EXPERIMENTAL AND NUMERICAL PREDICTION OF INDOOR AIR QUALITY

C. Teodosiu¹, S. Laporthe¹, G. Rusaouen¹ and J. Virgone¹

¹Centre de Thermique de Lyon (CETHIL), UPRES A CNRS 5008
Equipe Thermique du Bâtiment, Institut National des Sciences Appliquées
(INSA), Bât. 307, 20 avenue A. Einstein 69621 Villeurbanne Cedex – France

ABSTRACT

This paper is based on a dual approach (experimental and numerical) in order to predict the indoor air quality for small ventilated enclosures. The experimental part employs a ventilated test room and a tracer gas technique (constant method as gas injection) to estimate the diffusion of a pollutant. The gas used is the sulphur hexafluoride (F₆S). The numerical approach is a CFD simulation, adding a convection – diffusion equation (to determine the local mass fraction of the pollutant) to the equations normally used to solve a turbulent flow. As the injected quantity of the gas is extremely low, the convergence of the pollutant transport equation can be only reached after an important CPU. Therefore, we propose a strategy for the initialization of the problem in terms of tracer gas concentrations using the experimental data. This allows us to obtain important savings in time simulation. The experimental and numerical concentration tracer gas fields are compared for isothermal and non-isothermal conditions. Further, in order to characterise in a more general manner the ventilation efficiency and the indoor air quality of the two cases studied, we evaluate the ventilation efficiency index based on the experimental and CFD values. Moreover, we add to these results the values obtained by an improved zonal model. The results achieved reveal a good agreement between the experiment and CFD calculation. On the contrary, there are important discrepancies between the ventilation efficiency index values predicted by the zonal model and the values based on the experimentation.

KEYWORDS

Experimental cell, tracer gas, numerical simulation, indoor air quality, ventilation efficiency.

INTRODUCTION

Nowadays, it is known that we spend most of our time (90%) in the enclosed spaces so the indoor air quality becomes more and more an important parameter, especially for our health. On the other hand, it is obvious that one parameter which mainly determines the level of air quality in the indoor climates is the ventilation. This underlines the importance of the studies dealing with the efficiency of the
ventilation systems. Frequently, in this field of research, both experimental and numerical works are employed and our paper is based, too, on this dual approach. Using the tracer gas technique in a ventilated test room and, on the other hand, a CFD numerical simulation, we are able to have a complete description of a pollutant concentration field for the studied configurations. This allows us to quantify a ventilation efficiency parameter which express the potential of the tested ventilation system to evacuate pollutants.

EXPERIMENTAL SET-UP

The experimental set-up is the test room “MINIBAT” (CETHIL - INSA de Lyon, France). Figure 1 illustrates a simplified scheme of the experimental system. In fact, this installation includes two identical rooms (cell 1 and cell 2, $3.10 \times 3.10 \times 2.50$ m$^3$ each). A glass wall separates the cell 1 from an enclosed space (climatic chamber) whose temperature is controlled by the means of an air-treatment system. The temperature in this climatic chamber can vary between -10 and 30°C. The thermal guard is maintained at a uniform temperature of 20°C in order to represent adjacent spaces.

Our study used exclusively the cell 1 of MINIBAT. The ventilation system of this room has a fixed supply and a mobile extract. The results presented in this work were obtained for the configuration exemplified in the figure 1. Measurements were carried out using sensors (thermocouples) to determine wall surface and air temperatures in the enclosure. The experimental methodology allowed us too, to measure the air velocity field (using hot-wire probes), as well as tracer gas concentrations. In addition, near the centre of each zone, relative air hygrometry and operative temperature are measured. The air field parameters (mean velocity, temperature) and the gas concentrations were obtained in a vertical median plane, the measurements points representing a 10 cm $\times$ 10 cm mesh grid.

We used the tracer-gas technique for studying the indoor air quality. Certainly, this technique is the most widely used to predict the movement and quality of air within an enclosed space. Furthermore, procedures using tracer gases are the only ones that can be used experimentally to:

- characterise the ventilation systems (with regard to fluxes, flows, etc.)
- quantify the quality of the air in a space (by determining its age and studying the migration of pollutants).

