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Modelling of indoor air pollutants dispersion: new tools

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Abstract. Ventilation systems are used for create a thermally comfortable environment and good indoor air quality. It is therefore essential to have adequate tools for predicting the performance of these systems. Among the various approachs, the computational fluid dynamics could be a useful tool for the design of the ventilation system. When dealing with pollutants dispersion problems, a steady state averaged simulation can be misleading because it is not able to properly predict and model peak concentrations, which can be relevant even if temporary. An interesting approach is the use of LES (Large Eddy Simulations) simulations to obtain a better description of concentrations oscillations. In this framework, the aim of this work is the validation of simulation carried out using the FDS (Fire Dynamic Simulator) software with an actual case study, already studied with a mock-up. Secondly, two new configurations of the ventilation system are proposed, in order to stress the capacity of the software to describe complex and different features, classical of HVAC (Heating, Ventilation and Air Conditioning) systems. Interesting conclusions about efficiency are drawn from the comparison, highlighting the potentiality of the software.

1. Introduction

Ventilation is used in buildings for create a thermally comfortable environment and good indoor air quality. It is therefore essential to have adequate tools for predicting the ventilation performance of buildings: analytical models [1]; empirical models [2]; small-scale models [3]; real-time models [4]; multi-zone models [5], [6]; CFD models (Computational Fluid Dynamics). The last provide more detailed information on ventilation performance, representing a much more sophisticated tool than other models. Hayashi et al. [7] conducted a CFD analysis to examine the characteristics of a ventilation system in a closed environment, with a two-dimensional model. As for the three-dimensional CFD models Kassomenos et al. [8] analysed the dispersion of vinyl chloride monomer into a polyvinyl chloride pipe manufacturing plant. Siddiqui et al. [9] have proposed a model for a risk analysis in case of chlorine releases in an industrial environment. Predictive capacity of CFD models require a proper validation process, typically performed by reproducing experimental evidence; for this reason, Lee et al. [10] have validated their model with the estimated the concentration of a tracer gas, isobutene, using a small-scale model; Deevy et al. [11] have predicted the dispersion of a mixture of sulphur hexafluoride and helium in a thermally stratified room; Lambert et al. [12] have studied the release of carbon dioxide into a ventilated space.
Due to the high computational cost required, CFD simulations are often performed as RANS (Reynolds Averaged Navier-Stokes) simulations. When dealing with pollutants dispersion problems, a steady state RANS simulation can be misleading because it is not able to properly predict and model peak concentrations, which can be relevant even if temporary. An interesting approach is the use of LES simulations in order to obtain a better description of concentrations oscillations.

In this framework, the aim of this work is the validation of simulation carried out using the FDS (Fire Dynamic Simulator) software with an actual case study, already studied with a mock-up. Secondly, a comparison between two different configurations is performed, in order to stress the capacity of the software to describe complex and different features, classical of HVAC (Heating, Ventilation and Air Conditioning) systems. Interesting conclusions about efficiency can be drawn from the comparison, highlighting the potentiality of the software.

2. Materials & Methods

In this work the version 6.5.3. of FDS was used. FDS is a CFD modelling software developed by the BFRL (Building and Fire Research Laboratory) and NIST (National Institute of Standards and Technology), for the simulation of turbulent reactive flows (i.e., fire effects) through the solution of the transport equations using a LES (Large Eddy Simulations) approach. It is a low Mach solver designed to investigate fire behaviour and perform safety assessments [13]. Main advantages of the software are the low computational cost and the robustness of the algorithm; while the main drawback is related to meshing limitation: the geometry description with a rectilinear mesh is the only way to guarantee a high computational performance. Other details about the simulations (e.g., grid and boundary conditions) are discussed in the next section.

