

# Computational Fluid Dynamics prediction of indoor air quality

Raluca Teodosiu, Viorel Ilie, Catalin Teodosiu

**Abstract**—Accurate estimation of indoor air quality in enclosures is of major importance for achieving healthy indoor environment conditions. The CFD (Computational Fluid Dynamics) approach is currently one of the most used methodology in order to improve the indoor air quality in ventilated environments. As a result, the objective of this study is to evaluate the behavior of CFD simulations for the prediction of indoor air quality in a ventilated test room. The numerical model is based on convection – diffusion equations (to determine the mass fraction of the pollutant), added to the equations used to solve confined turbulent air flows. The computed values are compared with detailed experimental data from the literature, based on tracer gas technique to assess the diffusion of pollutants in a full scale test cell.

**Keywords**—indoor air quality, CFD modeling, ventilation

## I. Introduction

Most people are aware that outdoor air pollution can damage their health but many do not know that indoor air pollution can also have significant health effects. Recent studies of human exposure to air pollutants indicate that indoor levels of pollutants may be 2-5 times, and occasionally more than 100-1000 times, higher than outdoor levels. These levels of indoor air pollutants may be of particular concern because most people spend about 90% of their time indoors [1]. In addition, these indoor activities influence the composition of the indoor air by emitting volatile organic compounds (VOCs). As a result, indoor air is complex, with anywhere from 30 to 300 individual VOCs comprising a typical indoor air sample. The increasing number of different VOCs became the focus of attention in recent years as the question arises from the relationship between exposure to air pollutants and diseases. Indeed, exposure to volatile organic compounds (VOCs) has been associated with a range of adverse health effects (e.g. eye and nose irritation, allergy, liver and kidney dysfunction, neurological impairment, and even cancer) [2,3].

Consequently, the number of studies dealing with indoor air quality is continuously increasing nowadays.

---

Raluca Teodosiu, Viorel Ilie, Catalin Teodosiu  
Technical University of Civil Engineering Bucharest  
Romania

### Acknowledgments

This work is supported by the Romanian National Authority for Scientific Research, CNDI– UEFISCDI as part of the research program PN-II-ID-JRP-RO-FR-2012-0071.

In addition, the CFD (Computational Fluid Dynamics) technique has been increasingly used in the last decade as a pertinent numerical tool to assess the indoor air quality [4-8].

In line with this, the objective of this study is to predict the indoor air quality for small ventilated enclosures, based on CFD approach. It is worthwhile to mention that the numerical results are thoroughly validated based on detailed experimental data. Consequently, we first present the experimental set-up, followed by the description of the CFD modeling. We conclude with comprehensive experimental – numerical comparisons in terms of pollutant concentrations in the ventilated enclosure.

## II. Experimental set-up

This study is exclusively based on the experimental program performed in [9] on indoor air quality and efficiency of ventilation systems. This work was chosen as it provides complete experimental data (boundary conditions required by the numerical approach and indoor air pollutant concentrations required by the model validation).

The experimental set-up is based on a full-scale test room ( $3.10 \times 3.10 \times 2.50 \text{ m}^3$ ), provided by a mixing ventilation system – Fig. 1.

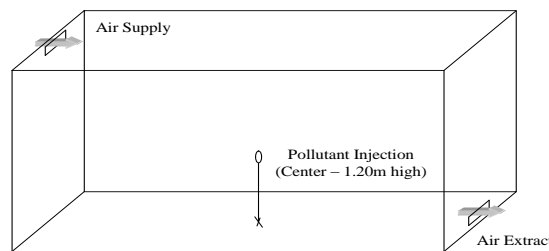


Figure 1. Experimental set-up [9]

In study [9] the tracer gas technique was used for investigating the indoor air quality. This method is the most applied to measure the quality of air within an enclosure. The tracer gas used was the sulphur hexafluoride ( $F_6S$ ) based on a constant injection method (continuous injection at a constant rate throughout the measurement time). The  $F_6S$  gas was constantly injected (0.7 ml/s) into the middle of the experimental room at a height of 1.20 m (Fig. 1).

The experimental procedure allowed measuring the gas (“pollutant”) concentrations in a vertical median plane of the test room, the measurements points representing a  $10 \text{ cm} \times 10 \text{ cm}$  mesh grid.

