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# AN INTRODUCTION TO THE CFD CAPABILITIES IN CONTAM 3.0

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## ABSTRACT

CONTAM is a multizone airflow network computer program for building ventilation and indoor air quality analysis. The program was recently enhanced to incorporate CFD capabilities for both external and internal environmental analysis. This paper introduces the CFD features implemented within the most recent version, CONTAM 3.0. The external CFD link predicts wind pressure coefficients and contaminant concentrations for airflow paths at the building surface. A converter computer program translates the wind pressure coefficients and contaminant concentrations to the CONTAM data format. The ability to embed single CFD zone within a CONTAM network model has also been implemented. This enables the detailed modeling of a zone, in which the well-mixed multizone assumption is too broad but uses the multizone approach for the rest of a building. This paper used a generic residential house model to demonstrate how the new CFD features enrich the existing CONTAM capabilities for indoor air quality analysis.

## INTRODUCTION

One of the most used building ventilation tools for bulk air analysis is multizone network airflow model. In a multizone model, airflow and species transport are calculated between the rooms of a building and between the building and the outdoors. The so-called well-mixed assumption is used to make the bulk analysis possible. Under the well-mixed assumption, a building is subdivided into zones with homogeneous air properties and species concentrations. When air and species properties are highly non-uniform, the well-mixed assumption may fail. For such situations, a tool to calculate detailed air properties, such as computational fluid dynamics (CFD), is needed. Compared to a multizone model, CFD is more computationally intensive and is less often used for whole-building analysis or long-term time-dependent simulations. For building ventilation design and indoor air quality (IAQ) analysis, the multizone and CFD models are not conflicting methods but can be integrated to take advantage of the benefits offered by each.

Schaelin et al. (1994) proposed a "method of detailed flow path values" to improve upon the well-mixed assumption. The method used CFD to calculate local pressures, velocities, and contaminant concentrations near flow paths and using them as inputs to multizone simulations. They demonstrated the method through manual exchange of boundary conditions between two stand-alone programs and showed promising results. Soon thereafter, Clarke et al. (1995), and Negrao (1998) started to implement an automatically coupled CFD and network model inside their building simulation program Environmental Systems Performance, Research version (ESP-r) (Clarke 1985). Their pioneering work provided one of the earliest coupled CFD and network models. Later, some applications of coupled CFD and multizone methods and some experimental studies were conducted by Srinivas (2001), Yuan and Srebric (2002), and Jayaraman et al. (2004). Their studies showed that coupling a CFD model with a multizone model could obtain more realistic predictions of airflow and contaminant transport in buildings with large spaces. However, these studies were mostly research-oriented and did not provide a general purpose design tool for the public. Currently, some commercial software is available with integrated building energy simulation and CFD capability, but they are not specifically developed for building ventilation and IAQ analyses.

Aiming at developing an open source tool for building ventilation design and indoor air quality analyses for the general public, this study has coupled CONTAM (Walton and Dols 2008), a multizone network software program developed at the National Institute of Standards and Technology (NIST), with CFD0, a CFD software with an indoor zero turbulence model (Chen and Xu 1998). CONTAM is a popular tool to determine building air infiltration, exfiltration, and room-to-room airflows driven by wind pressures on building exteriors, buoyancy effects related to the indoor and outdoor air temperature difference, and mechanical ventilation. It also predicts the dispersal of airborne contaminants and can be used to calculate the personal exposure to these contaminants for risk assessment. CFD0 was a CFD program originally developed for ASHRAE project

RP-927 (Chen et al. 1999), and improved by Wang (2007). Wang and Chen (2007) studied the solution characteristics of integrated multizone and CFD models, developed the coupling methods, and validated the coupled CONTAM and CFD0 program. In this paper, we further implemented the coupling methods in a new version of CONTAM to be released as CONTAM 3.0. This paper first introduces the schematics for the two methods of linking CONTAM and CFD0, i.e. the external link for performing external airflow analysis, and the internal link for embedding a CFD0 zone within a CONTAM airflow network. A demonstration case of a generic single family house is presented for the analysis of indoor contaminant transport.

