied zone ($0 - 1.8 \text{ m}$ above the floors) in the rooms and the atrium. The mean wind speed was assumed to be at a constant of 10 km/h from the west, the mean outdoor air temperature to be 15°C , and the mean relative humidity to be 70% . This study also assumed that a gaseous contaminant (hereafter C1) was released by a terrorist in the northeast corner of the atrium on the ground floor (Figure 1(c)) at a constant rate of $1.0 \times 10^{-5} \text{ kg/s}$. Since the C1 concentration cannot be uniform for such a large atrium, the well-mixing assumption would not work well. This study therefore selected the central atrium as the CFD zone and applied CONTAM to the remaining zones in the building.

RESULTS AND DISCUSSION

Steady Airflow and Steady Contaminant Transport

The coupled CONTAM-CFD0 simulations were first used for airflow and contaminant transport in the building under steady state. CFD0 divided the central atrium into $104 \times 27 \times 40$ (X×Y×Z) grid cells. CONTAM used the orifice equation (Walton and Dols 2003) for the airflow paths of the remaining zones. The convergence criterion was 0.1% for the CFD0 calculation and 1% for the coupled simulation. Twenty-five iterations between CONTAM and CFD0 were required for convergence. The total computing time was about 72 minutes on a 2.0 GHz Pentium IV PC.

Figure 2 compares the net airflow rates of the paths of the atrium calculated with the CONTAM-CFD0 model (with coupling) and with only CONTAM model (CONTAM alone). Here “net airflow rate” refers to that for paths with bi-directional airflow (both inflow and outflow through a path), the airflow rate was reported as the sum of the inflow and outflow. The atrium had 44 airflow paths (14 paths on each floor and two at the atrium top). Figure 2 shows only the airflow paths connecting the atrium to the ambient (Path 1 and 2), and paths connecting neighboring zones and the atrium. When the mass conservation for each neighboring zone of the atrium was obtained, the flow from neighboring zone to outdoors equals that of the path connecting to the atrium. Therefore, we did not show the airflow rates of the outflows from neighboring zones to outdoors in Figure 2. Except for the paths at Levels 2 and 3, the flow rates through some paths at Level 1 and through the two paths at the atrium top (the red numbers in Figure 2) are significantly different with the coupled program and multizone model alone. If a positive value is for inflow to the atrium and a negative one for outflow, the inflow through Path 1 increased from 4.1 kg/s to 7.0 kg/s. The airflow rate of Path 1 was considerably different from Path 2 after the coupled simulation, which can be explained by the changed airflow directions of Paths 63 through 66 and 78 through 81. Figure 2 shows that with the multizone simulation, the total flow rate of Path 63 - 66 and Path 78 - 81 together was about +2.5 kg/s (inflow to the atrium) while the flow rate of these paths was -1.9 kg/s (outflow from the atrium). The resulting difference of Path 1 (inflow to the atrium) and Path 2 (outflow from the atrium) was about $1.9 + 2.5 = 4.4$ kg/s with the coupled simulation, considering the airflows of the remaining paths changed relatively small after the coupled simulation as shown by Figure 2.