It is worthwhile to mention that the tests taken into account correspond to typical situations of mixing ventilation systems in small enclosures at very low room air changes per hour (e.g. rooms in dwellings or small offices). It is known that these configurations are frequently critical in terms of indoor air quality because of the VOCs significant indoor emissions and reduced ventilation fresh air flow rates. In order to meticulously test the relevance of the developed numerical model, the experimental conditions chosen in this study cover two situations: cold air supply and isothermal air supply in the room, according to the mean air room temperature (Table I).

TABLE I. EXPERIMENTAL CONDITIONS

Test	Air supply parameters	
	Temperature (°C)	Air changes per hour (h <sup>-1</sup> )
Cold air supply	11.2	1.05
Isothermal air supply	22.3	1.06

### III. Numerical prediction of the „pollutant” concentration field

As this study is focused on the modeling of indoor air quality rather than the CFD model itself, we present simply the key features of the numerical method in Table II. All the numerical investigations presented in this work are based on a general-purpose, finite-volume, Navier-Stokes solver (Fluent 15.0.0).

Concerning the numerical description of the air transport and diffusion of the „pollutant” in the room, we integrated in the CFD approach an equation (1) which represents the conservation of F<sub>6</sub>S species concentration in the two species „mixture” air-tracer gas.

$$\frac{\partial}{\partial x_i} (\rho u_i m_i) + \frac{\partial}{\partial x_i} J_{i,i} = S_{i,i} \quad (1)$$

where the first term in the left represents the convective term (xi – the x, y and z directions, respectively; ρ - the fluid density and u<sub>i</sub> –the velocity components) and the diffusion flux of species i’, J<sub>i,i</sub>, appears as a sum of two factors (2):

$$J_{i,i} = - \left( \rho D_{i,m} + \frac{\mu_t}{S_{ct}} \right) \frac{\partial m_i}{\partial x_i} \quad (2)$$

The first factor represents the mass diffusion flux due to concentration gradients, with D<sub>i,m</sub> the diffusion coefficient of the species i’ in the mixture; the latter one denotes the mass diffusion in turbulent flows or turbulent diffusion term added to the laminar diffusion term, with S<sub>ct</sub> the turbulent Schmidt number and μ<sub>t</sub> the turbulent viscosity. Finally, S<sub>i,i</sub> represents the term source and its value is equal to the injection flow rate

of tracer gas (F<sub>6</sub>S) that takes place in the middle of the test room - see the previous section.

It is worthwhile to mention that (1) is similar to classic convection-diffusion equations. In fact, it has the same form as the other equations describing the conservation of a variable within the computational field (mass, momentum, energy, turbulent quantities for the transition SST k-ω model – turbulent kinetic energy, dissipation of turbulent kinetic energy, intermittency and transition momentum thickness Reynolds number).

TABLE II. CFD APPROACH MAIN ELEMENTS AND HYPOTHESIS

Feature	Description
Fluid	Air – F <sub>6</sub> S mixture (density: ideal gas law for incompressible flow; viscosity and thermal conductivity: ideal gas mixing law based on kinetic theory; specific heat capacity: mass fraction average of the species heat capacities); F <sub>6</sub> S mass diffusion coefficient in the mixture: constant value (1.05 x 10 <sup>-5</sup> m <sup>2</sup> /s)
Flow	Three-dimensional; steady; non-isothermal; turbulent
Computational domain discretization	Finite volumes; unstructured mesh (tetrahedral elements); optimum mesh size (grid independent solutions); 1300000-1400000 cells
Turbulence model	Transition Shear Stress Transport (SST) k-ω
Numerical resolution	Segregated implicit solver; diffusion terms: second order central-difference scheme; convective terms: second order upwind schemes; velocity-pressure coupling: SIMPLE algorithm; convergence acceleration: algebraic multigrid (gradient method, Green-Gauss cell based)
Air supply boundary conditions	Velocity – fixed value across the diffuser (ratio of the measured air flow rate to the diffuser free area); temperature – uniform value (based on experimental data); turbulence quantities – uniform specification, defining two parameters (turbulence intensity and hydraulic diameter)
Air exhaust boundary conditions	Longitudinal exit velocity from mass balance; transverse velocity components are set to zero; gradients normal to flow direction of the other variables are also set to zero
Wall boundary conditions	Velocity – no slip boundary conditions; temperature – fixed values at wall internal surfaces (based on experimental values)

Concerning the initialisation of the calculations, the entire computational domain (the test room) was initialized in term of „pollutant” F<sub>6</sub>S mass fraction using the mean value based on the measurements. This method allowed us achieving important savings in time simulations.