3. Results and discussion

The case study simulated in this paper is that proposed by Rota et al. [14]; in which they have considered a ventilation system designed to reduce the risk to health in an industrial warehouse where calibration of thermocouples was carried out involving the use of alcohol baths (usually ethyl or methyl alcohol), which, by evaporation, dispersed within the working environment. The baths were placed in one half of the room, the rest was used for assembling and dismantling the thermocouples. In this type of working environment, it was not possible to apply a local ventilation system since it could have altered the calibration process.

Mock-up in scale 1:10, made of polymethyl acrylate, consisted of a base of 1.6 (L) x 0.8 (W) m with walls high 0.4 m. To create different airflow conditions within the room, the model had two openings on the rear wall, which represented windows of 0.1 (W) x 0.2 (H) m and one aperture, the door on the front wall of 0.2 (W) x 0.3 (H) m. At the centre of the ceiling there was a circular hole of 9 cm in diameter, connected to an intake system, which represents the ventilation system. The four diffusers simulating the thermocouple calibration counters, consisted of rectangular elements of 0.1 (L) x 0.2 (W) x 0.1 (H) m, each with two slots of 0.01 (L) x 0.16 (W) m placed on the upper base, through which tracer gas, ethane, was flowing.

The experimental tests have been carried out on three different cases, modifying the number of active pools and the opening of the windows, while the door on the right and the intake duct were always open; in the first case the two windows were closed and only two baths were in operation (Case 1), in the second case the other two tanks had been activated (Case 2), and in the third the windows had been opened (Case 3).

The concentration of ethane inside the mock-up has been measured at a constant height of 0.17 m, corresponding to the breathing height; the gas has been sampled by the use of long-needle semi-automatic injection syringes inserted into the simulation room by small sampling ports placed on the roof, arranged on two rows and numbered progressively, as in Figure 1, and then it has been analysed in a gas-chromatographic system Since the geometry of the room was symmetrical with respect to the vertical plane (from the door to the wall between the windows), the reference work contained ethane concentration measurements performed only in one half of the simulation chamber (as in Figure 1). Five measurements have been made for each sampling point.

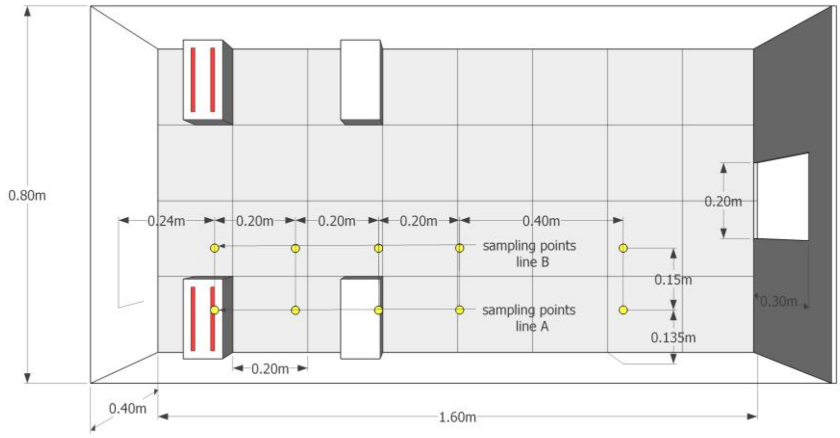

Figure 1. Position of samplings, top view [14].

The mock-up geometry was reproduced in FDS without any modification except: providing doors with a minimum thickness to allow the software to resolve the incoming streams from the opening, and making square the ventilation duct via the equivalent area to improve the solution through the square cells (as sketched in Figure 2). Uniform mesh was selected, with cubic cells of side 1 cm.
For the sake of brevity, only the Case 1 will be considered in this work; the relevant input data are reported in Table 1.