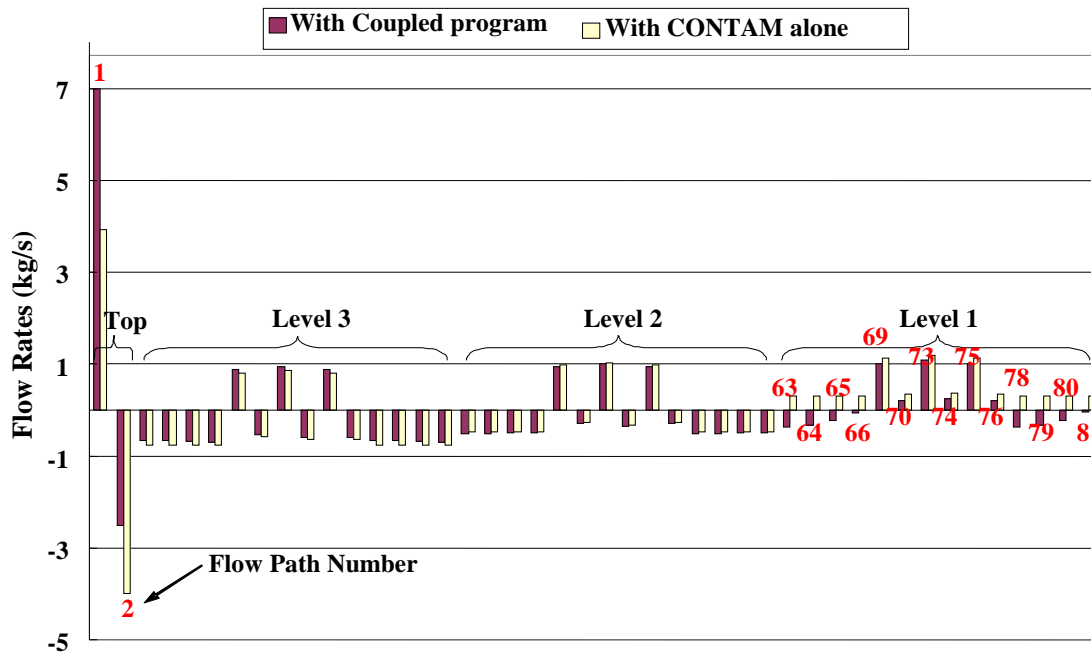


Figure 2. Comparison of net airflow rates of the atrium paths with the coupled CONTAM-CFD0 program and with CONTAM alone.

The changes of airflows with the coupling could be explained by the non-uniform distribution of temperature and pressure inside the atrium. Figure 3 illustrates the airflow and temperature distributions at section Y=5.5 m in the atrium (The CONTAM zones are also shown in the figure for comparison). Due to the buoyancy effect, the west wind from the top-left in the atrium with a temperature of 15°C traveled downwards after entering Path 1. The cold air then flowed along the atrium floor and rose at the right end of the atrium so that a huge recirculation zone was formed in the atrium. The temperature difference was about 4°C in the horizontal direction and 3°C in the vertical direction. Therefore, the assumption of uniform air temperature is not good for this case.

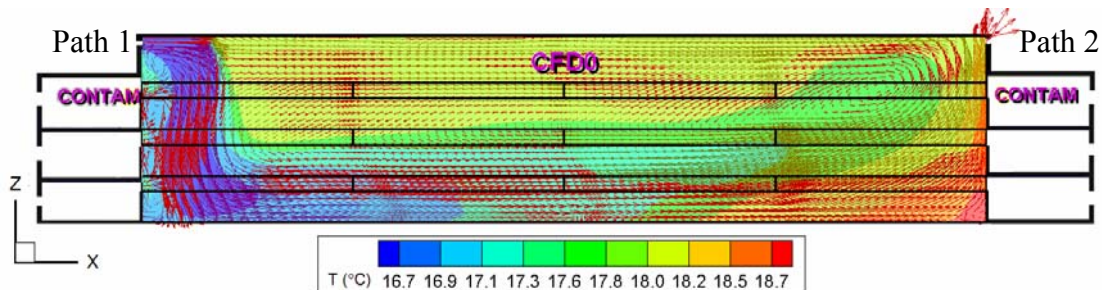


Figure 3. Velocity distribution and temperature contour at the middle vertical section of the atrium (Y=5.5m).

The significant changes in airflow rate, especially the change of flow directions, greatly affected the contaminant transport. Figure 4 illustrates the results of C1 concentration at four horizontal planes in the atrium. The positions of the planes are shown in Figure 5. With CONTAM alone, all the neighboring zones of the atrium in Figure 4(a) had zero C1 concentrations because the atrium has only inflows from all the neighboring zones. With coupling, the flows at Paths 63 through 66 and 78 through 81 became outflows for the atrium, so the C1 concentrations were non-zero for the neighboring zones 1 through 8. The closer the neighboring zone was to the source, the higher the C1 concentration of the neighboring zone.

Besides the global airflow directions, the detailed airflow pattern also played an important role for contaminant dispersion in the building. Although the airflow directions in Figure 4(b) and Figure 4(c) do not change after the coupled simulation, the airflow pattern inside the atrium caused poorly-mixed C1 concentration. The coupled simulation was able to calculate more detailed and likely accurate C1 concentrations than CONTAM alone. The airflow pattern can also cause highly non-uniform distribution of C1 concentrations inside the atrium. For example, the C1 concentration marked by the red circle in Figure 4(c) was lower than the surroundings, which could be explained by the airflow pattern in Figure 5. At the circled region, the fresh air moved upwards so the concentration inside this region at the P3 plane is lower than the surroundings. The same reason can be applied to the circled region in Figure 4(b). The impact of airflow patterns on the C1 distribution can further be observed for the P4 plane in Figure 4(d). The fresh air moved downwards after entering the atrium for about five meters and the air flowing leftward at the right side of the atrium top (Figure 3). Therefore, the C1 concentration at the right of the atrium top was higher than that at the left.