### IV. Results

The concentration field for the „pollutant” (tracer gas) is our principal interest in this study. As a result, we present numerical – experimental comparisons of F<sub>6</sub>S concentrations in the median vertical plane normal to the air terminal devices. Moreover, we selected three sections in this plane in order to facilitate the comparisons. These sections are positioned at 1.0, 1.8 and 2.7 m, respectively, from the test room air supply.

In general, we note that the numerical model leads to results in good agreement with experimental data. Concerning the isothermal case (Fig. 2), for the sections at 1.0 m and 2.7 m, there are only 4 points out of 50 where the difference is greater than 10%. However, for these 4 points (including only one in the last section, at 2.7 m), the difference is no more than 19%. On the other hand, at 1.8 m, there are most important discrepancies in 6 points between 1.1 m and 1.6 m on the height. It seems that the numerical model is too diffusive in this region close to the injection point. Nevertheless, the overall tendency of the concentration field is well predicted.

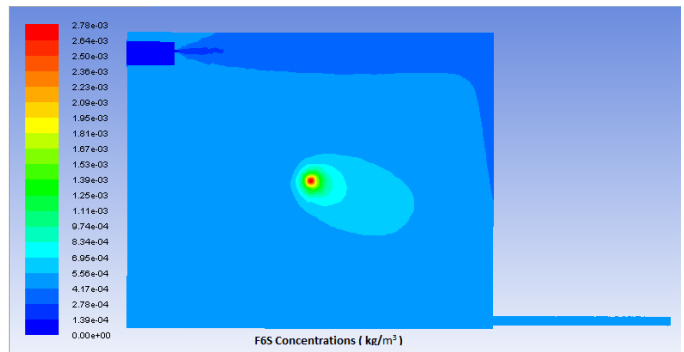


Figure 3. Tracer gas concentration field (isothermal air supply case)

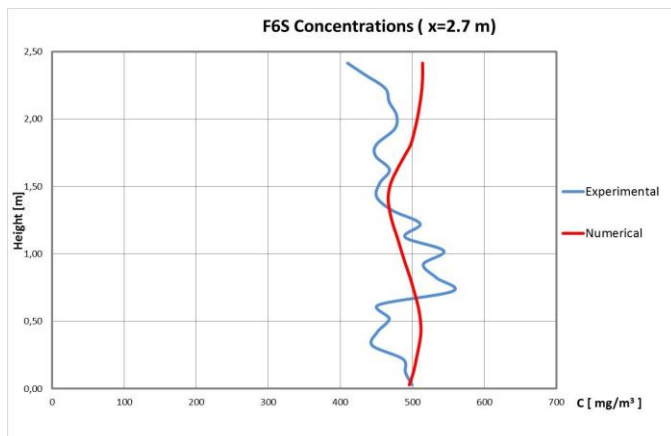
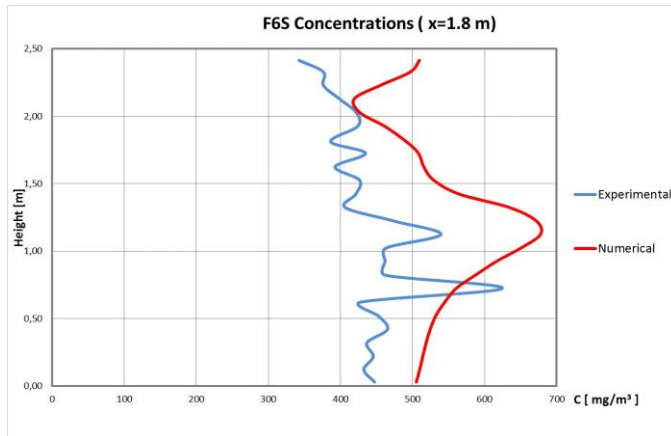
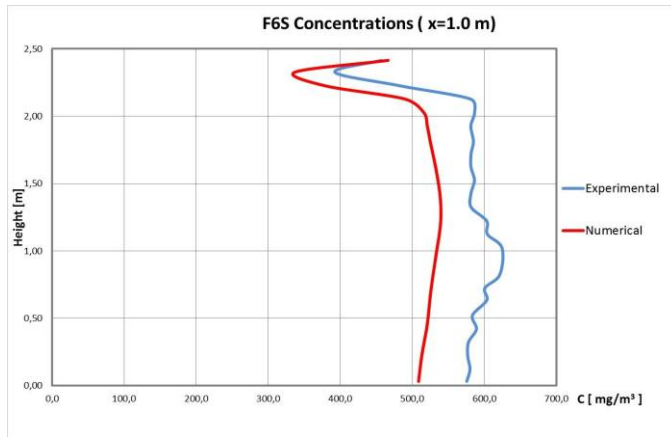