The tracer gas used in this study is the sulphur hexafluoride (F$_6$S). We have preferred F$_6$S as tracer gas Laporthe (to be published) mainly because of the sensibility of the Briel and Kjaer measuring system – Briel & Kjaer (1991). There are various ways of injecting a tracer gas into an experimental cell.
Hannion (1994), and we used in this study the constant method. This method consists of introducing the tracer gas continuously at a constant rate, throughout the measurement period; the mixing of the air in the test room should be sufficient to homogenise the concentration of the tracer gas. Moreover, the gas was injected (0.7 m/s) into the centre of the experimental cell at a height of 1.20 m. The injection procedure used a small ball in which a large number of small holes had been made in order to assure as much as possible an uniform gas introduction.

**NUMERICAL MODEL**

**Tracer gas concentration field prediction**

The calculations were carried out by the means of a CFD code, Fluent (version 5.0), Fluent (1998). In conjunction with the equations that governed a turbulent non isotherm flow (conservation of mass, momentum and energy as well as the transport equations of turbulent kinetic energy and its rate of dissipation in the case of a two-equation turbulence model), an equation which represents the conservation of species concentration is solved. This partial differential equation has the same form as the other equations describing the conservation of a variable within the computational field. Hence, the convection-diffusion equation for predicting the local mass fraction of the pollutant, $m_i$ (here sulfur hexafluoride, F$_6$S) takes the following form – equation (1):

$$\frac{\partial}{\partial x_i} \left( \rho u_i m_i \right) + \frac{\partial}{\partial x_j} J_{i,j} = S_i,$$

In equation (1), the first term in the left represents the convective term (where $x_i$ – the x, y and z directions, respectively; $\rho$ - the fluid density and $u_i$ - the velocity components) and the diffusion flux of species $i$, $J_{i,j}$, appears as a sum of two factors: $J_{i,j} = -\left( \rho D_{i,m} \frac{\partial m_i}{\partial x_j} + \frac{\mu_i}{S_t} \right)$; the first one represents the mass diffusion flux due to concentration gradients, with $D_{i,m}$ 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 $S_t$ the turbulent Schmidt number and $\mu_i$ the turbulent viscosity. Finally, $S_i$ represents the term source and its value is equal to the injection flow rate of sulfur hexafluoride that takes place in the middle of the test room - see the precedent section.

Consequently, the fluid is taken into account as a mixture of two species: air plus tracer gas (with air as bulk species). The properties for the mixture were defined as follows - for more details see Fluent (1998):
- density: ideal gas law for an incompressible flow
- viscosity and thermal conductivity: ideal-gas-mixing-law, the solver computes the values of these properties based on kinetic theory
- specific heat capacity: mass fraction average of the pure species heat capacities
- mass diffusion coefficient: constant value for the F$_6$S mass diffusion in the mixture (1.05 x $10^{-5}$ m$^2$/s).

Concerning the physical properties for the mixture constituents, constant values of specific heat capacity, thermal conductivity and viscosity were imposed for the air, as well as for the tracer gas.

**Main physical and numerical hypothesis**

In order to predict the flow in the test room presented at the previous section, the following physical assumptions were taken into account:
- fluid movement: 3D, incompressible, turbulent, (non) isotherm, steady
- near wall approach: two-layer.
Regarding the main numerical aspects of our simulations, briefly, they were as follows:
- computational domain discretisation: tetrahedral control volumes
- diffusion terms: second-order central-differenced
- convective terms: second-order upwind scheme.

**Initialisation of the calculations**

Firstly, the simulations were carried out initializing the concentration tracer gas field with zero values everywhere in the computational domain. In this model, we had only the term source imposed in the equation (1). Unfortunately, judging the convergence of our computations, we noticed that the evolution of the tracer gas transport equation residual (the imbalance summed over all the computational domain, for an exact definition of residuals – see Fluent (1998)) had not yet been 'stabilized'. This fact is illustrated clearly in the figure 2 where the progress of this residual is presented in function of the iterations completed.

![Figure 2: F6S Residual Evolution (zero initializing values)](image1)

![Figure 3: F6S Residual Evolution (mean experimental data as initializing values)](image2)

Subsequently, we tried to find out a method for accelerating the convergence of the equation (1). Therefore, we initialized the entire computational domain in term of pollutant (F6S) mass fraction using the mean value based on the measurements carried out in the vertical median plane of the experimental cell. The residual evolution obtained in this situation is shown in the figure 3. We observe that the convergence is reached after a reduced number of iterations. This allowed us to achieve important savings in time simulations. Therefore, this approach was employed further in our simulations.