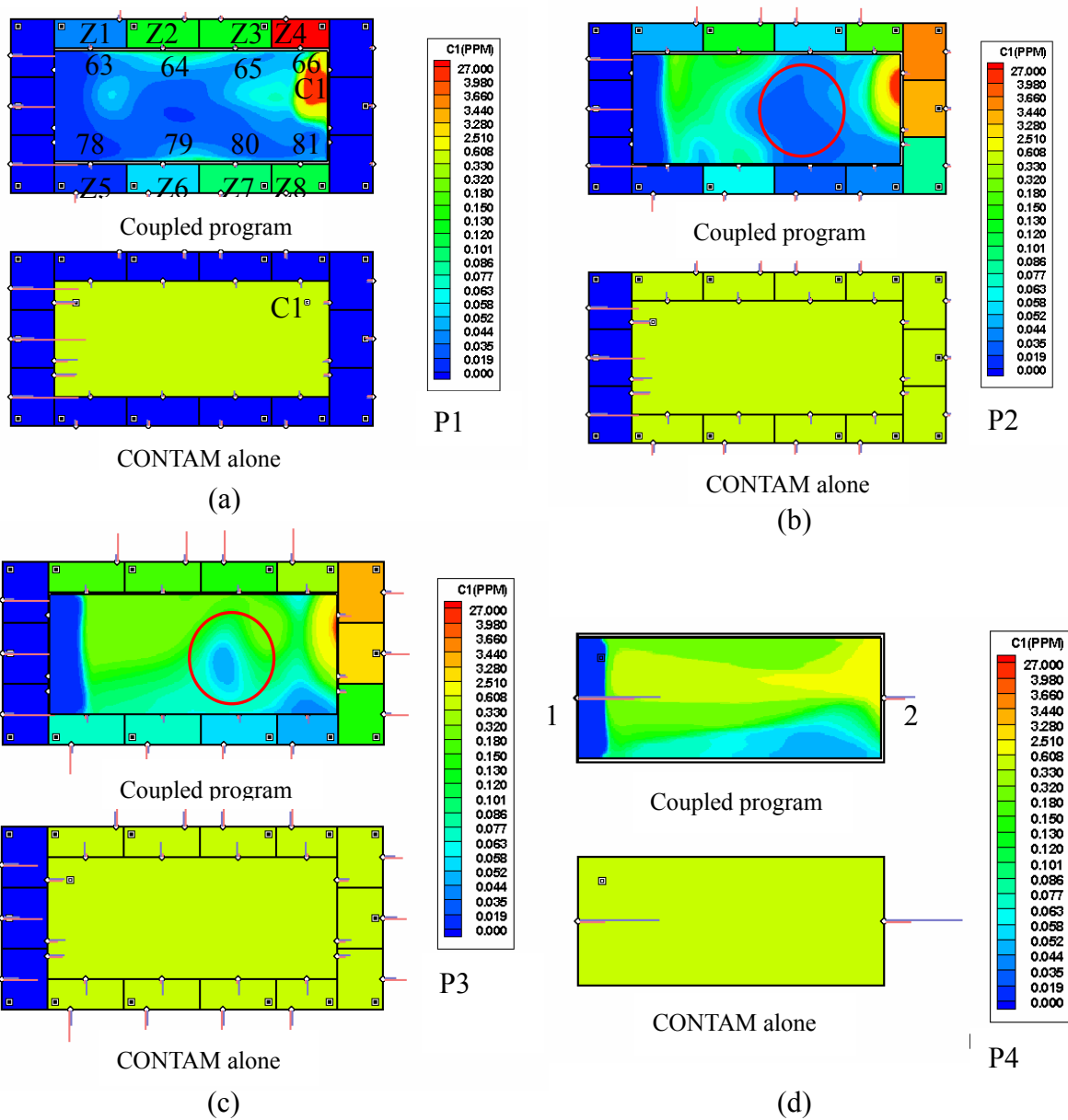


Figure 4. Comparison of C1 concentrations with the coupled program and CONTAM alone at (a) Plane 1 (P1, Z = 2.35 m); (b) Plane 2 (P2, Z = 5.05 m); (c) Plane 3 (P3, Z = 7.75 m); and (d) Plane 4 (P4, Z = 10.45 m) (The plane locations were defined in Figure 5).

