

On-Site Experimental Validation of a Coupled Multizone and CFD Model for Building Contaminant Transport Simulations

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ABSTRACT

Previous studies indicated that the coupling of multizone and CFD (Computational Fluid Dynamics) models can provide a good compromise between the accuracy and required computation time. The results show that the coupled model predicts contaminant distribution more accurately than multizone model alone for the zones close to the contaminant source location. For all other zones, the multizone models performed similarly or slightly better than the coupled model. The computational time of the coupled model is lower when compared to CFD alone and higher when compared to multizone alone. These observations show tradeoffs between accuracy and calculation speed. This paper presents results of on-site field experiments conducted to further validate the performance of the coupled model. In a real office space, contaminant concentration, temperature, and HVAC supply airflow rate are measured to validate the coupling method with a newly proposed indirect validation method. This method is composed of an experimental validation for the CFD model, and a numerical validation of the coupled multizone and CFD model. Overall, the conducted validation shows that the coupled multizone and CFD model gives good results. Therefore, the developed indirect validation method can be applied to other studies to evaluate the performance of multizone or coupled multizone and CFD models.

INTRODUCTION

The two most widely used types of computer methods for building airflow and contaminant transport simulations are multizone and computational fluid dynamic (CFD) models. Multizone models usually treat a single zone (room) as a node that has connections to the other nodes by flow paths. The

model calculates macro-scale bulk airflow and contaminant transport in and between the zones. On the other hand, CFD models divide the domain of interest, usually a single room, into smaller control volumes and calculate detailed micro-scale velocity, temperature and concentration distribution within the domain (room). The two models are similar in the principles of mass conservation, but CFD also solves the momentum conservation equation. Furthermore, these two airflow models use different transport equation solution procedures, discretization methods, and boundary condition specifications. Due to low computation demand, multizone models are widely used for bulk flow movement and contaminant transport calculations in entire buildings, while CFD models are typically used for calculations of microscopic airflow, temperature and contaminant distributions in a single space.

With perfect air mixing in zones, multizone models are applicable to each zone in a building. The perfect mixing assumption is acceptable in spaces where no major contaminant sources exist and the room air is completely mixed by the ventilation airflow jets. Therefore, the concentration within a single zone can be assumed to be uniform with the perfect mixing assumption. However, in the zones with contamination sources or ventilation other than mixing, the assumption of concentration uniformity is crude and can possibly lead to erroneous overall calculations. If the contaminant transport at the source is not correctly predicted, the distribution within the building and personal exposure in different parts of the building cannot be correctly calculated. To solve this problem, coupling methods have been proposed to combine the strengths of the multizone and CFD models, while mitigating their respective inherent weaknesses. In the present study, the coupled model used commercial PHOENICS CFD software

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(CHAM 2005), and CONTAMW multizone program (Dols and Walton 2002). Finally, this coupling method is experimentally validated using an indirect validation method.

Based on experiences from the previous studies (Schaelin et al. 1993, Negrao 1995, and Musser 2001), Yuan and Srebric (2002, 2004) as well as He and Srebric (2004), this study further developed and applied the idea of validating coupled multizone and CFD model. The coupled model consists of three steps illustrated in Figure 1. First, a multizone flow model is applied to the entire building to establish airflow rates and contaminant transport among the zones. Then, a detailed CFD model is applied only to the zones with the contamination sources. In this step, the predicted non-uniform airflow and concentration distributions are calculated and transferred to the multizone model as fluxes for the final third calculation step. At the interface surface between CFD and multizone models, the averaging of CFD results is necessary if multiple control volumes are adjacent to a single zone in the multizone model. The final step is a multizone model that excludes domain simulated by CFD. The three steps can be a part of an iterative loop, but normally very few iteration steps would be needed for convergence of iterations (Yuan and Srebric 2004). In the present study, the convergence was achieved in only two iterations.

The coupling strategy, presented in Figure 1, has also a potential for computational time savings. With this method, most of the complex CFD simulation steps are replaced by simple multizone calculations and the coupled model is usually much faster than the CFD model alone. Furthermore, defining the simulation model is relatively simple because specification of complex boundary conditions such as walls, windows, inlets/outlets is largely simplified by the use of a multizone model. However, the results of multizone model very much depend on boundary conditions, and, therefore, Furbringer et al. (1999) addressed the need for user-friendly tools and guidelines for the analysis of simulation output of multizone programs. There are several recent studies on the coupling of different CFD and multizone programs (Clark 2001, Musser 2001, Gao 2002), and many experimental validations of multizone programs (Emmerich 2001). However, only a few experimental validation studies are available to examine the performance of the coupled multizone and CFD models. The first study to validate coupled multizone and CFD model compared in details the temperature profiles and near-wall heat transfer (Negrao 1995), but did not validate the coupled model for contaminant concentration profiles. Another recent study included the validation of concentration