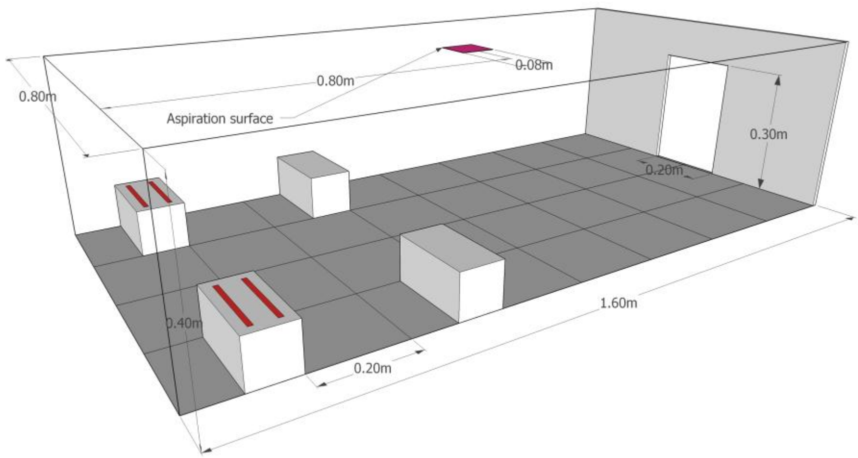

Figure 2. Geometry used in FDS for reproducing the mock-up Case 1.

Table 1 Input parameters of experimental test and simulations.

	Ethane mass flow rate [kg/s] per bath	Aspiration rate [m/s]	Aspiration volumetric flow rate [m^3/h]
Mock-up	1.1e-6	4.5	100
FDS	1.1e-6	4.5	100

Due to the high turbulence levels, a punctual monitor was supposed to be not suitable for a realistic description, thus in the simulations volumetric concentration monitors were used; this means that the simulation data are the mean, with the error bars, obtained among the values of the cells contained inside a volume centred in the experimental sample point, with a side of 4 cm (i.e., the mean on 64 cells).

To compare the results obtained from the simulations with the corresponding experimental ones, they were mediated on time, being the LES simulation transient. The mean time was obtained for each position, on the output values provided by the software, from the time the system reaches the stationary state, t_{ss},(around 100 s) until the simulation is completed (t_{fin} = 300 s).

Once obtained the mean value from FDS, the comparison with the experimental data was performed and sketched in Figure 3 and Figure 4.

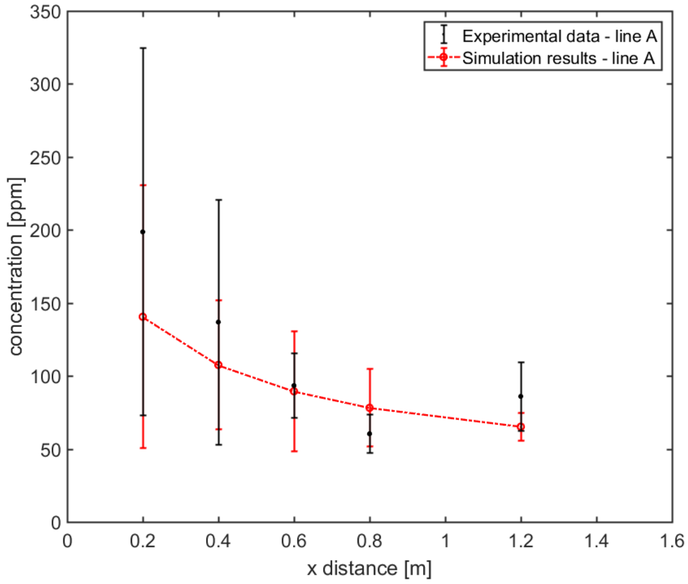

Figure 3. Comparison between experimental measurements and FDS predictions for the mock-up Case 1 at y = 0.135m (line A in Figure 1).

