

Article



Comparison of CFD and Multizone Modeling from Contaminant Migration from a Household Gas Furnace

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Abstract: In Central and Eastern Europe, a growing popularity of gas heaters as the main source of heat and domestic hot water can be observed. This is the result of new laws and strategies for funding that have been put in place to encourage households to stop using coal and replace it with cleaner energy sources. However, there is a growing concern that gas furnaces are prone to malfunction and can be a threat to occupants through CO (carbon monoxide) generation. To see how a faulty gas furnace with a clogged exhaust may affect a household, a series of multizone and computational fluid dynamics (CFD) simulations were carried out using the CONTAM software and CFD0 editor created by the National Institute of Standards and Technology (NIST). The simulations presented different placements of the furnace and ventilation outlet in an attached garage. The results showed how the placement influenced contaminant migration and occupant exposure to CO. It changed the amount of CO that infiltrated to the attached house and influenced occupant exposure. The results may be used by future users to minimize the risk of CO poisoning by using the proper natural ventilation methods together with optimal placement of the header in the household.

Keywords: indoor air quality; carbon monoxide; CONTAM; CFD0

1. Introduction

Coal consumption secures more than 50% of needs of the Polish economy for primary energy carriers, and the consumption of hard coal alone amounts to 70–80 million tons [1]. Additionally, in Poland, coal consumption makes up an exceptionally high level of economy energy security. In 2013, coal (both hard and brown) accounted for approximately 54% of the primary energy consumption and almost 90% of electricity production [2]. In the same year, approximately 11 million tons of hard coal was used in households [2].

To counteract coal consumption, there has been a growing trend for replacing coal furnaces for gas ones to improve air quality. Thanks to government funding and the growing social awareness, the replacement of coal furnaces to gas ones have increased. The aim is to limit emission from households and, in consequence, improve the air quality [3]. However, in Poland it is common that furnaces are located in an attached garage if there is no special boiler room, which can contribute to contaminant migration into an attached house.

In a house, an attached garage can be a significant contaminant contributor to the indoor environment without a furnace, let alone with one [4–12]. The contaminants from a starting car or chemicals alone can influence the air quality within an attached household. If the gas furnace were to malfunction and the fume exhaust not work properly, there is a risk of CO (carbon monoxide) poisoning. Carbon monoxide is an odorless, tasteless, poisonous byproduct of partial combustion of fossil fuels that is a leading cause of brain injury and death due to suicidal attempts or accidental exposure [13,14]. Its high mortality is associated with impaired functioning of the red blood cells to transport oxygen to the tissues in the body [15–17].



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Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/). To study how the location of a furnace, compared to the location of the airways, influences the contaminant migration, a series of multizone and computational fluid dynamics (CFD) simulations were carried out using the CONTAM with the CFD0 application.

CONTAM is a multizone indoor air quality and ventilation analysis computer program designed to determine airflows, contaminant concentrations, and migration, as well as personal exposure. It has the ability to calculate building airflow rates and relative pressures between zones as well as determining the variation in ventilation rates, for determining the distribution of ventilation air within a building [18]. It calculates contaminant concentrations that can be used to determine the indoor air quality (IAQ) performance of buildings before they are constructed and/or occupied, to investigate the impacts of different design decisions/methods concerning ventilation systems [19]. Predicted contaminant concentrations can also be used to estimate personal exposure based on occupancy patterns [18]. CONTAM has been used for multiple analysis, including infiltration calculations [20–23] and contaminant transport [24–28], as well as occupant exposure and comfort [29]. It is a valid tool for the assessment of a chosen ventilation system and can help to counteract the risks of poor IAQ. One limitation of CONTAM as a multizone program is that each zone is assumed to be at a uniform contaminant concentration [18].

On the other hand, CFD simulation programs are a powerful tool for estimating the airflow patterns and thermal environment of various heating, ventilation, and air conditioning (HVAC) systems in a very detailed way. They have been used for the estimation and control of the indoor environment and space ventilation when using different ventilation systems [30–33]. Furthermore, they have been used to analyse the influence of structures on airflow [34–37] and contaminant migration [26,38,39]. The limitation of CFD programs is that they are usually limited to a closed zone and it is not possible to provide results for an entire structure.

Because both multizone and CFD programs are well-researched instruments to predict contaminant migration as well as occupant exposure, in this study, it was decided to couple the multizone capabilities of CONTAM with the CFD methods of the CFD0 editor to estimate the contaminant infiltration of CO from a faulty gas furnace in a garage into an attached house.

