PRESSURE BOUNDARY CONDITIONS IN MULTI-ZONE AND CFD PROGRAM COUPLING

Zhiqiang (John) Zhai, Ph.D.
Department of Civil, Environmental & Architectural Engineering, University of Colorado
428 UCB, Engineering Center, ECOT-441, Boulder, CO 80309-0428 USA
Email: John.Zhai@Colorado.edu

Yang Gao
Select Energy Services, Inc.
24 Prime Parkway, Natick, MA 01760-1528 USA
Email: ygao@selectenergysi.com

Qingyan (Yan) Chen, Ph.D.
Ray W. Herrick Laboratories, School of Mechanical Engineering, Purdue University
585 Purdue Mall, West Lafayette, IN 47905-2088, USA
Email: yanchen@purdue.edu

ABSTRACT

Multi-zone and CFD airflow models are two important tools for the study of indoor environmental quality. The coupling of these two programs can provide a complementary and thus more accurate prediction of airflow in buildings with an acceptable computing cost. This paper reports the process to couple a multi-zone and a CFD program through pressure boundary conditions at room openings. The study developed a new algorithm to handle pressure boundary conditions in CFD. The algorithm allows the specification of a static or total pressure condition for a particular opening in CFD. It can automatically determine whether the pressure should be treated as total pressure (inflow) or static pressure (outflow) based on whether the airflow enters or leaves the space. To achieve a stable solution during the iterative calculation, special numerical relaxation methods have been used in the implementation of pressure boundary conditions. The validation and application studies show that the pressure boundary treatments and the coupling algorithm are sound.

INTRODUCTION

Study of indoor air quality needs the information of airflow in buildings. A multi-zone airflow simulation program, such as CONTAM (Stuart Dols 1997), can provide the distribution of airflow and contaminant concentration in a building. However, the program treats an indoor space as a zone in which the contaminant concentration is assumed to be uniform. For large indoor spaces, such as atria, lobbies, etc., the uniform assumption is not acceptable. On the other hand, Computational Fluid Dynamics (CFD) can give a detailed distribution of airflow and contaminant concentration for a building. But the computing time for an entire building is too long to be accepted for practical studies. A solution to the dilemma is to use a CFD program for indoor spaces where contaminant concentration is not uniform and a multi-zone program for the rest spaces of the building.

This coupling approach links the two programs through boundary conditions at large openings (i.e. mass flow rates and/or pressures at openings) (Negrao 1995). It is straightforward to specify mass flow rates as boundary conditions in a CFD program. Pressure boundary condition usually receives more attentions in the context of compressible flows. For incompressible flows (such as flow in buildings), a pressure condition is not needed at a boundary if velocities can be specified because they are interrelated. This works well for mechanically ventilated buildings where flow rate from air supply diffusers are known and flow direction can be predetermined. However, for many other types of flows in a building, pressure at boundaries can be determined but not the velocities. A typical example is natural ventilation in a building where pressures at open windows are known but the ventilation rate needs to be determined. Hence, to be able to specify pressure boundary conditions in a CFD program is important.

Very few studies of pressure boundary conditions are available for incompressible flow. Earlier work was performed by Gresho and Sani (1987) and Kobayashi et al. (1993). Some recent investigations include the

development of finite difference schemes based on local pressure boundary conditions (Johnston and Liu 2002) and the study of stability of pressure boundary conditions for time-dependent incompressible flows (Petersson 2001). Kelkar and Choudhury (2000) presented a method for the prediction of incompressible flow in domains with specified pressure boundaries. Their study indicates that the knowledge of the flow direction is essential to specify correct pressure boundary condition since inflow and outflow should be treated differently. However, flow direction at a specific pressure boundary is not always known a priori in reality and the corresponding pressure boundary condition needs to be applied iteratively depending on the flow direction. For instance, if a room has several open windows facing different directions, it is difficult to estimate the flow directions in some of the windows.

The objective of this paper is to develop a method to specify suitable pressure boundary conditions in CFD for large openings. The pressure boundary conditions can then be used to couple the multi-zone and CFD programs. The developed method has been demonstrated by applying it for three case studies.