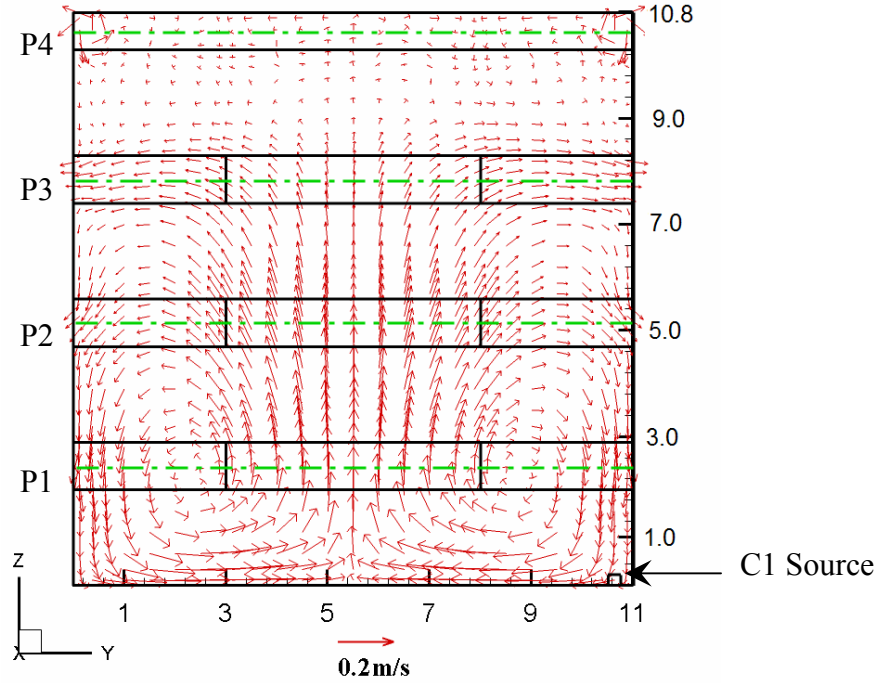


Figure 5. Velocity distribution at cross section $X = 30$ m.

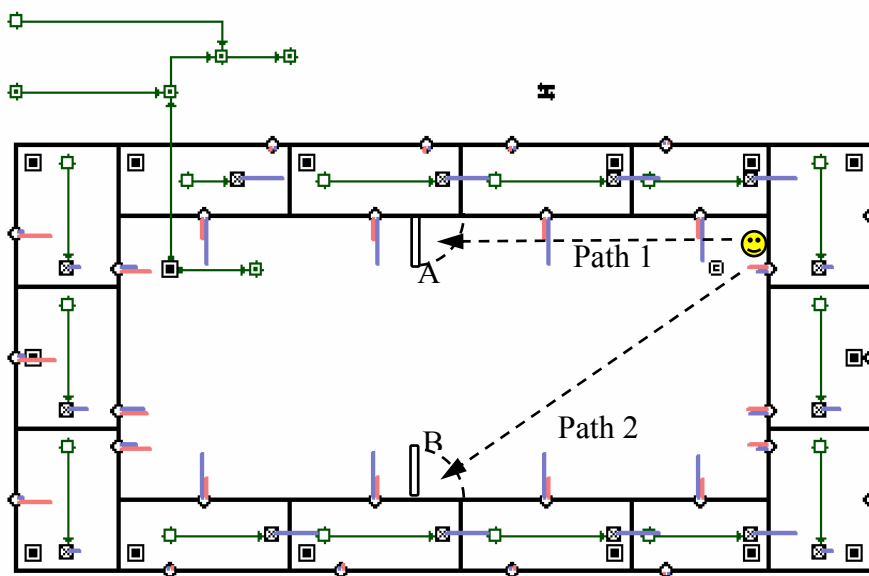
With the coupled multizone-CFD model, the results obtained seem more accurate compared with those simulated by the multizone model alone. In terms of computing time, this study did not simulate the whole building with CFD0, since the current version of CFD0 can only simulate buildings with cuboid shape. However, the coupled simulation used CFD for only one zone (the atrium). It would require much less computing time, compared with that if the CFD is applied to the whole building.

Transient Airflow and Transient Contaminant Transport

In reality, both the airflow and contaminant transport in the three-story building can be transient. The coupled CONTAM-CFD0 model can calculate transient airflow and contaminant dispersion. The calculated results can be very useful to evaluate the placement of contaminant sensors, for assessing the effectiveness of using emergency ventilation, and for developing strategies to evacuate the building occupants in case of a contaminant release.