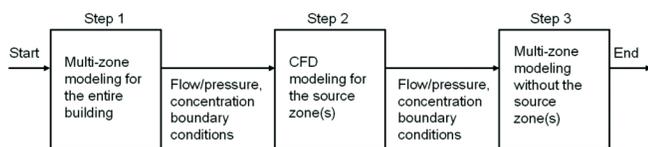


Figure 1 The tested coupling of multizone and CFD models.

profiles (Wang and Chen 2007), but used an environmental chamber partitioned into four sections to represent multiple zones. Thus, the present study proposes an experimental method conducted to validate the accuracy of a coupled multizone and CFD model for concentration profiles in real building environments with on-site experiments.

DEVELOPMENT OF AN INDIRECT VALIDATION METHODOLOGY

An evaluation of the accuracy and effectiveness of the coupled multizone and CFD model is undertaken. The results obtained by multizone method, coupled method, and experimental values are compared within the calculation domain. A straightforward approach is to compare data obtained by three methods within each space, which we called direct validation as shown in Figure 2. This method is considered accurate because it gathers and compares data from three different methods directly. However, for this direct comparison, an averaged concentration from experimental data is needed, which makes the measurement very complex and difficult. An experimental concentration measurement takes only point values at fixed locations, while the real building spaces are usually large with non-uniform temperature and concentration distributions. If an average value within a space is required, the space has to be divided into small cells (0.2 m or less). Within each cell, temperatures and concentrations should be measured to obtain averaged values for the entire space or each zone within a building. This would drastically increase experimental time, difficulties of equipment control, and the cost of the experiment. Therefore, an indirect validation method is used in this study.

To effectively validate the coupled method using typical space concentration sampling equipment, an indirect validation approach is proposed for the comparison. The indirect validation decomposes the validation into two steps as shown in Figure 2. The first step is comparing point measured temperatures/concentrations with point temperatures/concentrations from full-scale CFD at the same locations. The objective of this step is to prove the full-scale CFD prediction of the temperature and concentration distributions to be accurate. Once the accuracy of CFD simulation is evaluated, the second step is a comparison among averaged full-scale CFD, multizone, and coupled models. This comparison is valid only in the case that the full-scale CFD is proven to be a valid substitute for the experimental data.

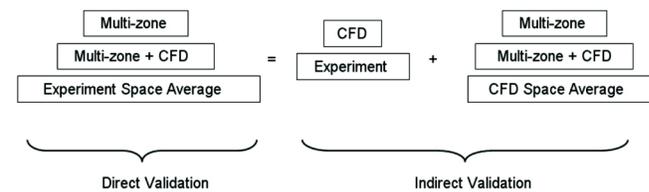


Figure 2 Two possible validation methods for a coupled multizone and CFD model.



Figure 3 The office photo with the on-site measurement instrumentation.

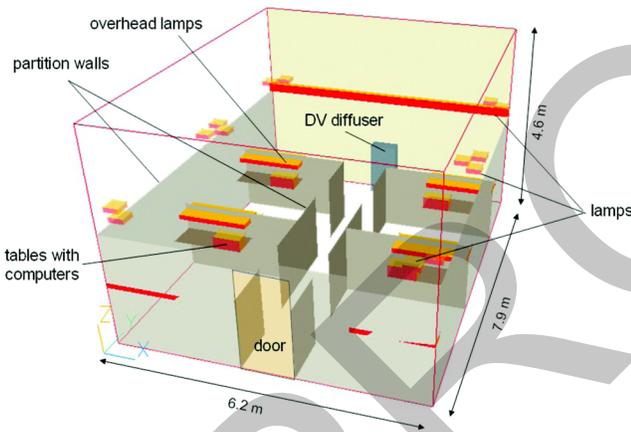


Figure 4 The cubicle office layout with displacement ventilation diffuser and major heat sources.

ON-SITE MEASUREMENTS

Experimental measurements were conducted in an interior cubicle office with displacement ventilation system as shown in Figure 3. Vertical partitions divided the lower part of this area into four large and two small cubicles. The large cubicles had two, and the small cubicles had one working stations per cubicle including computers and lamps, which are presented in Figure 4. During the measurements, occupants were not present, and the major heat sources were computers and the lighting. Table 1 lists the objects and heat sources located in the cubicles during all of the experiments.