PRESSURE BOUNDARY CONDITIONS IN THE COUPLING OF A MULTI-ZONE AND A CFD PROGRAM

Generally, coupling between a multi-zone program and a CFD program can be done by transferring airflow information from the CFD model to the multi-zone model, and transferring air pressure from the multi-zone model to CFD as boundary conditions. The transfer can be performed either manually (e.g. Schaelin et al. 1993 and Musser 2001) or automatically (Negrao 1995). Negrao (1995) coupled a CFD solver with the ESP-r program that has a multi-zone airflow model. The conflation technique essentially treated the airflows across the openings as sources.

The present study couples a multi-zone program, CONTAM, with a CFD program, MIT-CFD. Since CONTAM does not use source term in the mass balance equation, the coupling approach should be different from the one proposed by Negrao (1995). Coupling of the two programs requires matching the mass flow equations in CONTAM with the momentum equations in MIT-CFD at the inlet and outlet openings. In a coupled simulation, CFD is applied to a zone that has a non-uniform contaminant concentration. The MIT-CFD cells at the openings of the zone are linked to other zones computed by CONTAM. The information of mass flow rate and pressure is exchanged between those CFD cells at the openings and their adjacent CONTAM zones.

Figure 1 illustrates how the two programs are coupled in a four-zone apartment. This example assumes that zone 2 has a non-uniform contaminant distribution so that MIT-CFD is applied for the zone. Zone 2 has three openings: A, B, and C. CONTAM is used to calculate airflow in the other three zones. Since CONTAM assumes uniform total pressures in the neighboring zones of the CFD domain, it is reasonable to assume that the total pressures at the openings are the same as those in the adjacent zones. i.e: $P_A = P_1$, $P_B = P_3$, $P_C = P_4$. The pressure obtained from CONTAM at those zones can be used as boundary conditions for MIT-CFD to calculate the flow through those openings in zone 2. If the flow from opening A is inflow and from openings B and C is outflow for the CFD zone, total pressure must be imposed as boundary condition for opening A and static pressures for openings B and C, as will be explained later on. The total pressure, P_o, is the sum of static pressure, P, and dynamic pressure:

$$P_o = P + \frac{1}{2}\rho U^2 \tag{1}$$

where ρ is air density and U is air speed. The mass flow rates calculated by MIT-CFD at the three openings are used in CONTAM to calculate the total pressures in the other three zones. Obviously, this would require iterations between MIT-CFD and CONTAM to reach a converged solution.
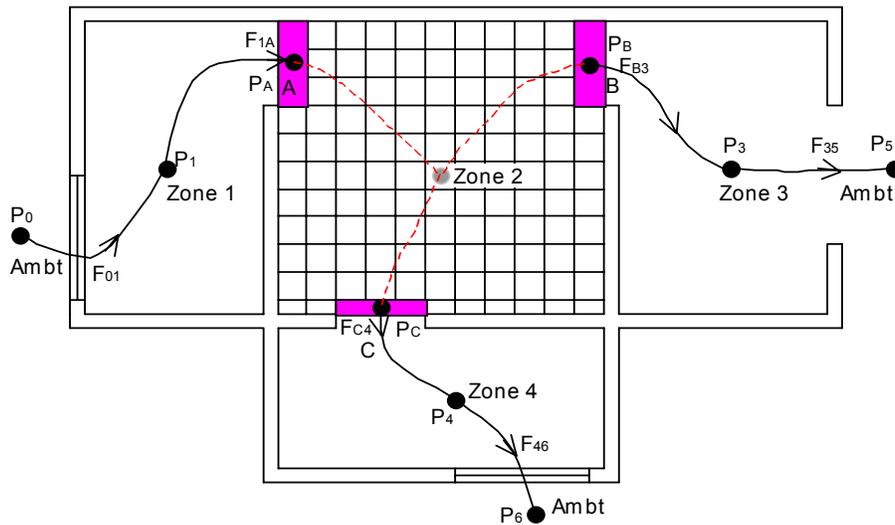
Figure 1 Illustration of the coupling between CFD and CONTAM

(1) Static Pressure Boundary Conditions

MIT-CFD uses the pressure-velocity correction algorithm of SIMPLE (Partanka 1980) and a non-staggered grid system (velocity and pressure are stored at the same central computing points of each grid cell). The program hence solves static pressure field in a calculation. If static pressure can be obtained from a multi-zone program and is used as boundary conditions for openings, the airflow rates and directions at the openings can be directly determined by local pressure gradients. The mathematic descriptions of this pressure boundary condition are:

$$P = P_{neighboring-zone} \tag{2}$$

$$\frac{\partial \phi}{\partial n} = 0 \tag{3}$$

where ϕ represents temperature, contaminant concentration, and turbulence properties at the boundary surface and n denotes the direction normal to the surface.