## METHODS OF CONTAM AND CFD0 INTEGRATION

The incorporation of CFD0 into CONTAM 3.0 provides two major capabilities: linking the effects of wind pressure and outdoor contaminant concentrations with CONTAM's indoor simulations, and embedding the detailed CFD zones within the CONTAM airflow and contaminant transport network.

### Linking of CFD and CONTAM for building exterior simulations

Wind pressure is the major driving force for air infiltration through a building envelope. Wind pressure, as a function of wind speed, wind direction, building configuration, and local terrain effects (ASHRAE 2009), can be accounted for by CONTAM with one of three options: specifying wind pressure to be constant, implementing surface averaged wind pressure profiles for each envelope penetration, and using spatially and time varying wind pressures based on an external Wind Pressure and Contaminant (WPC) file. The WPC file provides exterior pressure and/or contaminant concentrations time histories for every flow path that connects to the ambient zone including duct terminals and outdoor air intakes of CONTAM's simple air handling systems. It allows for the use of general, spatially varying wind pressure and ambient contaminant concentrations such as those from wind tunnel experiments or atmospheric models, e.g., plume or puff dispersion simulation tools (Walton and Dols 2008). A general approach for handling the variable effects of wind is the use of a local wind pressure coefficient, $C_P$, which is a function of local wind pressure, $P_w$, undisturbed wind speed, $U_H$, and wind pressure, $P_H$, at a reference height H in the far airflow field.

A rough estimate of average wind pressure profile over each side of a building surface can be obtained from empirical or experimental studies, such as Swami and Chandra (1988), as a function of wind direction relative to a building surface, i.e. "relative wind direction". However, surface-averaged wind pressure coefficients may be insufficient for air infiltration predictions (Gao 2002). In fact, air movement around buildings is a three-dimensional turbulent flow, so wind pressures could vary significantly even over a single building surface. To address the variations of wind pressure coefficients over a building surface, the most reliable means of determining $C_p$ for a specific building are through on-site measurements or wind tunnel studies (Persily and Ivy 2001). However, the measurements can be expensive, and sometimes technically difficult. Hence, numerical simulations, such as using CFD, of turbulent flows around buildings seems a better option as demonstrated by Gao (2002) and Jiang (2003). More importantly, using CFD for simulating external contaminant release near buildings can provide detailed profiles of contaminant concentration on building exteriors, which is useful to study the impact of outdoor air quality on an indoor environment (Wang and Emmerich 2009).

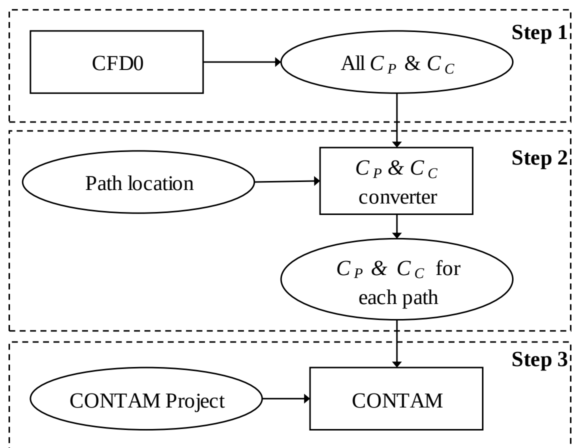



*Figure 1 Schematic of the link between CONTAM and CFD0 for building external airflow and contaminant transport simulations*

One of the new features of CONTAM 3.0 is the external CFD link, which calculates a profile of wind pressure coefficients for each building penetration. The use of wind pressure coefficients avoids extra CFD runs that would be required to obtain wind pressures when the wind direction or speed changes. The external CFD0 link is comprised of three steps as shown in Figure 1. First, CFD0 calculates airflow and contaminant transport outside a building and creates a file with all wind pressure coefficients ($C_P$) or contaminant concentrations ($C_C$). A separate computer program then searches in the files for the values of $C_P$ or $C_C$ for each specific airflow path, for which a location is defined in the CONTAM project. The program then converts the values to a CONTAM library file with $C_P$ or $C_C$ values for all envelope airflow paths. Finally, when a CONTAM simulation is performed using a CONTAM weather file, the appropriate $C_P$ or $C_C$ for each envelop airflow path is applied for each wind direction and simulation time step.