The concentration source was represented by a controlled flow rate of SF₆ (sulfur-hexafluoride) tracer gas. The space had only one supply diffuser, so the tracer gas penetrated all cubicles. As shown in Figure 5, the SF₆ source was located

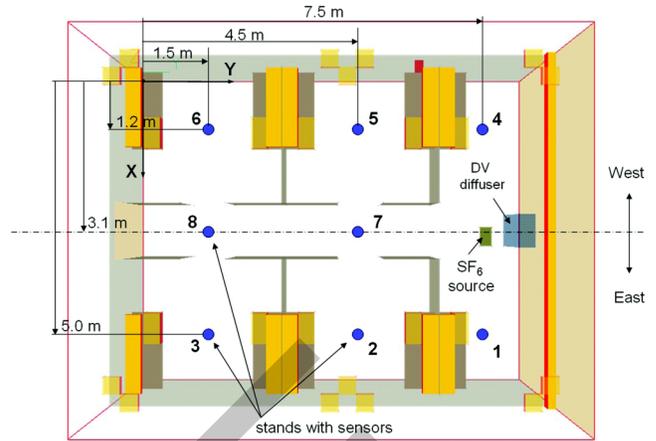


Figure 5 Locations of the seven temperature and SF₆ measuring stands in the cubicles.

Table 1. The Objects and Heat Sources Located in the Cubicles During the Experiments

Object Name	Number of Objects in the Space	Convective Heat Source (each)
Ceiling Lamps	14	40 W
Side Lamp	1	160 W
Computers	10	72 W
Overhead lamps	10	25 W
Partitions	10	—
Tables	10	—
Book shelves	10	—
Total Internal Convective Heat Sources		1690 W

the floor level at a rate of 28.5 ml/min. The source was not located on the centerline of the diffuser. Instead, it had an offset of 0.2 m to the east side of the diffuser to create an asymmetric SF₆ distribution that is more challenging for validation of the coupled multizone and CFD model. The concentration of SF₆ for the east area (zones 1, 2, and 3) and west area (zones 4, 5, and 6) of this cubicle office was considerably different. Concentration is measured in all of the six cubicles, three east and three west cubicles, and at two locations in the corridor. Figure 5 marks the locations where the stands and the sensors were positioned with the blue dots. Sensor stands were located in the middle of cubicles and each stand carried sensors for temperature, velocity, and concentration measurements at 0.8, 1.5, and 2.4 m from the ground. Totally, 25 SF₆ sampling tubes were located in the cubicles; 24 probes were located in the cubicle area, and 1 additional probe was located in the supply duct. In the cubicle area, velocity and temperature sensor were placed in the same locations as the 24 tubes for SF₆ sampling. Also, the temperature of supply air was measured.

Instrumentation

The SF₆ tracer gas system used in validation was composed of three functional subsystems: gas releasing system, automatic sampling system, and gas analyzing system. The gas releasing system discharged a solution of 0.1% SF₆ in nitrogen with an accuracy of 3%. The sampling system consisted of a series of nylon tubes and air pumping devices. Tubes were fixed in the space at the sampling locations, and were connected to the sampling device located outside of the experimental area. The gas analyzing system was a tracer gas monitor based on gas chromatography, and it measured the sample concentration with an accuracy of 3% in the range of 100 ppt (parts per trillion) to 10 ppb (parts per billion).

For the air temperature and velocity measurements, 24 low velocity omni-directional probes with temperature sensors were distributed within the experimental area. Velocity was measured with an accuracy of 0.02 m/s, while the temperature probes had an accuracy of 0.2°C. Also, temperatures of the floor and walls were measured with an accuracy of 0.5°C. In order to determine the flow rate of the supply diffuser, a Pitot tube was used for high air velocity measurement. Velocity was measured at 16 points in the rectangular duct cross-section, and the flow rate was calculated according to the measured velocity and the duct area.

Measurement Procedure and Results

To obtain quasi steady state airflow, temperature, and concentration distributions, the on-site measurements were conducted during the night (2:30 to 5:00 AM), when the internal heat gains and outdoor weather conditions are relatively stable. The night time experimental conditions enabled the experiences of the validation studies conducted in environmental chambers with tightly controlled environmental conditions to be transferred to the on-site experimentation, where the environmental conditions are influenced by air-conditioning operation, floor plan, thermal loads, human activity and infiltration. In our experiments, there were no human activities, infiltration was low, and the lighting plus equipment heat gains were dominant. Thus, during the measurement, the air-conditioning system was operating at relatively steady conditions. It is important that our experiments were conducted without adjusting any of the air-conditioning systems settings and without sealing or controlling any of the air pathways,

making the validation directly applicable to real building environments.