The numerical implementation of this static pressure boundary condition in MIT-CFD can be done as follows:

(1) Guess an initial pressure field and specify $P_2 = P_{neighboring\ zone}$ (as shown in Figure 2) at the first grid cells of the pressure boundary, as well as other boundary and initial conditions, solve the momentum equations for velocity components in the field (note that P_1 is the nominal pressure within non-staggered grid CFD and can be obtained through the extrapolation of interior pressures);

(2) Solve the pressure correction equation that is based on the continuity equation for the pressure correction term P' in the calculation domain except the first grid cells of the pressure boundary where P' = 0;

(3) Update P=P+P', velocity, and mass flow rates through each cell surface;

(4) Use the local mass conservation equation at the first grid cells of the pressure boundary to acquire the mass flow rate (velocity) at the opening. For example, $\dot{m}_{west} = \rho V_1 A_1 = \dot{m}_{east} + \dot{m}_{north} - \dot{m}_{south}$, as shown in Figure 2.

(5) Repeat from step (1) with the new pressure and velocity fields and iterate until a converged result is obtained.
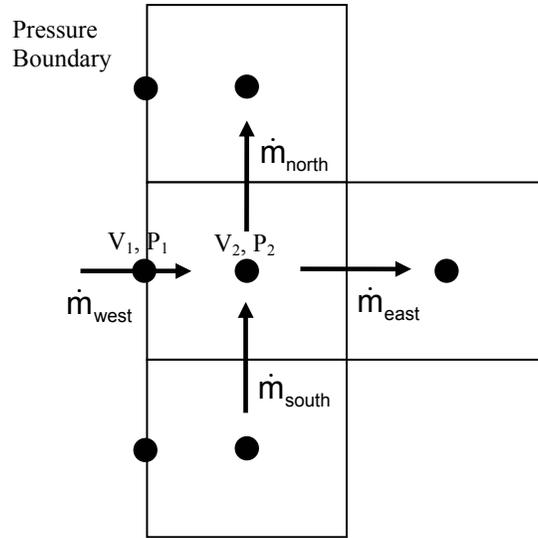
Figure 2 Schematic of pressure boundary treatment on a 2-D CFD grid

(2) Total Pressure Boundary Conditions

However, most multi-zone programs, including CONTAM, do not calculate static pressure but total pressure. Using total pressure in CFD as pressure boundary condition is not easy because airflow direction plays an important role. For airflow leaving a CFD zone, the flow dissipates its kinetic energy due to the viscous action. Thus, the static pressure at an opening is very close to the total pressure in the neighboring zone (Kelkar and Choudhury 2000). The total pressure can then be used as the static pressure at the exit opening:

$$P_{exit} = P_{neighboring\text{-}zone} \tag{4}$$

The numerical procedures described in the previous section can be used for the opening.

On the other hand, if the flow at the opening is an inflow to the space, the (static) pressure in the cross section at the opening will be the total pressure at the neighboring zone minus the dynamic pressure at the opening that is an unknown a priori. The relationship between them can be expressed as:

$$P_{neighboring-zone} = P + \frac{1}{2}\rho U^2 + \Phi \tag{5}$$

where Φ is pressure head lost due to the viscous effects. Therefore,

$$P = P_{neighboring-zone} - \Phi - \frac{1}{2}\rho U^2 = \alpha P_{neighboring-zone} - \frac{1}{2}\rho U^2 \tag{6}$$

where α is defined as pressure head lost coefficient. By using Equation (6), the update of air velocity for each iteration at the first cells of the pressure boundary will produce a new static pressure. The pressure can then be used to generate a new velocity with the numerical algorithm presented in the previous section until a converged solution is reached. In order to stabilize the iterative calculation, an under-relaxation factor λ can be used:

$$P^{n+1} = \lambda\left(\alpha P_{neighboring-zone} - \frac{1}{2}\rho U^2\right) + (1-\lambda)P^n \tag{7}$$

where n and n+1 represent the current and the next step of the iteration, respectively. For a simulation with total pressure conditions, the algorithm can automatically and dynamically judge whether to use Expression (4) or (6) for

the pressure boundaries according to the airflow status of entering or leaving the space that is determined by the simulation.

