New Method of Coupling Multizone and CFD for Building Simulation

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Abstract
Existing prediction tools of indoor environment such as Computational Fluid Dynamics (CFD) and multizone models each have their advantages but also their limitations. Therefore combining the two models could avoid their respective drawbacks and improve the accuracy of prediction of indoor air quality. This paper presents a coupling method which uses pressure differences output from a multizone model to link with CFD. The method is then applied to an example case with air infiltration and exfiltration, an open door, ventilation and a contaminant source. The outlined method models both small openings and large ones such as doors and windows and will be useful in the conception and design of advanced ventilation systems for residential and small office buildings at an improved accuracy with less computational burden.

Keywords: Coupling; CFD; multizone models; large openings; indoor air

1. Introduction
A good indoor environment design depends on being able to obtain through experiments or computational simulations parameters such as airflow pattern, velocity, temperature and contaminant concentrations. Factors such as long computing time, considerable labor output and varying accuracy can make experiments impractical. As for simulations, existing prediction tools such as Computational Fluid Dynamics (CFD) and Multizone models (COMIS [1], CONTAM [2] etc.), each have their advantages but also their limitations. Multizone models can simulate airflow and pollutant transport quickly by treating a building as a collection of well-mixed zones connected by flow paths such as doors, windows, HVAC ducts etc. However the well-mixing assumption in these models can lead to over-prediction and under-prediction of human exposure to pollutants when contaminant concentration in a space is not uniform. On the other hand CFD can give a detailed description of air velocity and contaminant concentration in a given area, but it is prohibitively time-consuming and labor intensive, and therefore difficult to model an entire building. This is why instead of analyzing the whole structure; CFD has been traditionally restricted to flows in single rooms or small sets of rooms where detail is desired. Therefore combining the two models could avoid their respective drawbacks and improve the accuracy of prediction of indoor air quality.

Many efforts have been made to try to take advantage of both models by integrating them. Schaelin et al. [3] proposed a method that can link results of CFD calculations with multizone models. In their study the well-mixing assumptions of multizone models were addressed by manually inputting detailed pressures, velocities, temperatures and contaminant concentrations of flow paths from CFD. Clarke et al. [4] and Negrao [5] succeeded in integrating an automatic airflow coupling inside ESP-r. Some other studies of coupling multizone network models with CFD programs are also found in the literature, e.g. Jayaraman et al. [6]; Musser [7]; Wang et al. [8]. However the previous studies are limited to simple airflow paths such as cracks or openings with small areas. None of the strategies could take into account coupling through large openings with bidirectional flow.

This paper will present a universal coupling method which can model both small openings and large ones such as doors and windows where bidirectional flow is significant. The method is then applied to an example case with air infiltration and exfiltration, an open door, ventilation and contaminant proliferation. The outlined method will be useful in the conception and design of advanced ventilation systems for residential and small office buildings.
2. Fundamentals of Coupling CFD and a Multizone Model for Building Airflow and Contaminant Transport Simulation

The coupling principle of CFD with multizone models is first to conduct a whole building simulation using a multizone model and then use its boundary conditions to apply CFD in a selected zone where the well-mixing assumption is not fulfilled. With the object of refining the entire calculation, the CFD result is then fed back into the multizone model. In order to illustrate the coupling strategy, the authors refer to Fig.1., which shows part of a multi-story building with an atrium (zone k) where the homogenous conditions of temperature, concentration, etc are not satisfied. Therefore the atrium is the selected zone where CFD will be applied. The solid arrows represent the multizone network of the whole building while the dotted arrows represent the effect of the CFD domain on the network model.