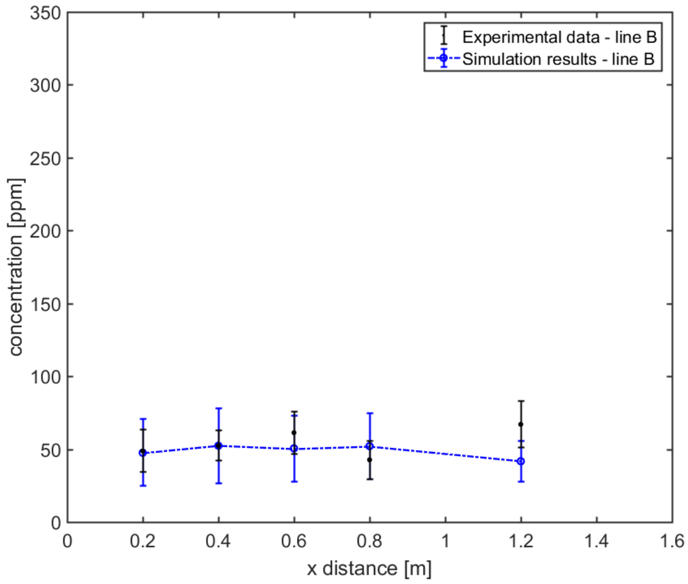

Figure 4. Comparison between experimental measurements and FDS predictions for the mock-up Case 1 at y = 0.285m (line B in Figure 1).

Good agreement between simulation predictions and experimental results was achieved, with a good consistency in both values and performance. Even better coherence is shown by the monitors located in the central part of the room (Line B of Figure 1) where lower concentrations were found.

It's worth spending a few words about the deviation of the results, both experimental and CFD, because highlight a very positive peculiarity of the software. It is possible to see that a really low reproducibility was obtained by the experimental tests even if all the precautions were taken in the measurement process. FDS results help to understand why measured values presented a high variability: the region of the mock-up in the tank area is strongly turbulent. This can be understood observing the deviation presented by the simulation results, which are of the same order of magnitude of the experimental deviations.
Moreover, the predicted concentration in the aspiration channel was validated with the experimental data. The comparison, reported in Table 2, is a further validation of the CFD simulations.

Table 2 Comparison between the concentration value of ethane at the intake system obtained during the experimental campaign [14] and the one obtained with FDS

	C_{exp}	C_{FDS}
Ethane concentration [ppm]	58	58.9

After the validation phase, two new configurations of the ventilation system were simulated. Keeping in mind that for the analysed case study (i.e., baths for calibration of thermocouples) it is not possible to position aspiration hoods directly upon the baths to avoid alterations to the calibration process, the two practical configurations, sketched in Figure 5, were studied and simulated.
In order to be able to compare the efficiency of the proposed solutions, the same tracer mass flow and the same number of ACH (Air Changes per Hour) were used in all the simulations, correcting the air flows.
The former (labelled as case N1) is characterized by a central channel of air emission and a certain number of exhaust hoods on the ceiling. This is a common solution applied often in huge environments, though to ensure a good air exchange; while in the latter (labelled as case N2) the air emission is obtained from a plenum posed on the ceiling and aspirations slits in the floor. On the other hand, this solution is frequently adopted when a strict control of pollutants is meant to be achieved; for example, in white and operating rooms.
These two configurations offer a presentation of various elements characteristics of a ventilation system such as air jets, hoods and plenum diffusers. The possibility offered by the software to model them should not be underestimated.
In Figure 6 an Figure 7 the comparison between the experimental data and the results obtained with the ventilation solutions N1 and N2 at the two sampling line are shown. Observing the results of N1, the higher levels of ethane calculated could be explained by the increased turbulence level in the room, which is generated by the jet air entries. This increased turbulence lead to an improved mixing in the volume, worsening the scenario by far. On the other hand, the second configuration (N2), exploiting a laminar airflow reduces the turbulence, preventing the pollutant mixing and allowing a timely aspiration of concentred puffs.
The N2 solution, with the laminar containment developed is absolutely more efficient. On the side of the modelling tool, the speed with which these scenarios can be analysed and understood are very well demonstrated. As an example, in Figure 8 are reported the visualization of the ethane concentrations for the three cases.