2. Simulations

The aim of the research was to see how the location of a gas furnace, with respect to the ventilation system, changes the contaminant migration from an attached garage. The furnace was assumed to be faulty, with a blocked furnace exhaust vent. To achieve this, the programs CONTAM and CFD0 software created by NIST were used.

Carbon monoxide was taken under consideration as it is the most lethal of the exhaust gases from a gas furnace. According to the World Health Organization (WHO), the limit of CO a person should be subjected to is less than 30 ppm in 1 h, or 50 ppm during the period of 8 h [40]. The effects of high carbon monoxide concentration are shown in Table 1.

CO Concentration (ppm)	Effect on the Human Body		
9	Maximum allowable concentration in living areas		
50	Maximum allowable concentration for a continuous 8 h period		
200	Headache, nausea, and dizziness after 2 h		
400	Headache, nausea, and dizziness—life-threatening after 3 h of exposure		
800	Dizziness, nausea, and convulsions within 45 min, death within 2 h		
1600	Dizziness, nausea, and convulsions within 20 min, death within 1 h		
3200	Dizziness, nausea, and convulsions within 5–10 min, death within 30 min		
6400	Dizziness, nausea, and convulsions within 1–2 min, death within 10–15 min		
12,800	Death within 1–3 min		

Table 1. CO concentrations and their effect on the human body.

Multizone simulation programs such as CONTAM have a series of limitations and assumptions [41]:

- The concentration of contaminants, room pressures, and temperatures are uniform in each zone.
- Transport of contaminants along each flow path between zones is instantaneous.
- The air is still in each zone, so the airflow through zones does not impact zone pressures.
- Wind pressures on a building's surface are uniform.

Despite these disadvantages, multizone modelling has the advantage to simulate large buildings with many different ventilation zones [42]. It also allows the modeling of infiltration as well as occupant exposure while the occupant is active and moves in and out of the zones [25].

When using CONTAM, the air that flows from zone 1 to zone 2 is calculated based on the pressure drop between zones, as is shown in Equation (1) [20]

$$F_{1-2} = f(P_1 - P_2) \tag{1}$$

where *F* is the mass flow (kg/s); P_1 and P_2 are the pressures in the zones (Pa).

The mass of air in a zone is given by the ideal gas law

$$m = \rho V = \frac{PV}{RT} \tag{2}$$

where *V* is the zone volume (m^3), *P* is the pressure in the zone; *V* is the flow (kg/s), *T* is the zone temperature, and *R* is the gas constant for air.

The same assumptions are used when the contaminant analysis is activated. The air is treated as a mixture of several different species. The inward airflow rate through one or more paths are calculated as:

$$\sum_{2} F_{1-2} (1 - \eta_2^{\alpha}) C_2^{\alpha} \tag{3}$$

where *F* is the mass flow rate between zones (kg/s) 1 and 2, η_2^{α} is the filter efficiency in the path, and C_2^{α} is the contaminant generation rate.

The above equations show that the program treats the airflow in a well-mixed way that influences the contaminant migration.

The layout in CONTAM of the house taken into consideration in this study is shown in Figure 1.



Figure 1. The layout of the house from the CONTAM application.

Each zone has a dedicated name and flow paths. The infiltration and weather conditions were constant for all the simulations, as the aim was to see the influence of the furnace and exhaust vent placement. Changes in air infiltration are individual for every building and location; the aim was to make a generic model where only the placement of the furnace would influence the results. The outside temperature was assumed to be -10 °C, to simulate winter conditions. Contaminants were only generated in the garage to reflect the faulty furnace. The contaminant taken into consideration was carbon monoxide, as it is the deadliest out of the contaminants. The CO generation rate was assumed to be 1×10^{-5} kg/s [43] at the temperature 800 °C [43], the indoor temperature was assumed to be 20 °C, while the outdoor -10 °C. The dimensions of the garage were 4 m \times 5 m \times 3 m. The same generation rate and dimensions were used for the CONTAM as well as the CFD0 simulations. Each zone represented in Figure 1 has multiple flow paths; the area of flow paths is shown in Table 2. The doors and windows, as well as natural ventilation, where all set as power-law models, meaning that the airflow was calculated according to the differential pressure across the flow path and the flow coefficient [18]. The same dimensions for the flow paths were used on the CFD0 simulations.