APPLICATIONS OF THE PRESSURE BOUNDARY CONDITION TREATMENTS

In order to demonstrate the ability of MIT-CFD to handle various pressure boundary conditions, this section uses the program for three different case studies. The cases are:

- Airflow in a 90-degree planar branch;
- Hybrid-ventilated room with two open windows;
- Coupled simulation of CONTAM and MIT-CFD for a building with several zones.

(1) Airflow in a 90-degree Planar Branch

Airflow in a 90-degree planar branch as shown in Figure 3 is selected to show how MIT-CFD could deal with the pressure boundary condition at exit openings. This case has been extensively studied (e.g. Kelka and Choudhury 2000). The width of the main branch, W, is the same as that of the side branch. This study used a uniform grid distribution of 90x60, and assumed a laminar, uniform velocity profile for the air entering the main branch for simplicity. Uniform static pressures of zero were assumed at the two exits to test the performance of the pressure boundary condition setting. A range of Reynolds numbers from 10 to 400 ($Re=WU_c/\nu$, where U_c is the inlet centerline velocity, and ν is the kinematic viscosity) were studied to evaluate the sensitivity of the flow.
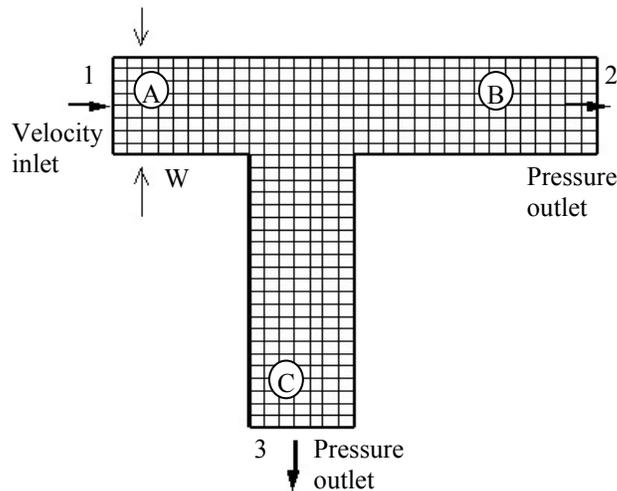
Figure 3 Configuration of a 90-degree planar branch

Figure 4 shows the predicted streamlines by MIT-CFD for Re = 10 and Re = 300. Compared with the results obtained by Kelkar and Choudhury (2000), MIT-CFD generates similar streamlines. Flow separates from the lower wall of the side branch at higher Reynolds numbers. The size and extent of flow separation are the same as those from Kelkar and Choudhury (2000).

Figure 5 further compares the fraction of mass flow rate versus Reynolds numbers of the present study with those obtained by Kelkar and Choudhury (2000) and Hays et al. (1989). The comparison shows that the fraction of mass flow in the main exit branch changes from 0.5 (equal flow split) at creeping flow rates to about 0.9 at Re = 400. The results from the three studies are similar, although larger differences were found in the region where Reynolds numbers are between 50 and 200. The differences may be attributed to the use of laminar, uniform velocity profile in this study rather than a fully developed, parabolic-shape one. The study verified that the pressure boundary conditions used in MIT-CFD are able to generate acceptable results.