Temperatures and local air velocities were continuously recorded for the entire duration of the experiment. For concentrations, three groups of repeated samplings were conducted, each collecting the data for all of the sampling points. Each of the three samplings lasted approximately 50 minutes including the preparation and transition time between two consecutive data points. The flow rate of the supply air was measured twice during the experiment, once before taking the SF₆ samples and the other after taking all of the samples. The temperature, concentration and flow rate sampling procedures were carefully selected to insure high accuracy of the measured data. The following sections describe sampling procedures for each of the three parameters: temperature, concentration and airflow rate.

Temperature: The air velocity and temperature system recorded the temperatures and velocities every five minutes during the experiment. The variations of temperatures during the experiment were less than 0.2°C, which was in the range of accuracy of the measurement system. This low temperature variation also indicated that the HVAC operation conditions varied little during the experiment and the quasi steady state thermal conditions was reached. Table 2 lists the temperatures of the 24 measured points.

Concentration: To eliminate the experimental errors as much as possible, the concentration was sampled three times during the experiment. Figure 6 shows the three groups of measurements. For most of the positions, all three measurements were in agreement. Only at position 1 and 14 is there a larger discrepancy in consecutive measurements. The sample point 1 is very close to the concentration source, and, therefore, even a very small change of airflow direction creates a change in measured concentration. A possible reason for discrepancy at point 14 is the measurement error. By averaging two closer data values and discarding the third one for each sampling location, the possible measurement error is decreased. The three groups of measurements are finally combined into one group of data used for further validation of CFD simulations.

Airflow rate: Two groups of diffuser flow rates were measured and calculated at the beginning, and in the end of the experiment according to the previously described method. The airflow rates were 0.27 and 0.25 m³/s respectively for the two measurements. The percent of difference is only 7.5%, which

Table 2. Measured Temperatures at the 24 Probe Locations

Point	Stand	T (°C)									
1	1	18.4	7	3	19.7	13	5	20.2	19	7	19.6
2		22.2	8		21.9	14		21.9	20		22.1
3		22.6	9		23.0	15		23.2	21		23.0
4	2	20.2	10	4	18.0	16	6	19.9	22	8	19.6
5		21.8	11		22.1	17		22.1	23		22.0
6		22.9	12		22.7	18		23.2	24		23.0

indicates the measurements are repeatable and also proves the HVAC system performance varied within acceptable range. The average value of the two measurements was used as an input parameter in CFD, multizone, and coupled simulations.

SIMULATION SETTINGS AND RESULTS

For the multizone model simulations, the cubicle office area was divided into two levels. The lower level extends from the floor level to the height of the partition (1.65 m). The upper level extends from the top of the partition up to the ceiling. Furthermore, each level is divided into 9 individual zones as shown in Figure 7. Therefore, the total number of zones used in the multizone modeling is 18.

In the coupled multizone and CFD model, the CFD domain covered zones 1, 4, and 7 in the lower level, and 10, 13, and 16 in the upper level. These zones included the area with the air supply diffuser and contaminant source. The detailed airflow simulation results in the vicinity of the contamination sources are crucial for the overall SF₆ concentration distribution calculations. The remaining zones are the domain of the multizone program, and the coupling procedure between multizone and CFD domain is described by Yuan and Srebric (2002).

According to the first step of the indirect validation method, a full-scale CFD simulation is conducted for the entire office floor covering all 18 zones. The office area

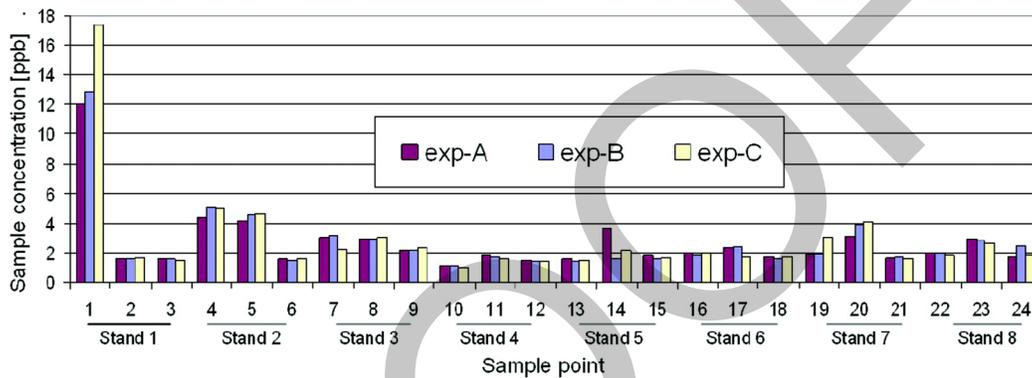


Figure 6 Three sets of the measured concentration data (exp-A, exp-B, and exp-C).