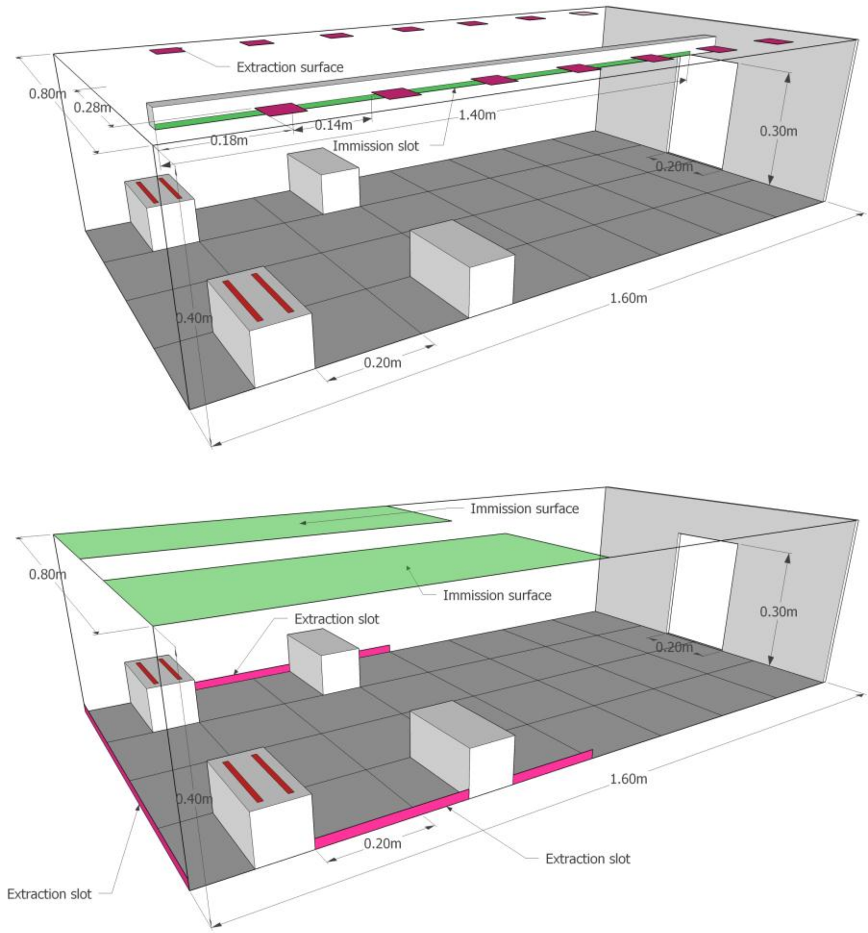

Figure 5. Sketches of the two new ventilation systems: N1 (top), N2 (bottom)

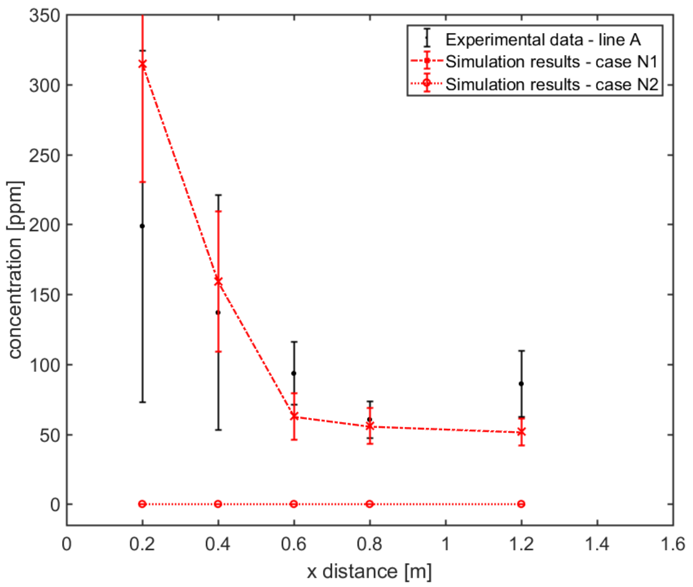

Figure 6. Comparison between experimental data and FDS predictions for the mock-up Case N1 and N2 at y = 0.135 m