The three-step procedure in Figure 1 provides a flexible external link between CONTAM and CFD0. It is recommended for studies of:

- Wind pressure and/or outdoor contaminant concentrations that vary with wind direction. In the first step, different wind directions can be defined, e.g. from 0˚ to 360˚ around the building. CFD0 will calculate and automatically save envelope $C_P$ or $C_C$ for all wind directions. When a CONTAM simulation needs to switch to different wind angles, it will interpolate the $C_P$ or $C_C$ values based on saved data without having to run the CFD simulation again.
- Parametric studies of variable locations of outdoor contaminant sources on indoor concentration levels. In the first step, CFD0 saves all calculated air properties and velocities at steady state, which can be reused if the locations of outdoor contaminant sources are changed, assuming such change will not affect the airflow field.
- Transient contaminant transport outdoors using previously-calculated external airflows at the steady state. Similar to the above feature, this option allows users to run a transient outdoor contaminant transport simulation using steady-state airflow results already available without the need to rerun the CFD calculations.

The external CFD link in CONTAM 3.0 has been successfully applied to the study of indoor exposure to carbon monoxide caused by operating gasoline-powered electric generators outside of a house (Wang and Emmerich 2009). This involved a study of many parameters including contaminant source location and weather conditions. The external CFD link helped to reduce the computational cost significantly.

## Embedding CFD zone within a CONTAM airflow network

The well-mixed assumption of multizone models could become less suited for zones with non-uniform distribution of air properties and contaminant concentrations (Wang and Chen 2008). An example could be a multi-story building with a large atrium. As a remedy, the large space can be handled by CFD0 and the rest of the zones in the building by CONTAM, while the two programs exchange information at the boundaries formed by the airflow paths between the CFD and CONTAM zones. To satisfy conservation equations on both sides of the boundaries, the process is often a two-way iterative procedure. This is different from the external link, where the values of $C_P$ or $C_C$ are passed one-way from CFD0 to CONTAM. Thus, the embedding of the CFD zone within CONTAM is a dynamic coupling method of the two programs.

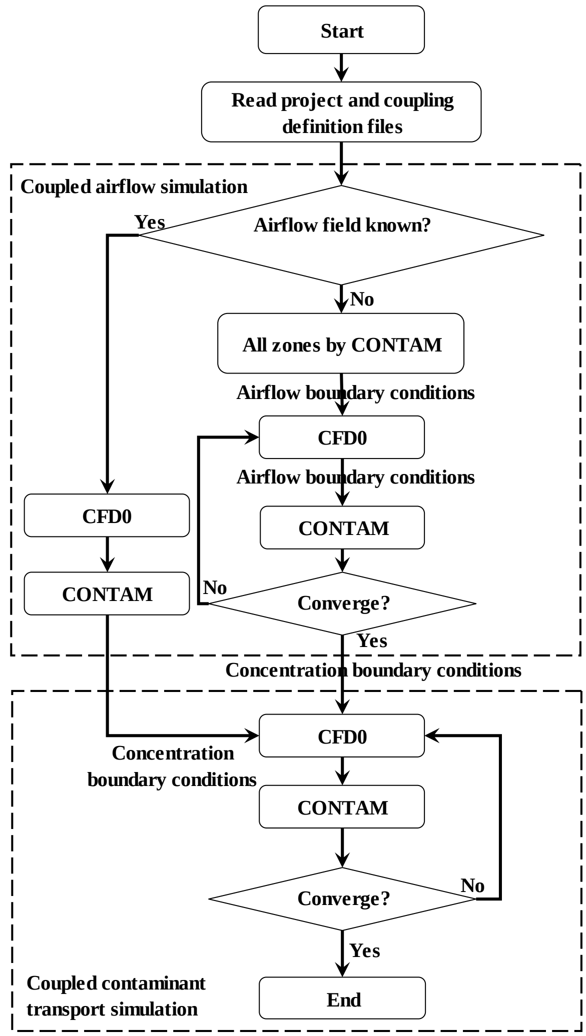



*Figure 2 Schematic of embedding a CFD zone within the CONTAM airflow network for simulations at steady state in CONTAM 3.0*