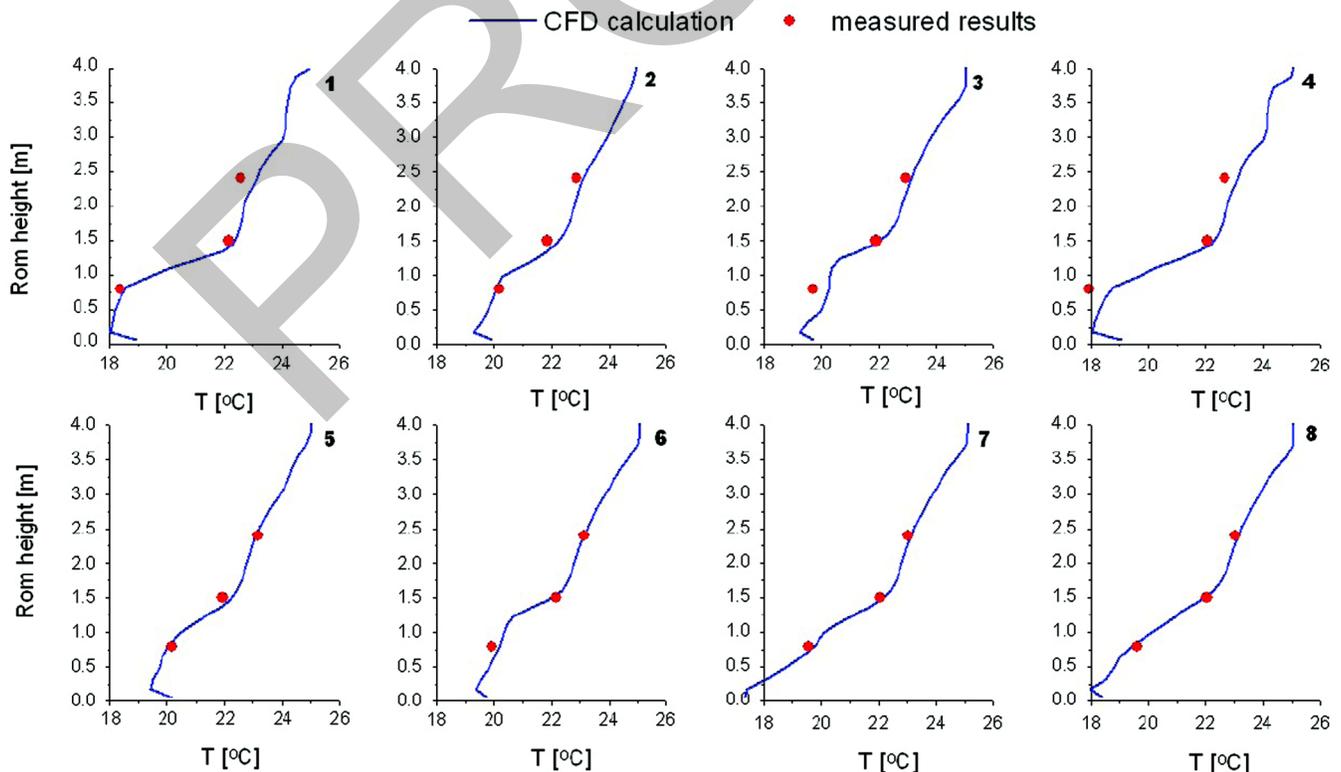


Figure 7 Locations of 18 zones for the comparison of CFD, multizone and coupled simulation results.