The multizone model calculates the mass continuity for zone j using this equation:

$$\sum_{i} \dot{m}_{ij} - \dot{m}_{jk} = b_{j} \quad (1)$$

where $\dot{m}_{ij}$ and $\dot{m}_{jk}$ represent the mass flow rate entering and leaving zone j respectively, while $b_{j}$ represents the source term of the equation. The flow connections $\dot{m}_{ij}$ and $\dot{m}_{jk}$ can usually be described by a non-linear relationship between the flow rates, pressure or temperature difference across the path. The relationship is generally an empirical function that can be found often in the literature. A very commonly used one is an exponential function in the following form:

$$\sum_{i} \dot{m}_{ij} = \sum_{i} C_{ij} (\Delta P_{ij})^{n_{ij}} \quad (2)$$

where $C_{ij}$ is the flow coefficient path; $\Delta P_{ij}$ is the pressure difference between nodes i and j; $n_{ij}$ is the flow exponential coefficient.

After linearization, an often-used expression in the multizone model for the airflow network is:

$$\sum_{i} \dot{m}_{ij} (P_{i} - P_{j}) - \dot{m}_{jk} = b_{j} \quad (3)$$

where, subscript $L$ denotes linearized coefficients and terms.

Since the above formulations are based on the perfect mixing assumption within the zones, when refinements concerning the airflow patterns and contaminant dispersion are necessary in some zones, CFD is then integrated into the flow network model. To do this, the network node representing the room where the well-mixing assumption is not fulfilled is replaced by updated connections to the new domain cells. Similarly the CFD model also involves the mass conservation principle in the calculated domain. For each cell in the CFD domain, to enforce mass conservation a pressure (or pressure-correction) equation is used.

$$\sum_{nb} a_{nb} P_{nb} - a_{p} P_{p} = b_{p} \quad (4)$$

where subscript $p$ denotes the node at which the equation is approximated and subscript $nb$ runs over the neighboring nodes. $a_{p}$ and $a_{nb}$ are the coefficients of the equation. Their expressions can be found in many CFD reference books; $P$ is the pressure or pressure correction depending on which algorithm is used. For SIMPLE, pressure correction is employed, for SIMPLER pressure is used. $b_{p}$ is the mass source term.

The coupling of CFD and multizone models is achieved by combining equation (3) and equation (4) into the following form:

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

where $C$ is the airflow coefficient matrix, $P$ is the pressure/pressure correction vector of zones and cells; $M$ is the flow rate vector of paths and cells at multizone and CFD zone interfaces; $B$ is the vector of mass source.

The coupled model can be solved iteratively by exchanging boundary conditions at the interface between the flow network and CFD model. The following two common boundary conditions can be used:

1) The network model imposes pressure at both the inlet and outlet nodes of the CFD domain, but up to now has been inapplicable to large openings with significant directional effects.

2) The network model imposes a velocity, but it is necessary to specify whether the flow is leaving or entering the calculation domain. It is difficult to model large openings with bi-directional flow if the above approach is used.

Considering that only the gradient of pressure affects the flow between zones, the authors developed a new method that uses the output pressure difference of the network model to compute the velocity at the CFD domain boundary. So this does not mean that pressure and velocity are imposed at the same time. The boundary velocity was computed using the output...
pressure difference from the multizone model.

To illustrate this method the authors shall consider
the near-boundary cell as shown in Fig.2.

For the near-boundary cell in Fig.2, the boundary
velocity interface between the multizone model and
CFD is computed using the following relation:

\[ U_b = \frac{1}{a_p} \left( \frac{P_p - P_j}{\Delta x} \right) \quad (6) \]

where \( P_p - P_j \) is the pressure difference between
zone \( j \) and the CFD domain zone, and is an output of
the multizone model. \( \Delta x \) is the distance between the
boundary face and the centre of the near-boundary cell.