Re=10   Re=300
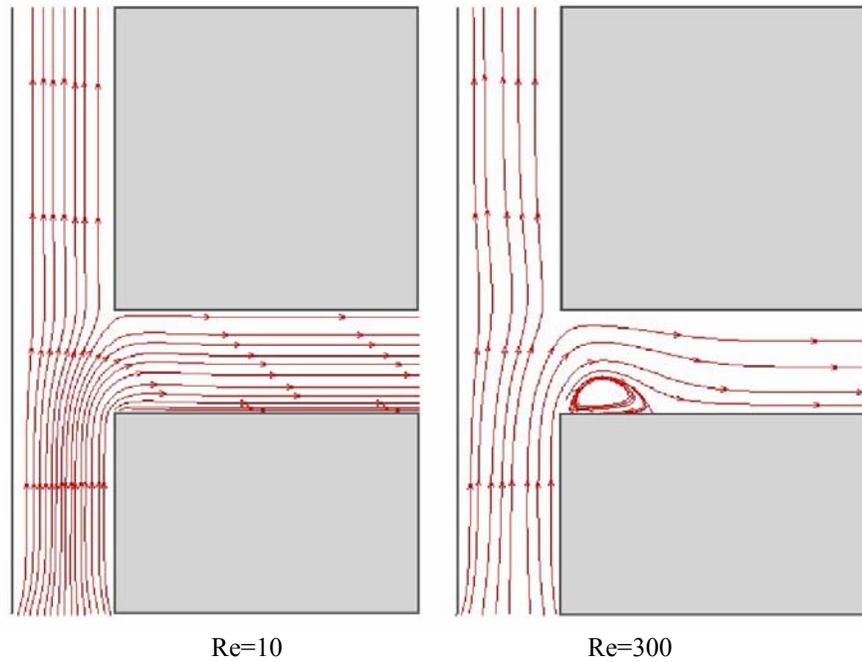
Figure 4 Contours of streamlines calculated by using MIT-CFD: (a) Re=10, (b) Re = 300
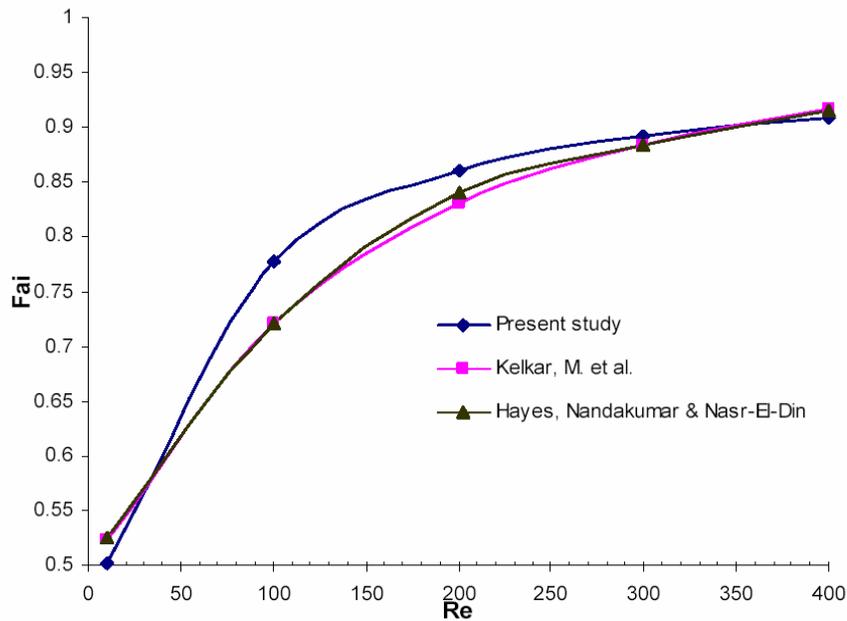
Figure 5 Fractional flow rate in main branch as a function of Reynolds number

(2) Hybrid-Ventilated Room with Two Open Windows

A hybrid-ventilated room with two open windows as shown in Figure 6 has been selected to show how MIT-CFD program can handle total and static pressure boundary conditions. The cubic room of 3m x 3m x 3m has a mechanical ventilation diffuser at the bottom of a wall supplying air at 1 m/s. Two open windows at the top of the opposite walls confront different pressures due to windward and leeward effects. The simulation assumed that the

windward window had a positive pressure of 1 Pa while the leeward window had a negative pressure of -1 Pa. The pressure boundary conditions were then specified as static one in one case and total pressure in another case. The simulation used a coarse grid of 10 x 10 x 12 and simulated the turbulent indoor airflow using a zero-equation turbulence model (Xu 1998). The current investigation did not consider the thermal effect. The computed results are compared with those obtained from a commercial CFD program, such as PHOENICS (CHAM 1999), in which the pressure at the two top openings is specified as total pressure.