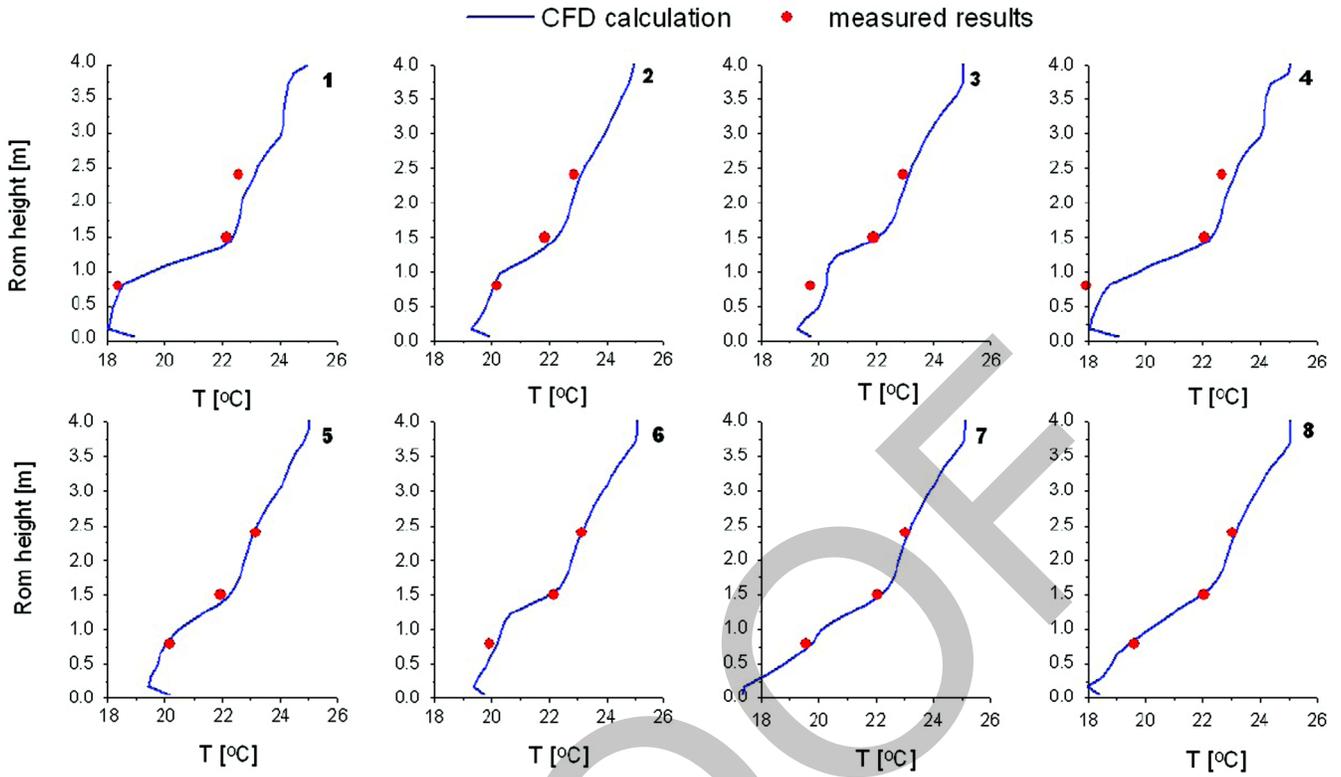


Figure 8 Measured and CFD data for temperature at 8 vertical positions in the cubicle office.