Figure 2. F<sub>6</sub>S Concentration vertical distribution (isothermal air supply case)

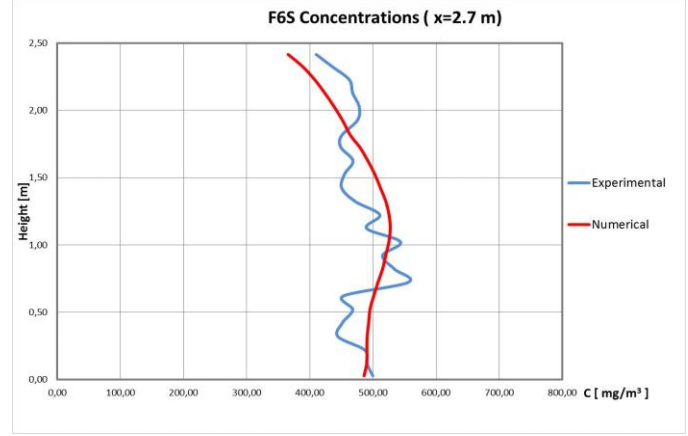
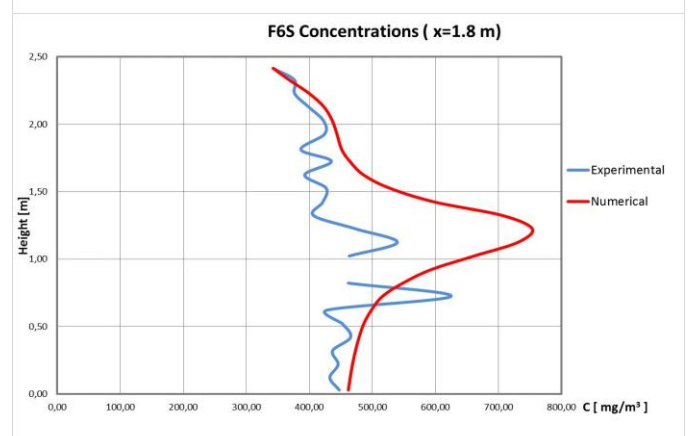
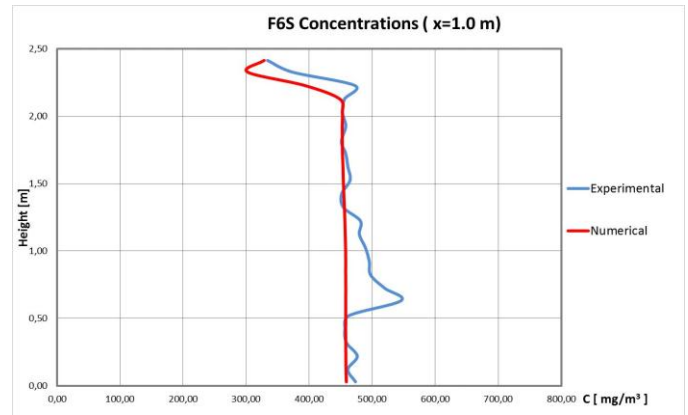


Figure 4. F<sub>6</sub>S Concentration vertical distribution (cold air supply case)

We add in Fig. 3 the general image of tracer gas concentration field in the median vertical plane based on the computed values for the isothermal air supply test.

For the more complex air flow which occurs in the case of a cold jet supplied in the room, the „pollutant” transport by the air is more visible, adding to the diffusion effects. All these phenomena are reasonable predicted, excluding the same region near the injection of the tracer gas (Fig. 4).