The study for transient state used a contaminant source for the building at the same location as that for the steady state in the previous section with zero source strength at time $t < 0$ and the same constant rate of 1.0×10^{-5} kg/s at time $t \geq 0$ (step function). As shown in

Figure 6, this case used a simple emergency ventilation system in the building. The system can supply clean outdoor air through supply vent to each room on each floor of the building and can extract air from the eight exhaust fans (EF) at the atrium ceiling. If the contaminant sensor in the building detected an internal contaminant release at a concentration higher than a certain level, for example, 0.1 ppm in this case, it would activate the emergency ventilation. Based on suggestion from Klotz and Milke (2002), the total flow exhausted was designed to be 22 ACH (125,000 m³/h) for the atrium and the flow rate supplied through the room supply vent was 15 ACH for each of the remaining zones in the building (total 104,000 m³/h). The clean make-up air came from the openings on the building envelop and the two openings at the top of the atrium, Paths 1 and 2. Thus, the building was at negative pressure when the emergency ventilation system was on.



(a)

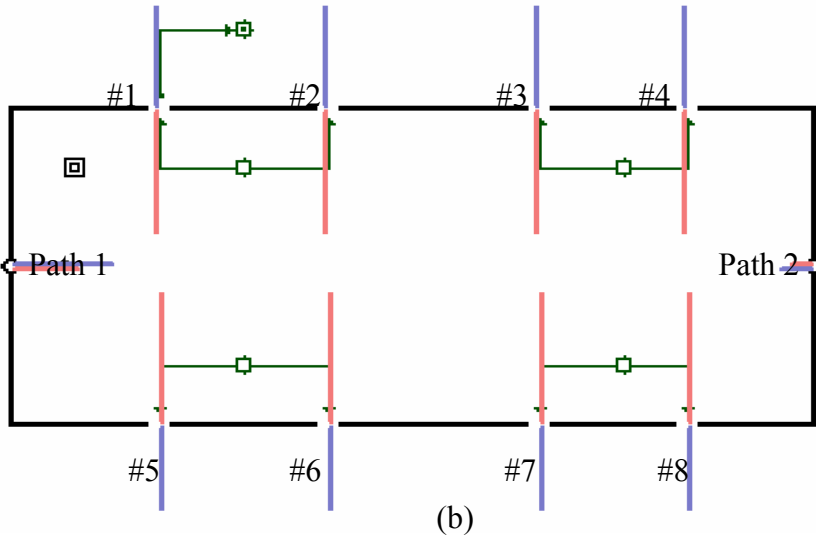
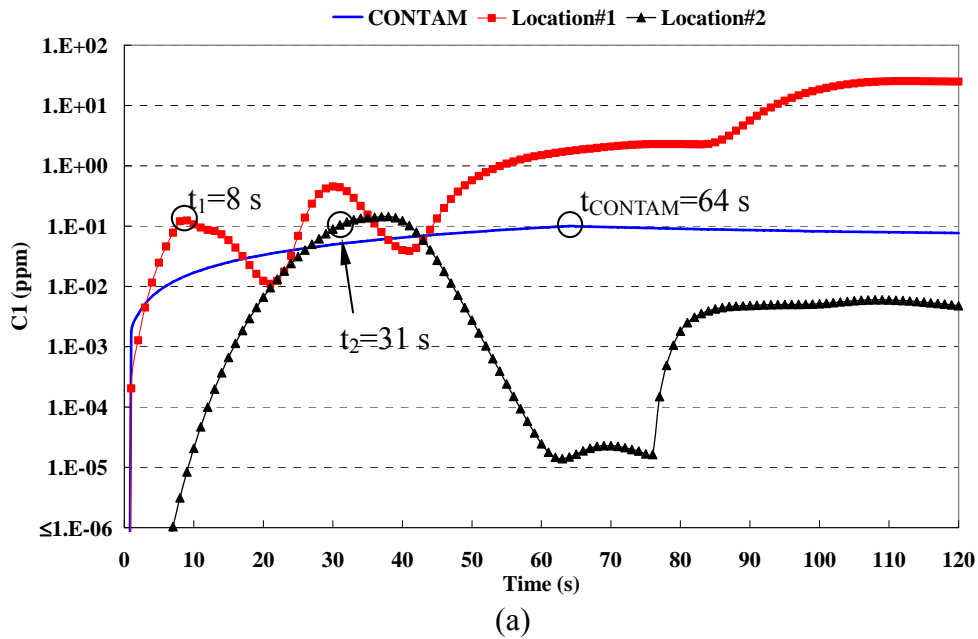


Figure 6. Emergency ventilation system and its airflow distribution calculated by CONTAM (a) at the first floor and (b) the atrium top.