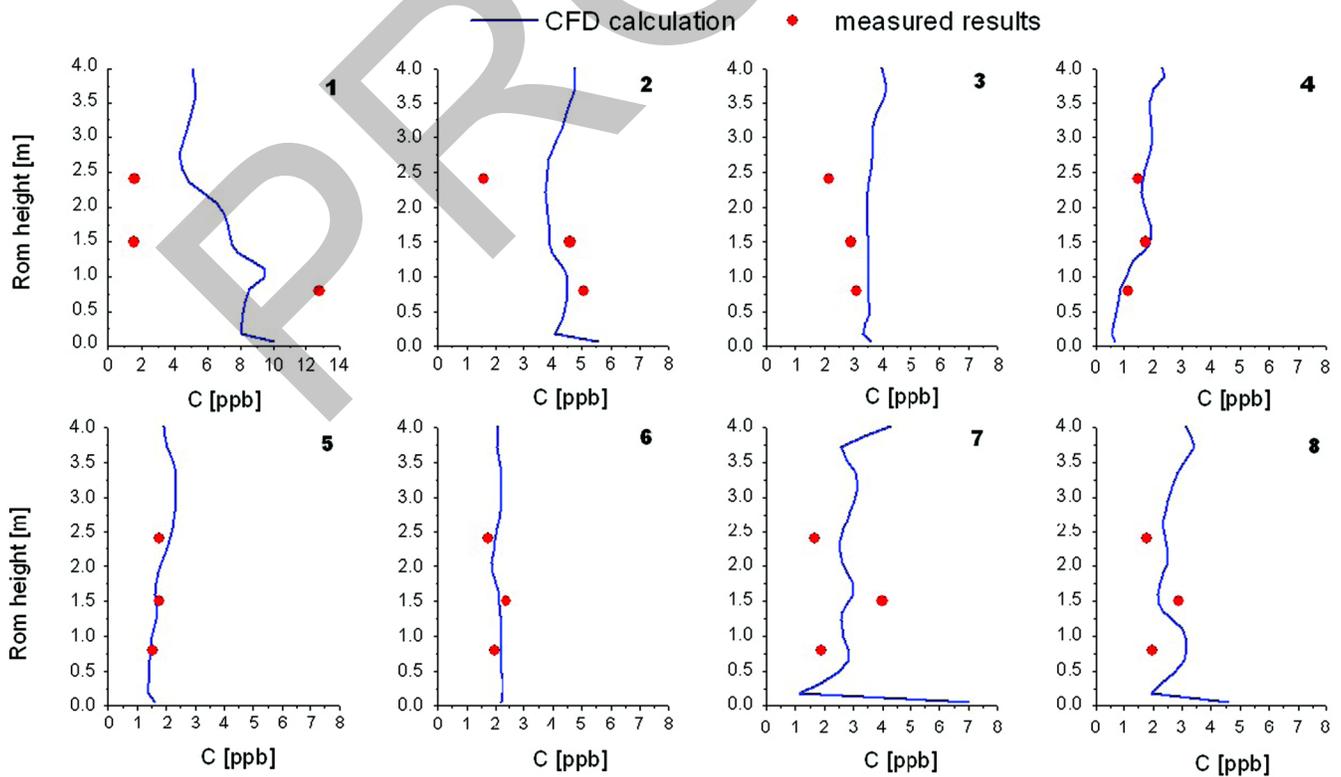


Figure 9 Measured and CFD data for concentration at 8 vertical positions in the cubicle office.

consisted of $46 \times 68 \times 31$ control volumes, and the RNG $k-\epsilon$ model was used to account for the turbulence of airflow. The wall and floor temperature measurements provided data for the CFD simulations. The floor was divided into 9 areas in accordance with the zone division in Figure 7. Since the airflow in the office cubicles was generated by buoyancy from internal heat sources, it was crucial to precisely define internal heat sources based on the power consumption of lamps and computers. In the CFD domain, these sources were defined as surface heat flux sources.

Comparison of CFD with Experiment Results

In the first step of the indirect validation procedure, temperatures and concentrations were compared for CFD and experimental data. The temperature is first validated to prove CFD prediction accuracy, because an inaccurate temperature distribution strongly affects the concentration and airflow rate predictions. Figure 8 shows the result of the temperature validation. The calculated vertical temperature distribution is presented for eight stand positions (refer to Figure 4) accompanied with experimental results. As shown in Figure 8, 20 out of 24 points have the temperature difference between calculated and measured data in the range of air temperature measurement accuracy (0.2°C). The valid CFD prediction of temperature distribution is necessary for accurate concentration calculations, especially for rooms with buoyancy driven flow such as in the analyzed case of displacement ventilation.

Figure 9 shows the validation of CFD concentration results. Even though agreement between measured and CFD predicted results is not as good as for the temperature distribution, CFD successfully predicted most of the concentrations in the cubicle office. At several points, the disagreement is larger, but for most of points, the difference between calculated and measured results is within 20%. Considering the complexity of the on-site measurements and the sensitivity of concentration distribution calculations, the simulation results can be considered as being really good. The fact that the local CFD and the experimental point data agree enough to accept the CFD predictions as accurate enables the second step of the indirect validation. In this second step, the full-scale CFD data represent the field measured data.

Comparison Between CFD, Multizone, and Combined Methods

In the second step of the indirect validation, the simulation results by CFD, multizone, and coupled methods are compared in each zone. The comparison results were expected to have the same characteristics as shown in our previous study (Yuan and Srebric 2002). This study has demonstrated that the coupled method provides reliable and fast results.

The comparison of the averaged CFD concentrations, multizone concentrations, and coupled model concentrations are shown in Figure 10. The coupled model shows advantage over the multizone simulation in zones covered by CFD calculations, which are zones 1, 4, 7, 10, 13, and 16, representing approximately twenty percent of the calculation domain. On the other hand, the multizone model performs similarly or slightly better than the coupled model in the rest of the calculation domain. Interestingly, the highest and the lowest concentration zones, zone 1 and zone 4, are adjacent to the source zone 7, as shown in Figures 4 and 7. Zone 1 is located at the floor level on the east side closer to the position of the contaminant source, while zone 4 is located symmetrically on the west side of the source zone. The asymmetry of the concentration in this case was nicely captured by the coupled method, while the multizone method failed to predict the asymmetry due to its inherent assumption of the uniform concentrations in each simulation zone. Nevertheless, the multizone model performed well outside of the immediate vicinity of the source zone. Even the buoyancy driven transport of contaminants with displacement ventilation can be captured with the multizone simulations as long as the temperature field is correctly specified or calculated.