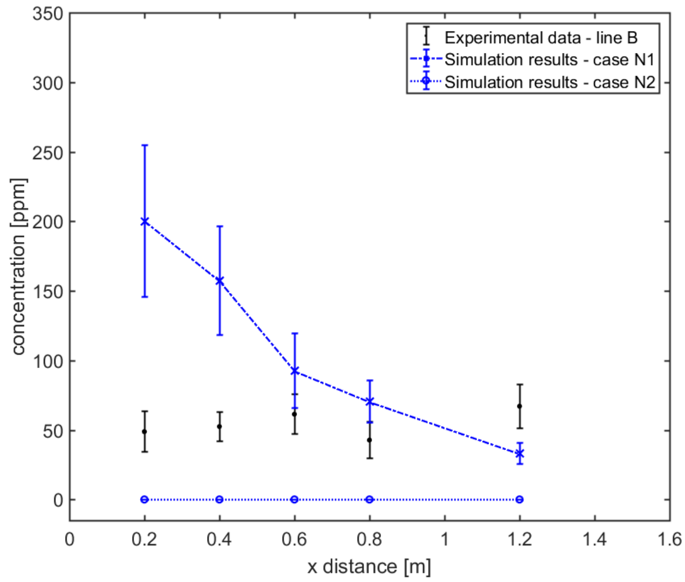

Figure 7. Comparison between experimental data and FDS predictions for the mock-up Case N1 and N2 at y = 0.285 m

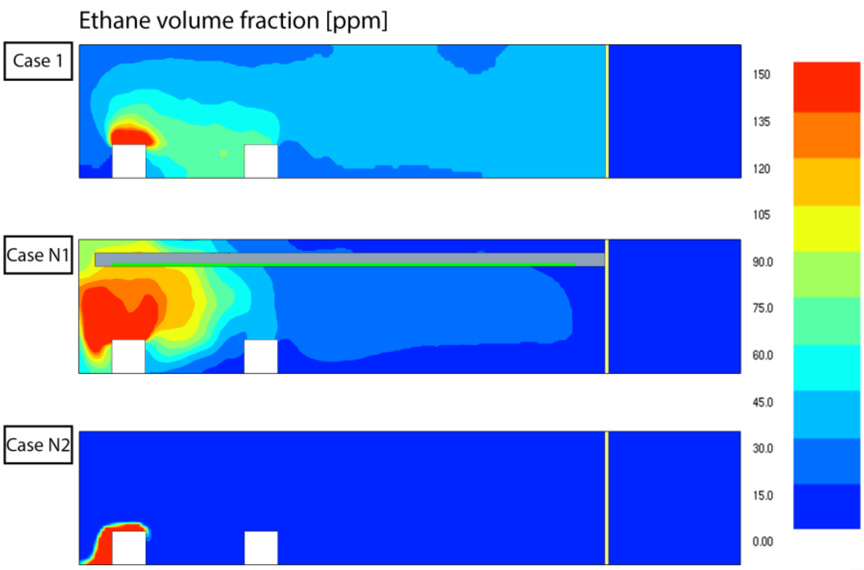

Figure 8. Ethane concentrations contours for the three cases: base case, N1 and N2

4. Conclusions

In the first part of this work a specific validation process was undertook with good results, highlighting that FDS, used in this work, undoubtedly represents an effective tool for analysing fluid-dynamic problems concerning the transport and dispersion of pollutants in confined environments.
The possibility offered to understand physical phenomena could be really useful in industrial practice to address some actual problems in ventilation design.
In the second part of the work, two alternative configurations of the ventilation systems were proposed; this has enabled to prove the effectiveness of FDS during the phase of the design of the plant as it allows easily evaluating the performance of any ventilation system and monitoring the most important parameters.

5. References

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