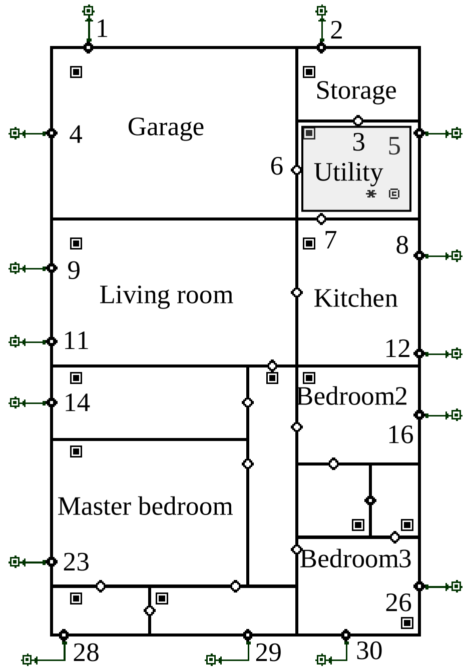
Given that the boundary conditions are exchanged iteratively between CONTAM and CFD0, the dynamic coupling procedure can be unstable if the boundary conditions are exchanged incorrectly (Negrao 1998; Bartak et al. 2002). Wang and Chen (2007) suggested that the exchange of pressure boundary conditions between the two programs can achieve an unconditionally stable solution, whereas other ways of information exchange, such as mass flow rates, may lead to solution divergence. Figure 2 shows the two-step schematic for coupling CONTAM and CFD0 programs in CONTAM 3.0 for a simulation at steady state: coupled airflow simulation and, if necessary, coupled contaminant transport simulation. If an airflow result is available from a previous coupled calculation, it can be imported directly to save computational cost. Otherwise, the coupled program performs a fully coupled procedure for airflow prediction. The fully coupled procedure obtains initial values of air pressures and flow rates for all zones by running a CONTAM simulation for the whole building. With boundary conditions from CONTAM, CFD0 calculates the airflow in the CFD zone and feeds boundary conditions back to CONTAM. The iteration continues until the convergence of both sets of calculations. If a coupled simulation of contaminant transport is needed, a similar iterative procedure is used except that the contaminant concentration is exchanged at each interface airflow path as opposed to the air pressures. When a coupled simulation is transient, the procedure in Figure 2 is repeated for each time step.

## DEMONSTRATION OF THE CFD CAPABILITIES

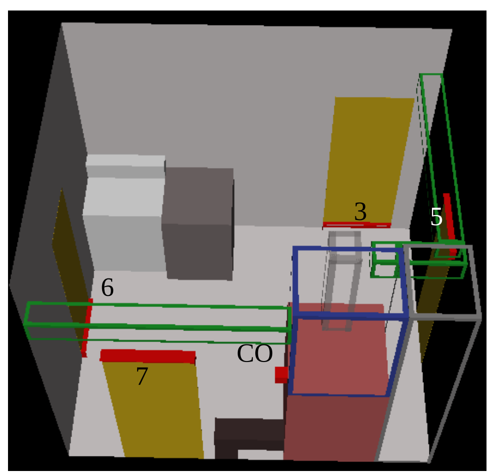
A generic low-rise residential house was selected to be modeled. Due to the page limit, this paper only demenstrated the embedding CFD zones within a CONTAM airflow network. A more detailed study for both external and internal CFD link can be found at Wang et al. (2010).

Figure 3 provides CONTAM and CFD perspectives of the house, which was 15.5 m × 7.4 m × 3.0 m (l × w × h) (the height excluding the slant roof). The internal CFD link is demonstrated by simulating the transport of carbon monoxide (CO) in the house produced by a faulty furnace in the utility room (the shaded zone in Figure 3(a)), for which the CFD model is shown in Figure 3(b). In order to investigate the effects of non-uniformity of CO concentration in the room, the utility room was selected to be simulated by CFD0, and the remaining rooms were simulated as well-mixed zones.