Windward
P=1Pa

Leeward
P= -1Pa

V=1m/s
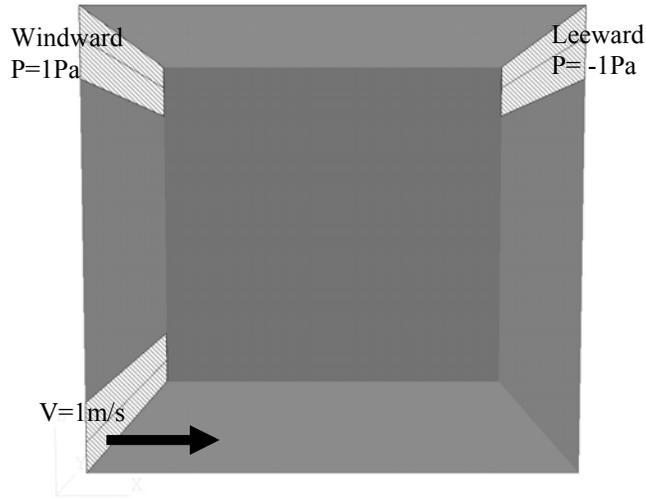
Figure 6 Sketch of the hybrid-ventilated room

Figure 7 compares the airflow pattern in the middle section of the room simulated by the current program with that by PHOENICS. The agreement is good except in the low-speed core. The MIT-CFD produced more complicated vortex structures in the core. This could be due to different methods handling inlet velocity. Table 1 compares the total mass flow rates through the room and the static pressure at the windward opening calculated with different methods. The mass flow rate calculated with the total pressure conditions by MIT-CFD is similar to that by PHOENICS. The current investigation assumed the pressure head lost coefficient α=1, which means that there is no pressure loss due to the opening geometry and friction. Therefore, the total pressure at the windward opening calculated by MIT-CFD is:

$$P_o = P + \frac{1}{2}\rho U^2 = 0.458 + 0.5 \times 1.2 \times 0.95^2 = 0.9995 Pa \qquad (8)$$

This verifies that MIT-CFD can correctly calculate the static, dynamic and total pressure.

The computed results also show that using static pressure boundary conditions will provide a quite different solution. The mass flow rate would increase by 20% due to the larger pressure difference between two windows. However, the simulation with static boundary conditions does not need to specify the pressure head loss coefficients. This is a nice feature since it is difficult to obtain the coefficients for most cases, which need to be determined from experiments.
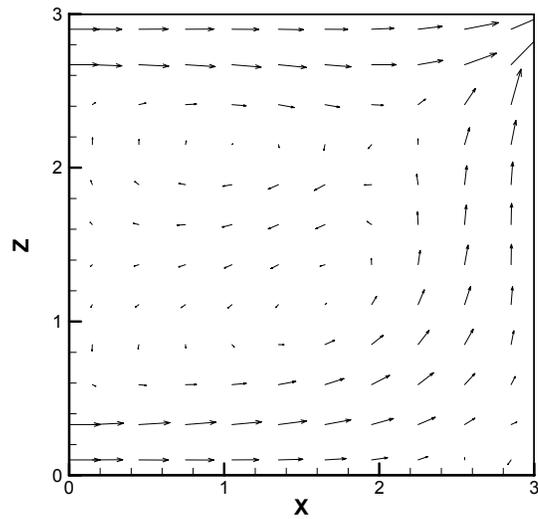
(a) by MIT-CFD
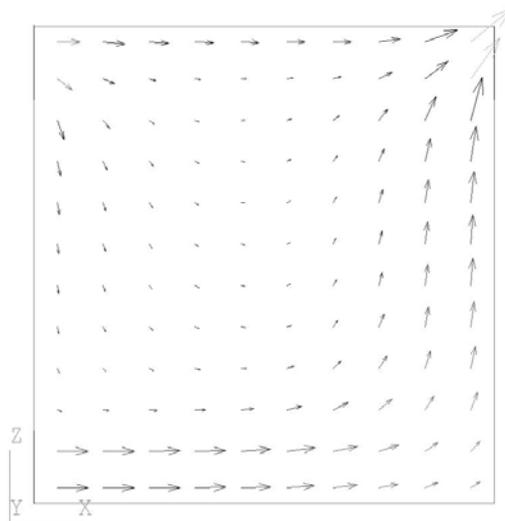
(b) by PHOENICS

Figure 7 Velocity patterns in the middle section of the room across the windows and fan with total pressure boundary conditions

Table 1 Mass flow rate and static pressure for the hybrid-ventilated room using different pressure boundary conditions