Zone	Room Volume (m ³)	Flow Path	Flow Path Area (m ²)	Exchange Rate (m ³ /h)	
		Garage door	0.02		
Garage	60	Door to the house	0.009	90	
		Natural ventilation	0.04		
		Window	0.005		
Kitchen and Living Room	60	Natural ventilation	0.04	70	
-		Door	0.009		
Room	18	Door	0.01	30	
		Window	0.005		
D (I	10	Door	0.01	50	
Bathroom	18	Natural ventilation	0.04	50	
Closet	18	Door	0.009	20	
		Window	0.005	30	

Table 2. Zone and	flow path	characteristics.
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CONTAM and CFD0 solve different sets of conservation equations. As shown above, CONTAM only solves air mass and contaminant conservation equations, while CFD0 solves the Reynolds-averaged Navier–Stokes equations.

CFD0 couples with CONTAM to generate a CFD simulation of a dedicated zone. The multizone model provides average characteristics of airflow and contaminants, while the CFD method predicts the three-dimensional distribution of these parameters. Incorporation of CFD0 into CONTAM allows the linking of information about the exterior wind pressures and outdoor contaminant concentrations to CONTAM's indoor simulations, as well as embedding detailed CFD zones into the CONTAM airflow and contaminant transport network.

In this study, the chosen CFD zone was the garage, and its layout on the CFD0 software can be seen in Figure 2.

CFD0 code is based on the finite volume method. In this method, the domain is divided into a set of small control cells, defined by a mesh. For the CFD0 code, only zero-equation and standard k- ε are available as turbulence models. For this study, the simulation was solved with the k- ε turbulence model and wall functions. The power-law option was selected, since it has been proven to produce useful results in flow simulations [44]. Boundary conditions were imposed by the CONTAM software for the coupled simulation (CONTAM \rightarrow CFD \rightarrow CONTAM). In this coupling method, CONTAM provides a pressure and contaminant boundary condition to CFD0, and the results from the zone are returned to CONTAM. It was selected for this research as it provides a stable and convergent coupling solution [44].



Figure 2. Computational fluid dynamics 0 (CFD0) wall frame of the garage.

In this study, equation residuals were used to assess convergence. The solutions were considered converged when the scaled residuals were less than 10^{-6} for the momentum, turbulence dissipation, energy, and species [45,46].

The CFD0 editor only allows one type of mesh: the hexahedral mesh, which was used in this study. The mesh used for the study had an element count of 1,000,000 elements. A mesh independence test was done using the mean velocity of the outlet vent in the garage, and is shown in Table 3.

Table 3. Grid independence test.

Number of Elements —	Average Air Velocity V (m/s)		Conversor co Bato (%)
	Calculated	Numerical	
500,000	0.625	0.724	13.67
1,000,000		0.634	1.42
1,500,000		0.638	2.03

Four different scenarios were taken into consideration while conducting the study:

- Case 1: The furnace was on the same wall as the door to the house.
- Case 2: The furnace was on the perpendicular wall in relation to the door to the house (opposite the garage door).
- Case 3: The furnace was on the opposite wall than the door to the house.
- Case 4: The furnace was on the opposite wall than the door to the house, but the outlet vent was on the same wall as the door.

For all cases in both the multizone and CFD simulations, the input parameters were identical; the only changes were in the location of the furnace and/or the ventilation grill. The timeframe for each simulation was 24 h.

3. Results

To determine if the placement of a faulty gas furnace, with respect to the natural ventilation system, influenced the contaminant migration into an attached house, a series of the simulation were carried out. The simulations were carried out for a period of 24 h to eliminate the influence of boundary conditions on the results.

First, the simulations were done primarily in CONTAM to see how the contaminant migrates from the garage into the living room. The results are shown in Figure 3. It shows that with the depleted air exhaust from the furnace, the contaminant concentration rises rapidly in the garage in a period of under 1 h. In the living room, the concentration rises to the level of 100 ppm. Both these levels are hazardous for occupants, and above the recommended safety levels. In the bedroom, as well as the closet, the concentrations are 55 ppm and 15 ppm, respectively, which is much lower than the first two rooms, but is still not an acceptable level. The closet and the bedroom had a similar concentration as they had the same flow paths and similar dimensions.



Figure 3. Results of the CONTAM simulation.

After obtaining the results from the CONTAM simulations, a series of CFD simulations were carried out using the CFD0 application. The garage was chosen as the CFD zone and four cases were taken under consideration, as stated in the previous chapter

In the first case, the furnace was on the same wall as the door to the attached house. The results are shown in Figure 4. It shows that the majority of the contaminant accumulate in the garage before exiting through the ventilation system. This is hazardous for occupants that would use the garage, as it can even lead to their death.