The following describes the inputs used to establish the test case. The utility room is 3.2 m × 2.6 m × 2.7 m (l × w × h) with a total CFD grid of 70 × 70 × 90. The ambient air temperature was set to be 25 ˚C and the wind was set to 10 m/s and from 30˚ relative to the north. The wind pressure profiles from the experiments of Holmes (1986; 1994) were used. The CO source strength was set to 126.6 g/h, which was determined from a suggested CO emission rate of 1 mg/kJ by a previous experimental study (Ryan and McCrillis 1994), and the suggested furnace power of 35.2 kW (120 000 Btu/h) from another study (Lee 1990). The furnace was also run under a 10-minute on/off cycle. Figure 3(b) illustrates the CO source location, the furnace, and the four airflow paths that are modeled as cracks located at either the top or bottom of the doors. The airflow was assumed to be steady, and the time-dependent transport of CO was simulated for two hours with a one-minute time step.




*(a)*




*(b)*

*Figure 3 (a) the CONTAM zone configuration with the shaded zone of the utility room and (b) the internal view of the utility room in CFD of the low-rise house with a slant roof*

The CFD0 simulation of the utility room used the CONTAM-predicted airflow rates for the door cracks as inputs. Table 2 provides the calculated airflow rates through the door. There were two air inflows to the room, air from the storage room through path 3 and from the outside through path 5. Most of the outflow goes to the kitchen through path 7 and the rest to the garage through path 6.

*Table 2 Predicted airflow rates of the airflow paths in the utility room (a negative value shows outflow from the room)*

| AIRFLOW PATH | PATH 3 | PATH 5 | PATH 6 | PATH 7 |
|---|---|---|---|---|
| Airflow Rate × $10^3$ kg/s (× $10^3$ $m^3$/s) | 6.6 (5.5) | 7.2 (5.6) | -1.1 (-0.9) | -12.8 (-10.6) |

With the calculated airflow rates as inputs, CFD0 calculated the time-dependent CO distribution in the utility room for the duration of two hours. Local values of CO concentration were provided near the airflow paths in the utility room for the CONTAM simulation of the rest of the rooms of the house. As shown in Figure 7, at end of the two-hour simulation time the CO levels in the utility room were non-uniform. The CO concentration was close to zero near paths 3 and 5 due to the inflow of uncontaminated air. Because path 7 was closer to the CO source than path 6, the local CO level near path 7 was higher. Moreover, the top portion of the room generally had higher CO levels than the lower one, which also contributed to the higher CO concentration near path 7 than path 6.

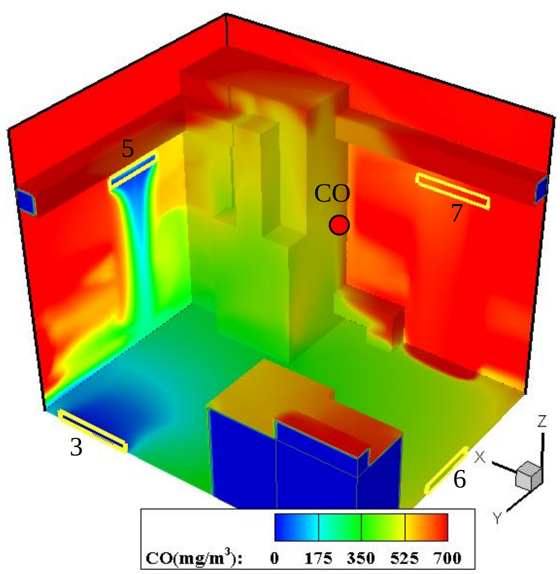



*Figure 7Distribution of CO concentration (mg/$m^3$) in the utility room at end of the two hour simulation time*

Figure 7 only shows one "snap shot" of the CO distribution at the end of the simulation. In fact, the transient CO distribution in the whole house was determined by many of these "snap shots" from the CFD calculation. Figure 8 illustrates how the CO levels in the rest of the house changed over time compared with that in the utility room. Room names followed by a parenthesized "CFD" refer to the results when the utility room was modeled by CFD0 and the rest of the rooms by CONTAM. When the whole house was simulated by CONTAM, the results were tagged by "well mixed".