Considering the calculation time of each method, presented in Table 3, the coupled method is three and half times faster than the CFD method. The computational advantage of the coupled model is due to the fact that the systems of the algebraic/differential equations is relatively small and much easier to solve, than the numerical procedure for the systems of partial differential equations associated with the CFD methods. In addition, the time required to set up a coupled model is much shorter than the time needed to set up a CFD model because the computation domain covered by the multizone simulation

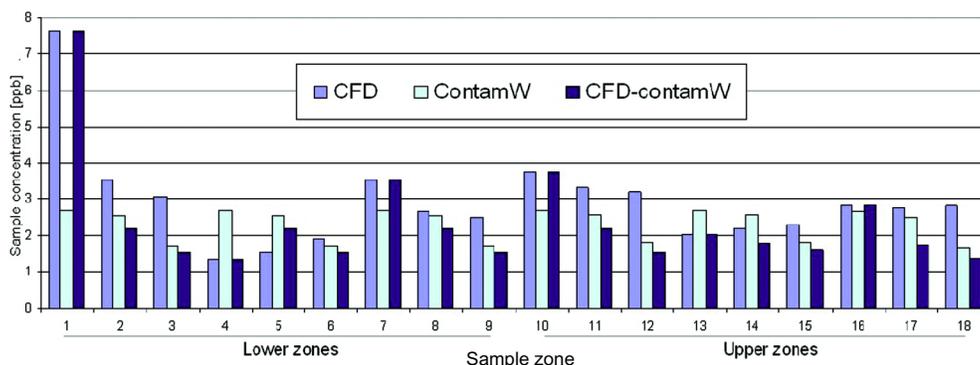


Figure 10 The comparison of CFD, multizone and coupled simulation results.

Table 3. The Computation Time for Different Simulation Methods as Executed on a PC (Pentium 5)

Model	Mesh Size	Computation Time
CFD Entire office	61 × 82 × 32	81432 s (~22.6h)
CFD Source zones	61 × 48 × 32	22958 s (~6.4h)
Multizone	18	<5 s

required only associated source/sink intensities, rather than a detailed geometry, detailed space layout, and detailed source/sink locations. Overall, the justification for use of either of the three models, CFD, multizone or coupled models, is case dependent. At present, users of the simulation models are responsible for making this judgment based on the tradeoffs between required accuracy and available computational time.

CONCLUSION

An on-site validation study of the coupled multizone and CFD model required development of an indirect validation approach, which enabled comparison of discrete experimental data points to calculated bulk airflow and contaminant concentrations. The indirect validation is divided into two separate steps. The first validation step checks the accuracy of the CFD modeling for the entire calculation domain. The main factors for accurate CFD modeling include not only the numerical decisions such as selection of turbulence models, grid distribution, and integration scheme, but also the boundary conditions necessary for accurate building representation. In our simulations, the boundary conditions were obtained from on-site measurements and a survey of the building office floor. The second validation step examines the accuracy of the coupled multizone and CFD model when compared to the validated CFD from the first validation step. The main factors to influence the accuracy of the coupled model are the accuracy of multizone prediction and the accuracy of the exchanged CFD-multizone boundary conditions. Future work can be conducted with these two different directions to enhance the accuracy of the coupled model for entire building simulations.

Through the two steps of the indirect validation, the accuracy of the coupled multizone and CFD model is proven to be better than the multizone model alone for the zones close to the contaminant source location. For all other zones, the multizone models performed similarly or slightly better than the coupled model. The computation time of the coupled model is greatly reduced when compared to the CFD model alone, and it is greatly increased when compared to multizone model alone. The coupled model can be a fast and reliable method in airflow and contaminant transport predictions for an entire building simulation. Nevertheless, the applicability of the three tested models, CFD, multizone and coupled models, is case dependent. Based on the tradeoffs between required accuracy and available computational time, users of these simulation models should make a decision which model represents the appropriate tool for a contaminant dispersion problem of interest. To support this important and challenging decision

making, the developed indirect validation method can be applied to other studies to evaluate the performance of multizone or coupled multizone and CFD models.

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