	MIT-CFD (Static pressure boundary)	MIT-CFD (Total pressure boundary)	PHOENICS (Total pressure boundary)
Total mass flow rate through leeward window (kg/s)	3.928	3.261	3.347
Static pressure value at windward window (Pa)	1	0.458	0.765

(3) Coupled Simulation of CONTAM and MIT-CFD for a Building with Several Zones

The last example is used to verify the algorithm of pressure boundary conditions for coupling CONTAM with MIT-CFD, through which MIT-CFD could use the pressures calculated by CONTAM to determine the airflow in a building zone more accurately. The building selected has been partitioned into four zones interconnected by openings as shown in Figure 1, where zone 2 has the similar configuration as 90-degree planar branch and is required for detailed airflow analysis. Thus zone 2 is simulated by CFD in the coupled program, while the other three zones are simulated using CONTAM. The coupled program starts with CONTAM simulation to obtain initial pressure results at the interconnected openings, which are fed to CFD solver as total pressure boundary using the above discussed algorithm. The CFD results are then passed back to CONTAM to update the simulation results for the entire building.

Figure 8 compares graphically the mass flow rates (blue bars) and relative pressure differences (red bars) obtained from CONTAM before and after the coupling. The longer the lines are, the larger the values are. The outflow from Opening B of zone 2 after the coupling is much larger than that before the coupling. Therefore, the airflow to zone 3 is much greater than that to zone 4. Because CONTAM itself cannot simulate momentum force but CFD can, the coupling results can be more reasonable. In the coupling, the pressure discharge coefficients in CONTAM are changed to obtain the same flow rates as MIT-CFD. With this approach, the pressure differences between zones would remain the same. Table 2 shows that the coupling changes the pressure discharge coefficients but not the pressure differences.

(a)   *(b)*
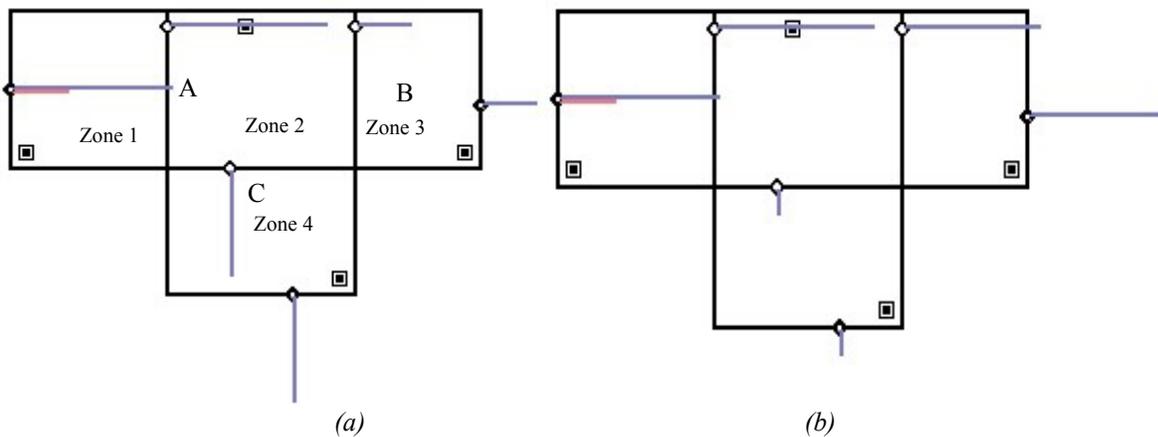
Figure 8 Airflow pattern calculated by CONTAM for the four-zone building: (a) before coupling with MIT-CFD; (b) after coupling with MIT-CFD

Table 2 The impact of coupling on airflow rates for different zones in the building

Airflow Path		Flow rate before coupling (kg/L)	Flow rate after coupling (kg/L)	Original pressure discharge coefficient kg/L·$(Pa)^n$	New pressure discharge coefficient kg/L·$(Pa)^n$	Pressure difference before coupling (Pa)	Pressure difference after coupling (Pa)
From	To						
Zone 1	Zone 2	0.005918	0.005918	1.0	1.0	0.000035	0.000035
Zone 2	Zone 3	0.001973	0.005096	1.0	2.582328	0.000004	0.000004
Ambient	Zone 1	0.005918	0.005918	0.01	0.01	0.350225	0.350225
Zone 3	Ambient	0.001973	0.005096	0.02	0.051647	0.009736	0.009736
Zone 2	Zone 4	0.003945	0.000822	1.0	0.208337	0.000016	0.000016
Zone 4	Ambient	0.003945	0.000822	0.04	0.008333	0.009725	0.009725