It was showed that CO levels in the utility room fluctuated every ten minutes with the on-off cycle of the furnace whether using CFD or not. The simulation with CFD predicted obviously fluctuant and higher CO concentration in the kitchen than that in the well-mixed case. Path 7, which connects the kitchen and the utility room, was very close to the CO source, so a fluctuation of CO strength could easily affect the CO level in the kitchen. The peak CO level near path 7 was around 2500 mg/$m^3$, which is more than three times higher than that near path 6. This shows the importance of the source location and the local concentration of CO near inter-zonal connections. Note that when the utility room was simulated as a CFD zone, the CO level of the utility room was spatially averaged over the entire room. Figure 8 also does not show the results of the bedrooms and the rest of the house because they were much lower compared to those of the three rooms shown in the figure.

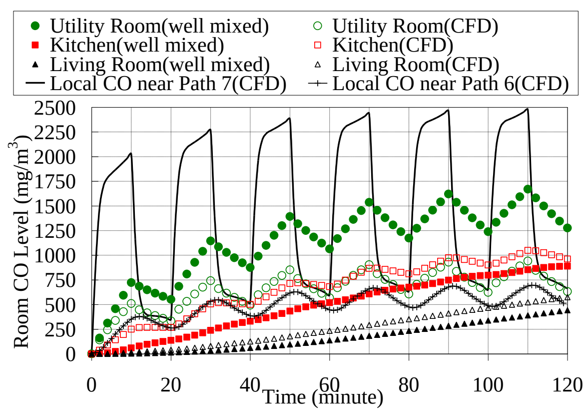



*Figure 8 Comparison of CO levels in the utility room, kitchen, and living room of the house with and without CFD simulations*

The CO levels in the non-source zones were similar in magnitude between the CFD and well-mixed case. However, the small difference in CO levels may be important with respect to occupant exposure. Based on the time and CO levels an occupant is exposed to, a clinical symptom of CO poisoning can be evaluated (NIOSH et al. 1996). In this study, a syptom of headache can be associated with the exposure to the CO level of 233 mg/$m^3$ (200 ppm(v)) for one to two hours.

When CO reaches 815 mg/m$^3$ (700 ppm(v)), an exposure to this level for one hour or more can cause more severe CO poisoning, such as progressively worsening symptoms of vomiting, confusion, and coma. The well-mixed simulation (without CFD) is shown to reach either of the two critical lines about 20 minutes later than that with CFD in both the living room and the kitchen. A period of 20 minutes may be crucial considering occupant safety and evacuation. Therefore, the capability of embedding a CFD zone within the multizone network provides a useful tool for the study of short-term exposure.

## CONCLUSION

This paper introduced implementations of the new CFD features in CONTAM 3.0 – the external CFD link for simulations of airflows around the building exterior, and the internal CFD link for embedding a CFD zone within a CONTAM airflow network. The external CFD link predicts distributions of wind pressures and contaminant concentrations outside a building for simulating their effect on indoor contaminant concentrations. The internal CFD zone enables the detailed calculation of air and contaminant concentrations within a room or region of a building for which the well-mixed assumption is insufficient, and the remaining rooms are handled with the well-mixed assumption that is typical of CONTAM. The new capabilities were demonstrated by modeling a generic low-rise residential house for the internal CFD link in CONTAM. It was shown that the embedded CFD zone is very useful for analysis of short-time contaminant transport, especially for evaluation of occupant exposure. Note that this paper is simply a demonstration of the new CFD capability in CONTAM 3.0. Further experimental studies are definitely needed. However, it is shown that the new CFD feature of CONTAM 3.0 provides a potentially useful capability for building ventilation design and indoor air quality analysis.

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