Suppose a contaminant sensor could be placed in three different locations as shown in Figure 1. Since Location #2 was vertically right above Location #1, they appear to be at the same location in the plan view of Figure 1(c). Apparently, if a sensor is placed very close to the contaminant source, it can respond very fast. However, CONTAM would predict the same response time for all the sensors placed in the atrium due to the well-mixing assumption. The coupled CONTAM-CFD0 program can evaluate the three sensor locations by predicting how the sensor responds to contaminant release. As shown in Figure 7(a), the coupled CONTAM-CFD0 model calculated very different response times for the three sensors. CONTAM calculated that C1 concentration in the atrium reached 0.1 ppm 64 s after the C1 release. The coupled CONTAM-CFD0 model determined that the sensor at location 1 would reach 0.1 ppm in as short as 8, and location 2 in 31 s, and location 3 more than 10 min, because the contaminant distribution was highly non-uniform. The C1 concentration calculated location 3 was not shown, since it was close to zero during the first 120 s after the C1 release. Sensors 1 and 2 were very close to the contaminant

source so their response time was short. Figure 7(a) also shows that the calculated C1 concentration by the coupled simulation increased steadily in the beginning whereas fluctuated dramatically after the emergency ventilation was on. It was caused by the significant change of airflow pattern caused by the emergency ventilation as shown by Figure 7(b). If the positive flow direction is +X for U, +Y for V, and +Z for W, all the velocity components U, V, and W at sensor location #1 reversed to negative flow after the emergency ventilation was on. Especially, the W velocity component changed so dramatically so that the fresh air from the neighboring zone of sensor #1 prevented the contaminant spreading upwards. Figure 8 provided a close look at the airflow pattern. At 22 s in Figure 8(b), sensor #1 was surrounded by air with low C1 concentration, which explains the lowest C1 level was obtained at the same time in Figure 7(a). The velocity components stabilized after 120 s. As a result, the C1 concentration reached the steady state too.



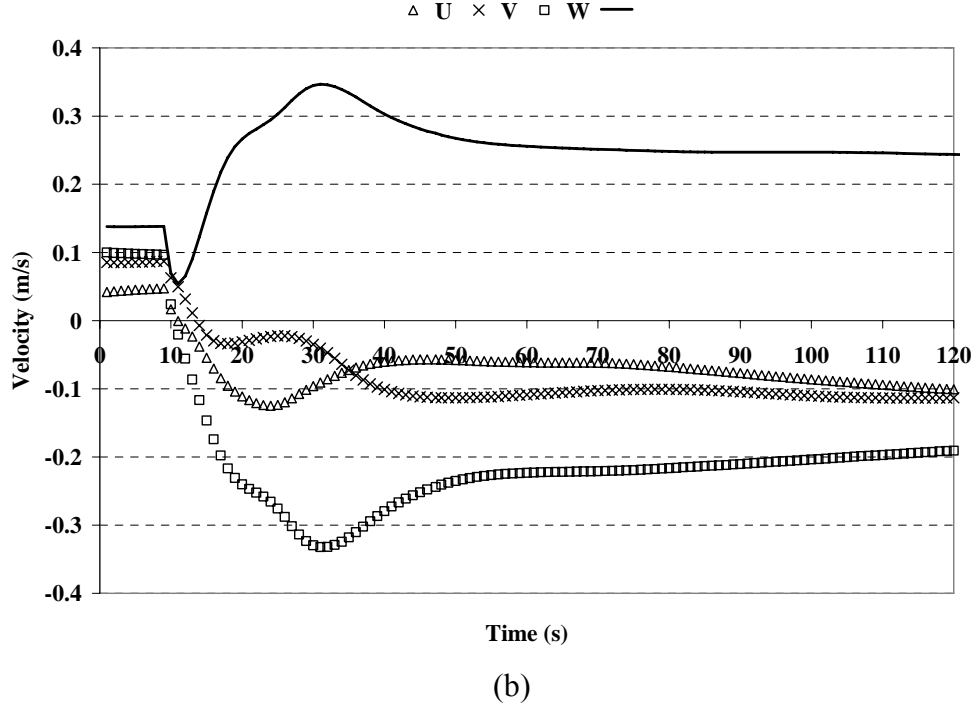


Figure 7. (a) C1 concentration computed by CONTAM and by the coupled CONTAM-CFD0 program at sensor 1 or 2 and (b) calculated velocity component U, V, W (positive in +X, +Y, +Z direction, respectively) and scalar velocity $\bar{v} = \sqrt{U^2 + V^2 + W^2}$ by the coupled program for sensor location #1.