\( a_p \) is the central coefficient of the discretized
momentum of cell \( P \) which is generally in this form:

\[ \sum_{nb} a_{nb} U_{nb} = -\frac{\Delta P}{\Delta x} \quad (7) \]

where \( nb \) denotes the neighboring cells and \( a_p \) is
equal to the sum of the neighboring coefficients \( a_{nb} \). \( \Delta P \) is the pressure gradient between cells. As \( a_p \) is not
known at the near-boundary cell face it is extrapolated
from the interior node of the CFD domain momentum
equation using a second order extrapolation. This
makes the boundary velocity part of the computational
domain of CFD, since its value is updated every time
the momentum's equation is calculated. The boundary
velocities determined in this manner need to be corrected
to satisfy the mass conservation; they are corrected in
such a way that the mass conservation of zone \( j \) of the
multizone side is satisfied. The implementation of this
method into the SIMPLE algorithm [9] can be done as
follows:

1. Solve discretised momentum equations
2. Compute boundary velocities
3. Correct boundary velocities
4. Solve pressure correction equation
5. Solve all other discretised transport equations

This method makes it easier to model large openings
with bi-directional flow such as doors or windows since
it takes advantage of their pressure difference profile,
an output of the multizone model. Since the velocities
determined using the pressure difference profile are
corrected before use in the continuity equation, there is
no problem of global mass conservation.

3. Application of the Method

3.1 Case description

The authors applied their method to a typical
example of a residential building, a schematic of which
is shown below in Fig.3.

The situation represented is a house with two rooms
connected by an internal door. Room 1 is assumed to
be a combination of a living room and kitchen and is
most likely where airflow patterns and contaminant
concentrations are not uniform; therefore it is chosen
for the CFD calculation. The dimension of room
1 is 7 m x 5 m x 2.5 m. The kitchen ventilation is
mechanically forced by an exhaust system above the
cooking range running at 200 m³/h. The cooking plate
is assumed to have a convective heat transfer of 500 W
to the air. For the cooking process a unit contaminant
source of 0.01 ml/s was assumed and adiabatic walls
were supposed for the CFD simulation. In order to
apply the authors’ method to a large opening, the
internal door between room 1 and room 2 is fully open.

3.2 Calculation procedure of the coupled program

The coupled program starts first by running a whole
house simulation using its multizone part in order to
extract boundary conditions for the CFD part which
analyses the selected room 1. The boundary conditions
used for the multizone part consisted of meteorological
conditions without wind, and an outside air temperature
assumed to be 20°C. Typical leakage data and exhaust
fan characteristics were considered to calculate the
values for the crack flow through the windows and the
effective flow rate through the internal door connecting
room 1 and room 2. The air in the second room was
22°C and at the beginning of the simulation the
contaminant concentration in it was zero.

The calculated air infiltration rate through the
windows and the effective flow rate through the
open door were both 100 m³/h; meaning that half of
the exhaust volume through the exhaust system was
infiltrated from the windows and the other half from
the adjacent room (through the door). In addition
to calculating the flow rate through the door, the multizone part of the program also gave the pressure differences on either side of it. To model the open door, it was described as a conjunction of parallel small openings, properly located with their height corresponding to that of the cells in the CFD domain, and with only a one-way flow allowed for each one. Each small opening was then described by a crack flow equation taking into account the local pressure drop. The figure below shows the pressure difference in relationship to the door height, as output of the multizone model part of the coupled program.

The pressure differences in relationship to the door height described in Fig. 4, indicate the bi-directional flow which is characteristic of large opening behavior. Here positive pressure differences mean that the flow is leaving the room, while negative pressure differences mean that the flow is entering the room. The pressure differences are used to calculate the boundary velocities at the door in the CFD calculation. For the CFD calculation part of the program, a zero-equation turbulence model for indoor airflow simulation [10] was used. The number of grid points used in the calculation was 24 in the y direction, 28 in the x direction and 17 in the z direction. Using the authors method as previously described in the SIMPLE algorithm, the velocity of the air flow at different heights of the door was computed using equation 6 and then corrected in a way that satisfies the mass conservation; meaning that the mass flow rate calculated with those velocities must equal the effective flow rate through the door calculated by the multizone part of the program.