We show also in Fig. 5 the overall distribution of the „pollutant” in the median vertical plane of the room, using numerical results for the cold air supply case. As it can be seen, the air flow in the enclosure is totally different and this has an impact on the F<sub>6</sub>S concentration field, too. It can be clearly noticed in Fig. 5 the recirculation region which occurs in the main room air flow. In addition, the jet area is characterized by low “pollutant” concentrations as this corresponds to the fresh air supply. On the other hand, for this situation, the convective phenomena are more important. Consequently, the mean tracer gas concentration in the median vertical plane is slightly greater in this situation. The same behavior was perceived based on the measured values.

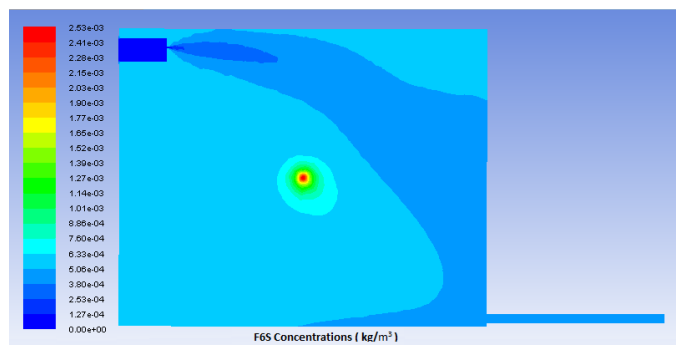


Figure 5. Tracer gas concentration field (cold air supply case)

## v. Conclusion

The model which has been presented leads to reasonable results for isothermal and non-isothermal conditions in ventilated spaces. Consequently, the CFD simulations (with convection-diffusion equations for the conservation of the pollutants, added to the basic equations governing the air flow) can be used for practical purposes dealing with the assessment of pollutant spreading in ventilated enclosures. This is mainly due to the proper estimation of the main driving air flows in the room (air jet and wall boundary layers), the convective phenomena being well “captured” by the numerical model. On the other hand, further analyses should be performed to improve the accuracy of the CFD model dealing with pure molecular diffusion of pollutants (especially for low quantities). In this context, the CFD approach should become in the near future the alternative to extremely difficult and expensive experimental investigations for studying the indoor air pollution.

Finally, in further work the CFD model, developed here only for the contaminant transport, should be integrated with VOCs sorption (adsorption / desorption) phenomena both in the building materials and in room air (e.g. taken into account

VOC emission materials with different emission rates and VOC adsorbent materials). Another perspective of our numerical model is to incorporate CFD computations for both indoor and outdoor environmental analysis (e.g. using data of wind pressure and outdoor contaminant concentrations to determine the pollutant quantity that enters inside).

## References

- [1] T. Hancock, Built Environment (Encyclopedia of Public Health), 2002. Retrieved June 19, 2014 from <http://www.encyclopedia.com/doc/1G2-3404000130.html>
- [2] US Environmental Protection Agency, Integrated Risk Information System (IRIS), 2014. Retrieved June 29, 2014 from <http://www.epa.gov/IRIS/index.html>
- [3] US Environmental Protection Agency, An Introduction to Indoor Air Quality: Volatile Organic Compounds (VOCs), 2012. Retrieved June 29, 2014 from <http://www.epa.gov/iaq/voc.html>
- [4] H. Haung, and F. Haghighat, “Modelling of volatile organic compounds emission from dry building materials”, Building and Environment, vol. 37(12), pp. 1349-1360, 2002.
- [5] L. Wang, D.W. Stuart, and Q. Chen, “Using CFD capabilities of CONTAM 3.0 for simulating airflow and contaminant transport in and around buildings”, HVAC and R Research, vol. 16(6), pp. 749-763, November 2010.
- [6] S.B. Poussou, S. Mazumdar, M.W. Plesniak, P.E. Sojka, and Q. Chen, “Flow and contaminant transport in an airliner cabin induced by a moving body: Model experiments and CFD predictions”, Atmospheric Environment, vol. 44(24), pp. 2830-2839, 2010.
- [7] L. Yang, M. Ye, and B.J. He, “CFD simulation research on residential indoor air quality”, Science of The Total Environment, vol. 472, pp. 1137-1144, February 2014.
- [8] Z. Ruining, X. Li, and J. Tu, “CFD study of the effects of furniture layout on indoor air quality under typical office ventilation schemes”, Building Simulation, vol. 7(3), pp. 263-275, June 2014.
- [9] S. Laporte, “Contribution to the qualification of ventilation system of buildings”, Ph.D. thesis, INSA Lyon, France, 2000.