By using the information from the sensors to activate the emergency ventilation, the building could be protected or unprotected depending on the sensor locations. When the contaminant sensor was at location #1, Figure 8(c) shows that the ceiling exhaust fans removed the contaminant effectively, make-up fresh air was drawn into the atrium through Path 2, and most areas of the building were well protected. When the sensor was placed at location 3, the ceiling fans were not activated even at the end of 10 min. The contaminant could disperse very far in the atrium from the source as illustrated by Figure 8(d). The C1 concentration was mostly more than 0.1 ppm. The building was not protected from such a terrorist attack if the emergency ventilation was not turned on.

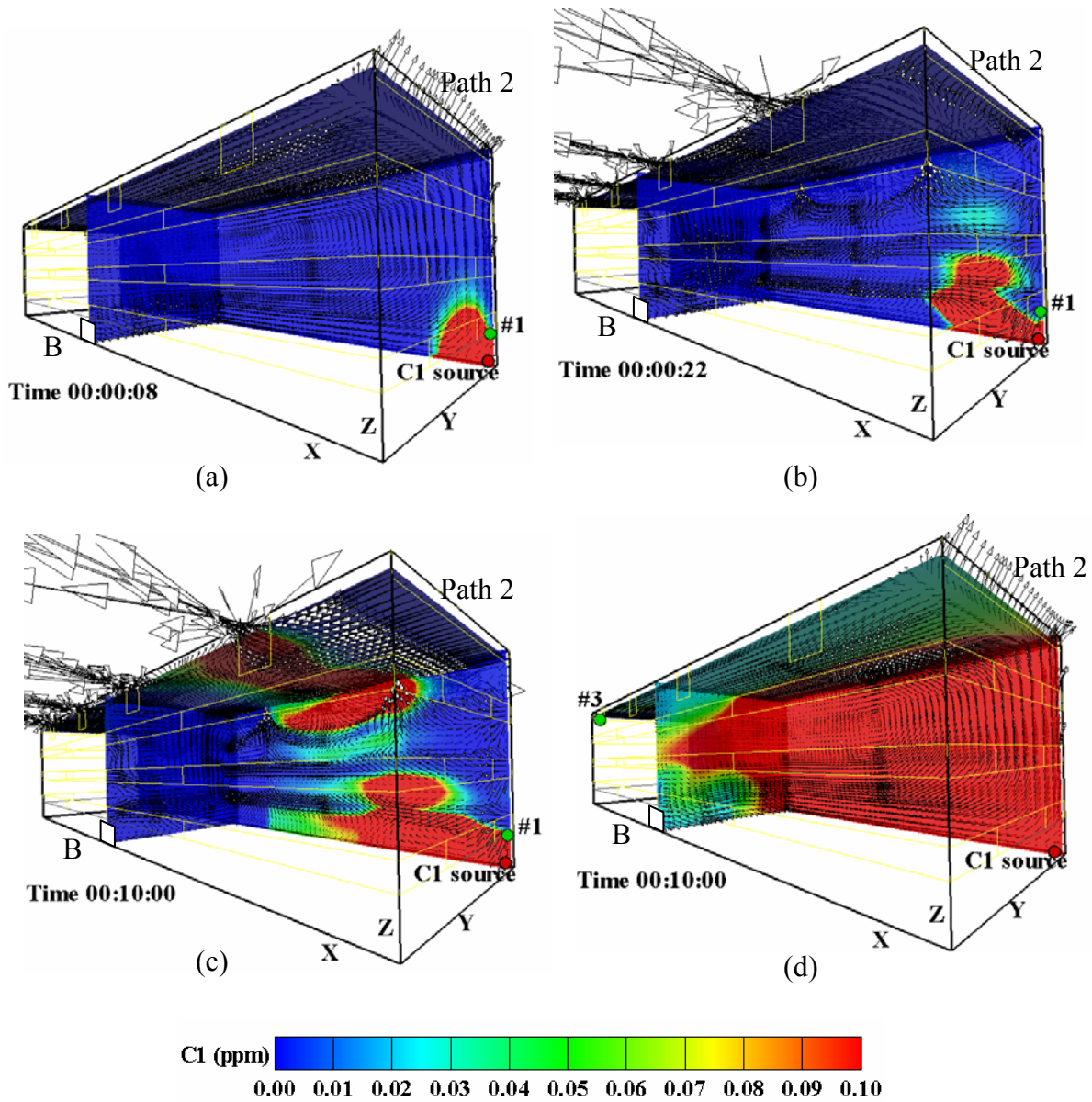


Figure 8. The calculated C1 concentration by the coupled simulation at the middle section of Door B ($X = 24$ m), the section across the C1 source ($Y = 10.5$ m), the middle plane of Path 2 ($Z = 10.45$ m) at (a) 8 s, (b) 22 s, and (c) 10 min for sensor location #1, and (d) 10 min for sensor location #3.