4. Results

Figs. 5. and 6. show the contour lines of the temperature and the contaminant concentration respectively at the plane y = 2.25 m, while Figs. 7. and 8. give them at the plane x = 3.9 m. Table 1 gives a comparison of the contaminant concentration of the multizone only simulation with the coupled multizone-CFD simulation. In the coupled analysis, the contaminant concentration in room 1 is a representative value taken at a height of 1.6 m while those of room 2 and the exhaust are the average values at the door and the exhaust outlet respectively.
5. Discussion and Conclusion

A method for linking multizone models with CFD through large openings using pressure differences has been presented. The accuracy of the results of multizone calculations is restricted by the assumption of homogeneously mixed conditions in each node. This condition is not fulfilled as shown by the stratification of the temperature and the contaminant concentration in Figs. 5 to 8. So the use of a multizone model to simulate the whole house would lead to a false prediction. Table 1 illustrates, compared to the coupled analysis, the over-prediction of the multizone model used to calculate the whole house in this example case. The multizone model gives a single value for the space, while the coupled analysis gives a different value for different zones or nodes.

This study confirms what is already known about the failure of the well-mixing assumption of the multizone model leading to over-prediction or under-prediction of contaminant in a space. Previous works were limited to modeling one-way orifice openings. The solution the authors propose in the outlined method shows its ability to model both small openings and large openings with bidirectional flow and therefore is universal.

|                | Multizone-only analysis | Coupled analysis |
|----------------|-------------------------|------------------|
| Room 1         | 0.18 ppm                | 0.10 ppm         |
| Room 2         | 0.15 ppm                | 0.09 ppm         |
| Exhaust        | 0.18 ppm                | 0.15 ppm         |

Table 1. Contaminant Concentration in Room 1, Room 2 and Exhaust

References

1) Feustel, H. E., and A. Rayner-Hooson. 1990. Fundamentals of the multizone airflow model COMIS. Technical Note AIVC 29. AIVC, Coventry, GB.
2) G. Walton and W. Dools. CONTAMW 2.1 User manual. 2003. NIST, Gaithersburg, MD, USA.
3) A. Schaelin, V. Dorer, J. van der Mass and A. Moser. 1993. A new method for linking results of detailed airflow pattern calculation with multizone models, Proceedings of the 13th AIVC conference on Ventilation for Energy Efficiency and Optimum Indoor Air Quality, Nice, France pp.63-76.
4) Clarke, J. A, Dempster W. M, and Negroo, C. O. R. 1995. The implementation of a Computational Fluid Dynamics algorithm within the ESP-r system. Building Simulation 95, Madison, pp.166-175.
5) C. Negroo. Integration of computational fluid dynamics with building thermal and mass flow simulation. 1998. Energy and Buildings. 27(2) pp.155-165.
6) B. Jayaraman, D. Lorenzetti, A. Gadgil. 2004. Coupled model for simulation of indoor airflow and pollutant transport. Report LBNL-56667 for contract DE-AC03-76SF00098. Lawrence Berkeley National Laboratory Raw, G. J, Aizlewood, C. E, Llewellyn, J, et al. 1999. Indoor air quality and health in 10 office buildings in the UK - a multi-disciplinary study. BRE Report 9911332.
7) Musser, A. 2001. An analysis of combined CFD and multizone IAQ model assembly issues, ASHRAE Transactions, 107(1) AT-01-13
8) L. Wang and Q. Chen. 2005. On the solution characteristics of coupling of multizone and CFD programs in building air distribution simulation. Proceedings of Building Simulation'05. V. Ill, pp.1315-1322, Montreal, Canada.
9) S. Patankar. 1980. Numerical Heat Transfer and Fluid Flow. McGaw-Hill Book Company, New York.
10) Q. Chen and W. Xu. 1998. A zero-equation turbulence model for indoor airflow simulation. 1998. Energy and Buildings. pp.137-144.