In the second case, the furnace was on the same wall exhaust vent—perpendicular in relation to the door to the house (opposite the garage door). The results are presented in Figure 5. Contaminants still flow into the house, but the majority flow directly into the outlet vent. Additionally, the majority of contaminants remain in one area of the garage and do not fill the room.

Figure 6 presents case 3, where the furnace was on the opposite wall than the door to the house. In this case, the contaminant accumulation is the lowest. The least amount of contaminants flow into the house, and the majority of carbon monoxide goes directly to the outlet vent.



Figure 4. CO distribution in the garage—case 1 (concentration of CO in kg/kg).



Figure 5. CO distribution in the garage—case 2 (concentration of CO in kg/kg).



Garage door

Figure 6. CO distribution in the garage—case 3 (concentration of CO in kg/kg).

In case 4, the furnace was on the opposite wall than the door to the house, but the ventilation grill was on the same wall as the door. The results are presented in Figure 7.



The contaminant accumulation, in this case, is the highest, as the carbon monoxide has to travel to the opposite wall to be extracted. This leads to high CO levels.

Figure 7. CO distribution in the garage—case 4 (concentration of CO in kg/kg).

The coupled results between CONTAM and CFD0 are shown in Figures 8 and 9. The results of the CFD simulations are directed to CONTAM, which uses the information for the multizone simulation of the house. Both in Figures 8 and 9, the black dashed line represents the simulation done only in CONTAM without the CFD0 application as a basis for comparison. As is shown in these figures, the connection with the CFD program, as well as the change of placement of the furnace, alters the concentration on CO, not only in the garage, but also the amount of the contaminant that flows into the house.

For the garage, as well as for the rest of the building, the worst case was case 4, where the furnace was on the opposite wall than the door to the house and the ventilation grill was on the same wall as the door to the house. The concentration in the garage grew up to 565 ppm and 165 ppm in the living room.



Figure 8. Coupled CONTAM and CFD0 results for the garage.



Figure 9. Coupled CONTAM and CFD0 results for the living room.

The case in which the least contaminants were transported into the house was case 3, where the furnace was on the opposite wall than the door to the house without changing the placement of the outlet vent. The concentration in the garage was just below 260 ppm, while in the living room it was around 75 ppm. All of these concentrations are still above the maximum safety levels, but for case 3, they are much lower than in the worst-case scenario, improving the safety of occupants as well as allowing them more time to notice the faulty furnace before permanently damaging the occupants' health.

As carbon monoxide is one of the most dangerous contaminants, it is important to create strategies to minimize its influence on occupants. The results prove that the placement of the furnace is vital and can influence contaminant migration. Such studies can be an important step before designing a house to improve ventilation strategies.

The results also show how the combination of the multizone program with a CFD application can impact contaminant concentration. While multizone programs can be helpful to estimate contaminant concentration, it is clear that CFD applications are more advanced and can predict the influence of small changes.

4. Conclusions

Research on the effects of furnace placement was conducted to see if it influenced the migration of carbon monoxide from a garage into an attached house, as well as its accumulation in the garage itself. The furnace and the outlet vent were moved for each case. Both multizone and CFD simulations for a period of 24 h were conducted.

The furnace was assumed to be faulty—lack of contaminant removal—to reflect a hazardous environment. Not only did CO accumulate in the garage, but it also leaked into the house, causing dangerous conditions for occupants. Four scenarios were taken into consideration. The best results were achieved when the furnace was on the opposite wall than the door to the attached house and the ventilation was not moved. The worst results were achieved when the furnace was on the opposite wall than the door to the attached house and the opposite wall than the door to the attached house and the opposite wall than the door to the attached house and the outlet vent was moved to the same wall as the door to the house. In this case, not only was the contaminant accumulation in the garage the highest, but the infiltration of CO into the living room was also the highest as well.

The results prove that the location of the furnace influences contaminant accumulation and migration. Such simulations can be an important tool when designing a ventilation system with respect to the furnace to improve the removal of dangerous substances.

The coupling of the multizone program with the CFD application allowed the analysis of the contaminant migration, as well as influenced the rest of the zones in the CONTAM

model. The results show that the connection of the two programs allows better results, reflecting the real conditions, and can be a valid tool for airflow and contaminant analysis.

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