**RESULTS**

In our experimental – numerical comparisons, the concentration field for the tracer gas was of primary interest. Hence, we present such comparisons obtained in a vertical plane normal to the centre line of the air terminal devices. Moreover, we selected three sections in this plane in order to facilitate the comparisons. These sections are positioned at 1, 1.8 and 2.67 m, respectively, from the test room air supply.

Figures 4 and 5 show the measured and computed results for an isothermal case and for an air supply temperature of 11.2 °C at 1 air change per hour. Regrettably, there is a lack of experimental data in certain points for the last section (figure 5, x = 2.67 m) - in the case of the cold jet. These problems occurred because of the tracer gas measuring system.

The evaluation of the results given in the figures 4 and 5 shows a good agreement between the measured and simulated values, even that some discrepancies exist in the upper part of the enclosure. Most important differences (10-20%) occur in a few points between 0.75 and 1.25 m.
This can be partially explained as an effect due to the measured values since variations from 400 mg/m³ to 650 mg/m³ or more, within 10 cm., are not plausible in the middle of the room, especially in our configurations which ensure an uniform air movement in the occupied zone.

In order to characterise in a more general way the ventilation efficiency and the indoor air quality of the configurations tested, we add to the results already presented, the values of an index $\varepsilon_c$, equation (2) that represents the capacity of a ventilation system to evacuate pollutants, Sandberg & Sjöberg (1983).

$$\varepsilon_c = \frac{C_e(\infty)}{C(\infty)}$$

$C_e(\infty)$ – pollutant concentration in the extracted air
$C(\infty)$ – mean pollutant concentration in the room

The above equation is applied in permanent mode (meaning constant outlet concentration). In the table 1, we show the values of this index, values obtained based on the experimental data (as a mean value all over the experimental mesh), as well as values achieved using the CFD model proposed in this paper. We add to these comparisons the ventilation efficiency index values obtained by the means of an improved zonal model Bouia (1993) applied in the study Castanet (1998) for the same configurations.

In building physics, the zonal model approach, that consists to split the room into different zones characterising the main driving flows, was initially used to predict the thermal behaviour of rooms but we can see its application frequently extended these days to ventilation systems and their efficiency.
For this reason, a direct comparison between simplified methods such as the zonal models and CFD computations in the field of ventilation efficiency is quite interesting.

Based on the results given in the table, we notice that the zonal model predicts more or less reasonable the $\varepsilon_c$ value for the non-isothermal situation as the cold jet penetrates in the occupied zone and that compensates somehow the diffusion of the gas in the enclosure which is not taken into account in this simplified model. On the contrary, in an isothermal situation (and for a hot jet too, see Castanet (1998)), the result given by the zonal model is far from the experimental value (48%). In the same time, the CFD computation carried out lead to a good agreement with the value based on the measurements (a difference of 17.5% for the isothermal case and 6.7% for the non-isothermal situation). This underlines the importance and the accuracy of the CFD technique for the studies dealing with the pollutant diffusion predictions in rooms.

**TABLE I**

<table>
<thead>
<tr>
<th></th>
<th>$\varepsilon_c$ - isothermal case (Re = 7100)</th>
<th>$\varepsilon_c$ - non isothermal case (Re = 7200 and Ar = 0.0134)</th>
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</thead>
<tbody>
<tr>
<td>Experimental</td>
<td>1.23</td>
<td>1.02</td>
</tr>
<tr>
<td>Zonal model</td>
<td>0.64</td>
<td>1.04</td>
</tr>
<tr>
<td>CFD</td>
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<tr>
<td>Zonal model</td>
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<td>0.97</td>
</tr>
<tr>
<td>CFD</td>
<td>1.02</td>
<td>0.97</td>
</tr>
</tbody>
</table>

**CONCLUSION**

This study emphasizes the important interdependence existing between the numerical model and the measurements in the domain of indoor air quality: the CFD simulations represent surely one way to correctly express the pollutant dispersion in the enclosures but these calculations must be based on several measured values in order to reach a more quicker convergence - especially while the pollutant quantities are not so important in the room. On the other hand, the comparison based on the results given by a zonal model, in order to describe in a general way the indoor air quality, illustrated the limitations of such an approach concerning the diffusion of a pollutant in enclosures.

**REFERENCES**