The coupled CONTAM-CFD0 simulations can also help to determine strategies for occupant evacuation. Suppose a building occupant was at the upper-right corner in

Figure 6(a). During the evacuation, he/she could leave the building through Door A by following Path 1 or through Door B by Path 2 as shown in

Figure 6 (a). Door A was closer to the occupant and could be the logical choice. In fact, Figures 8(b) and 8(c) illustrate that the dominant airflow pattern was along the X direction so that the contaminant was pushed further to the left end of the atrium other than the Y or Z direction. Even at the end of 10 min, the C1 concentration at the middle section of Door B ($X = 24$ m) was much lower than that of the section across the C1 source ($Y = 10.5$ m). Consequently, the occupant would exposure to more contamination by using Path 1 than that by Path 2, especially from $t = 10$ s to 16 s, shown in Figure 9. The accumulated exposure by using Path 1 is about twice as much as that by Path 2, which indicates that Door B was a better choice. Although the determination of evacuation strategies in real cases could be more complicated than this example and would need much faster simulation than those presented in this paper, this study shows that the coupled CONTAM-CFD0 simulation has the potentials for evaluating evacuation strategies. Note that the results in this paper depended on the certain design parameters, such as sensor response concentration, exhaust fan flow rate, and sensor locations. For example, we intentionally selected 0.1 ppm as the sensor response concentration to demonstrate the coupled multizone-CFD0 program. Users are advised to choose using the coupled multizone-CFD method when a multizone-alone simulation fails or when computational time and accuracy are equally important.

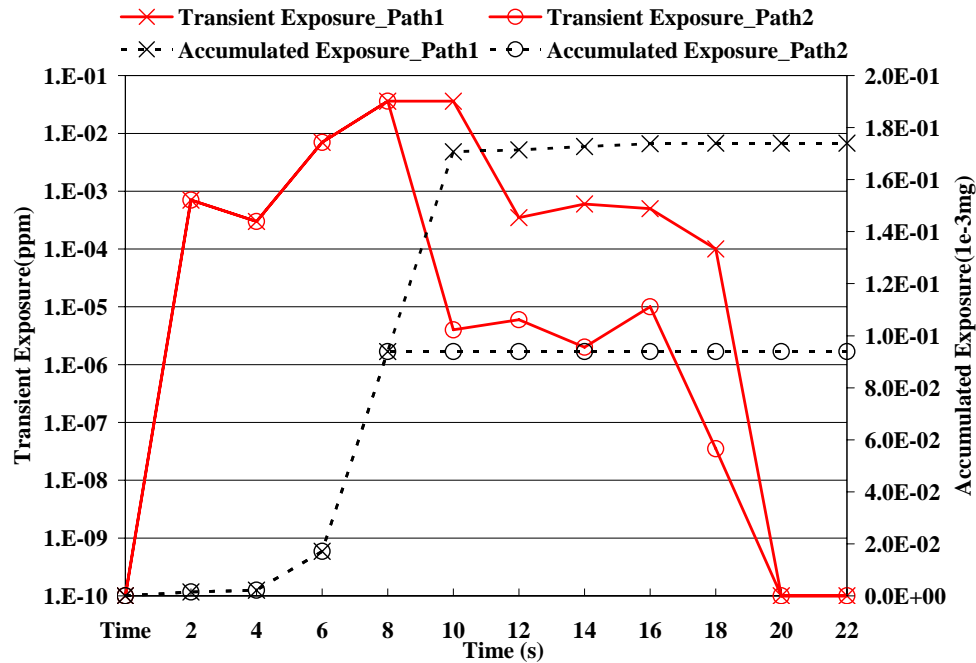


Figure 9. Personal exposures to C1 contaminant by using different evacuation paths.

CONCLUSIONS

This study applied a coupled multizone and CFD program to simulations of natural and emergency ventilations in a three-story building with a large atrium. It was showed that the coupled program can be used to evaluate placement of contaminant sensors and determination of occupant evacuation strategies. With a reasonable computing time, the program could provide details of airflow and contaminant distributions at both steady and transient states in a large space, where the well-mixing assumption of multizone model fails. The coupled multizone-CFD program has the strong potential of wider applications, such as optimization of contaminant sensor placements and occupant evaluation strategies, which require multiple test runs and huge computing time.

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