CONCLUSION

The coupling of a multi-zone airflow simulation program, CONTAM, with a detailed computational fluid dynamics (CFD) airflow program, MIT-CFD, can improve the accuracy of airflow calculated by the multi-zone program and reduce the computing cost by CFD. This study proposed a coupling method of these two programs through pressure and mass flow rate boundary conditions at openings. CONTAM can supply MIT-CFD pressures at the openings while MIT-CFD can provides CONTAM accurate airflow rates through the openings.

CFD simulation normally requires total pressure for inflow boundaries and static pressure for outflow boundaries. In order to determine whether an opening is an inflow or outflow one, iteration is needed in a simulation. This study has developed a new algorithm to handle the pressure boundary condition in MIT-CFD. The algorithm allows the specification of a static or total pressure condition for a particular opening in MIT-CFD. If static pressure is specified as boundary condition for an opening, its value is fixed at the opening while the mass flow rate through the opening is determined based on the local mass balance. If the total pressure condition is specified as boundary condition for an opening, the static pressure at the opening will be calculated iteratively by deducting the newly obtained local dynamic pressure from the given total pressure. The algorithm can automatically determine whether the pressure should be treated as total pressure or static pressure based on the airflow direction. To achieve a converged result, special numerical relaxation methods are necessary in the implementation of pressure boundary conditions. The case studies presented in the paper demonstrate the good performance of the algorithm and program developed.

REFERENCES

CHAM. 1999. PHOENICS Version 3.1. London, CHAM Ltd.

Gao, Y. 2002. Coupling of computational fluid dynamics and a multizone airflow analysis program for indoor environmental design. MS Thesis, Massachusetts Institute of Technology.

Gresho, P.M., and Sani, R.L. 1987. On pressure boundary conditions for the incompressible Navier-Stokes equations. International J. Numerical Methods in Fluids, 7:1111-1145.

Hays, R. E., Nandakumar, K., Nasr-El-Din, H. 1989. Steady laminar flow in a 90 degree planar ranch. Computers & Fluids, 17-4:537-553.

Johnston, H., and Liu, J. 2002. Finite difference schemes for incompressible flow based on local pressure boundary conditions. Journal of Computational Physics, 180:120–154.

Kelkar, K.M., and Choudhury, D. 2000. Numerical method for the prediction of incompressible flow and heat transfer in domains with specified pressure boundary conditions. Numerical Heat Transfer, Part B, 38:15-36.

Kobayashi, M.H., Pereira, J.C.F., and Sousa, J.M.M. 1993. Comparison of several open boundary numerical treatments for laminar recirculating flows. International J. Numerical Methods in Fluids, 23: 971-979.

Musser, A. 2001. An analysis of combined CFD and multizone IAQ model assembly issues. ASHRAE Transactions.

Negrao, C.O.R. 1995. Conflation of computational fluid dynamics and building thermal simulation. Ph.D. Thesis, University of Strathclyde, Glasgow, UK.

Patankar, S.V. 1980. Numerical heat transfer and fluid flow. Hemisphere, New York.

Petersson, N.A. 2001. Stability of pressure boundary conditions for Stokes and Navier–Stokes equations. Journal of Computational Physics, 172:40–70.

Shaelin, A., Dorer V., et al. 1993. Improvement of multizone model predictions by detailed flow path values from CFD calculation. ASHRAE Transactions, 93-7-4: 709-720

Stuart Dols, W., Walton, G., and Denton, K. 1997. CONTAMW1.0 user manual. Gaithersburg, MD, NIST.

Xu W. 1998. New turbulence models for indoor airflow simulation. Ph.D. Thesis, Department of Architecture, Massachusetts Institute of Technology, Cambridge, MA.

Zhai, Z., Hamilton, S.D., et al. 2000. Integration of indoor and outdoor airflow study for natural ventilation design using CFD. Proceedings 21st AIVC Annual Conference. Paper 13, The Hague, The Netherlands, September.