About Author (s):

**Catalin Teodosiu**



**Organizations and experience:** Vice-president of Romanian Association of Building Services Engineers (AIR) – Bucharest Subsidiary (from 2010); Assistant Professor (from 2007), lecturer (2004-2007), assistant lecturer (1996-1998) in Thermo-Hydraulic and Protection of the Atmosphere Systems Department, Faculty of Building Services and Equipment, Technical University of

Civil Engineering, Bucharest; assistant lecturer (2002-2004) in National Institute of Applied Science (INSA) Lyon; assistant lecturer (2001-2002) in University Claude Bernard – Lyon I; Ph. D. (1998-2001) in INSA Lyon; author or co-author of 4 books and university courses; over 55 articles in international and national journals and papers in peer-reviewed international conferences proceedings; over 30 international or national research-development-innovation projects (6 as project manager/responsible). Relevant research work:

C. Teodosiu, F. Kuznik and R. Teodosiu. *CFD modeling of buoyancy driven cavities with internal heat source – Application to heated rooms*. Energy and Buildings, 2014; 68:403-411

C. Teodosiu. *Modeling and simulation of technical systems in the field of building equipment* (216 pages), Matrix ROM, Bucharest, 2007 (ISBN 978-973-755-182-5)

C. Teodosiu, R. Hohota, G. Rusaoui and M. Woloszyn. *Numerical prediction of indoor air humidity and its effect on indoor environment*. Building and Environment, 2003;38(5):655-664

**Current research:** CFD (Computational Fluid Dynamics) modeling, focusing on turbulence models and integrated heat-airflow-moisture models; building simulation; high efficiency buildings





**Viorel Ilie**

**Organizations and experience:** Ph.D. Student (from 2013) - Thermo-Hydraulic and Protection of the Atmosphere Systems Department, Faculty of Building Services and Equipment, Technical University of Civil Engineering, Bucharest; M. Sc. degree in Energy Efficiency of Buildings (2011-2013), Technical University of Civil Engineering (Building Services Faculty), Bucharest. Relevant research work:

C. Teodosiu, V. Ilie and R. Teodosiu. *Appropriate CFD turbulence model for improving indoor air quality of ventilated spaces.* (submitted for publication in Mathematical Modelling in Civil Engineering, July 2014)

**Current research:** CFD (Computational Fluid Dynamics) modeling; ventilation systems efficiency.



**Raluca Teodosiu**

**Organizations and experience:** Scientific Secretary of Energy Auditors Order Romania, OAER (from 2011); Lecturer (from 2004) in Thermo-Hydraulic and Protection of the Atmosphere Systems Department, Faculty of Building Services and Equipment, Technical University of Civil Engineering,

Bucharest; assistant lecturer (2003-2004) in University Claude Bernard – Lyon I; Ph. D. (2000-2003) in INSA Lyon; over 40 articles in international and national journals and papers in peer-reviewed international conferences proceedings; over 10 international or national research-development-innovation projects (1 as project manager/responsible). Relevant research work:

R. Teodosiu. *Integrated moisture (including condensation) – Energy-airflow model within enclosures. Experimental validation.* Building and Environment, 2013; 61:197-209  
F. Kuznik, G. Rusaouen, R. Hohotă (Teodosiu). *Experimental and numerical study of a mechanically ventilated enclosure with thermal effect.* Energy and Buildings, 2006; 38(8):931-938

C. Teodosiu, G. Rusaouën and R. Hohota (Teodosiu). *Influence of Boundary Conditions Uncertainties on the Simulation of Ventilated Enclosures.* Numerical Heat Transfer, Part A : Applications, 2003;44(5):483-504

**Current research:** CFD (Computational Fluid Dynamics) modeling, experimental investigations concerning indoor air quality; thermal-aeraulic behavior of buildings; modeling energy consumption of buildings.