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Numerical and experimental analysis of flow and particulate matter dispersion in indoor environment

A Pini[1], I Musa[1], P Monti[1], G Leuzzi[1], A Di Bernardino[2], G Cattani[3], A Di Menno di Bucchianico[3], M Gherardi[4] and A Pelliccioni[4]
[1] DICEA, University of Rome "La Sapienza", Rome, Italy
[2] Department of Physics, University of Rome "La Sapienza", Rome, Italy
[3] Italian National Institute for Environmental Protection and Research, Rome, Italy
[4] INAIL-DIMEILA, Monteporzio Catone, Rome, Italy

Email: agnese.pini@uniroma1.it

Abstract. Reducing indoor particulate matter (PM) concentration is an issue of concern from an environmental point of view as the world's population spend only 4% of their time outdoors. Computational fluid dynamics (CFD) is a fundamental tool for predicting indoor pollutant dispersion and improving knowledge on how indoor and outdoor environments interact in terms of pollutant and momentum exchanges. In this paper, an unsteady CFD simulation has been carried out to investigate the airflow and PM concentration in a classroom of the University of Rome "La Sapienza". Wind velocity and PM concentration acquired during a field campaign conducted within and outside the building of interest have been used as input for the simulation and to test the model performance as well. The results show a reasonable agreement between measured and simulated concentration within the classroom and emphasize the major role played by the micrometeorology in PM concentration. The importance of the boundary conditions at the room openings has been also discussed.

Keywords: I/O particle concentration, indoor environment, CFD, particle dispersion modelling

1. Introduction

Particulate matter (PM) pollution is an issue of concern for the scientific community. It is known that long exposures to high concentrations of inhalable, i.e. fine and ultrafine, PM could affect human health. Monitoring PM concentration in indoor environment, where people spend most of their time, is therefore necessary. PM concentration within a confined environment depends on several factors, such as indoor and outdoor sources, building ventilation and micrometeorology [1] [2]. Furthermore, indoor air circulation is usually rather complex and accumulation zones with high concentration levels generally form. Computational fluid dynamics (CFD) has proven to be a powerful tool for investigating airflow and PM concentration in urban areas [3] and in indoor environments as well [4]. The availability of reliable and representative experimental input data for the numerical simulation is a prerequisite toward obtaining physically plausible results from CFD. On the other hand, data from field campaigns (or from laboratory experiments as well) are needed to evaluate CFD performance [5].

In this work, CFD simulations of the airflow and PM concentration fields within a classroom were carried out. Preliminary analysis performed in steady conditions for several configurations of the openings, i.e., windows and doors, were conducted to investigate the most common flow patterns occurring in the classroom. Field measurements of wind velocity and PM concentration, collected both in the classroom and outdoor, have been used as input for an unsteady CFD modelling of airflow and PM dispersion with a two-fold motivation. First, to test the capabilities of the CFD model to reproduce the PM concentration indoor and, secondly, to investigate the main flow characteristics as well as the role played by the external micrometeorology in realistic airflow fields.

2. **Material and methods**

2.1. Field data

Wind velocity and PM concentration have been measured simultaneously during the long- and short-term field campaigns conducted in the framework of the BRiC project #22 [6]. These campaigns have been carried out at the University of Rome "La Sapienza" from November 2017 and are still in progress. During the project, three Intensive Operating Periods (IOPs) lasting twelve hours each (0500–1700 local standard time) were performed, during which high-frequency data were collected outside and within the "E. Fermi" building (Fig. 1). For the present work, we used as input for the simulations data of wind velocity and PM concentrations measured during IOP#1 (21 July 2018) within and outside a classroom located at the second floor of the building. On the East side of the room there are nine windows (W1-W9), while two doors (D1 and D2) allow the passage to the hallway on the opposite side. The room is 3.85 m tall, while its area and volume are about 133 m^2 and 513 m^3, respectively.

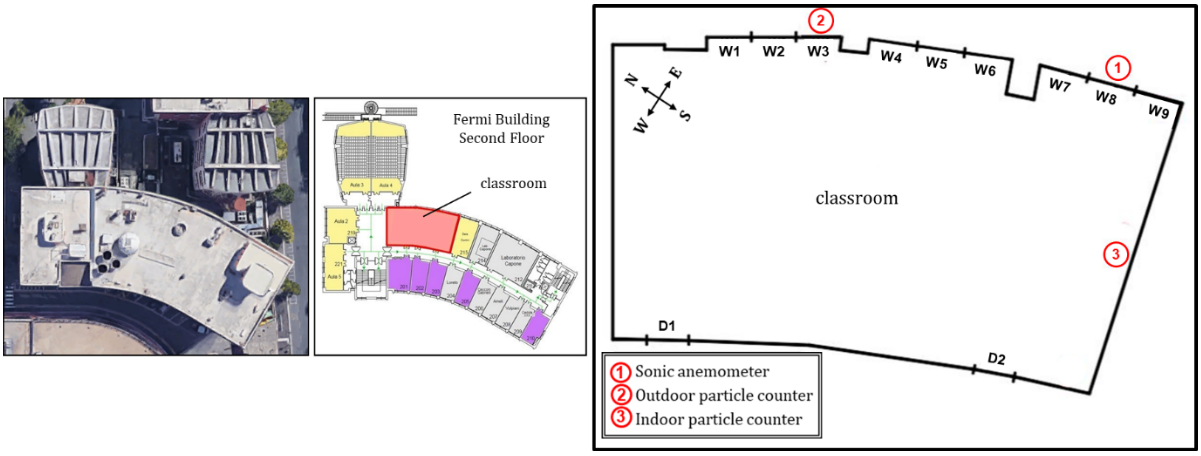

Figure 1. Aerial view (Google Earth) of the "E. Fermi" building of the University of Rome "La Sapienza" (left panel) and layout of the classroom (feature in red in the central panel). The map on the right panel shows an enlargement of the classroom. The numbers indicate the positions of the instruments. D1 and D2 denote room doors, while W1-W9 indicate the windows.

"La Sapienza" is located in the center of Rome, in a morphologically heterogeneous area with buildings of different heights and complex geometry. The diurnal cycle of the winds in Rome is considerably influenced by land- and sea-breeze regimes for a large part of the year [7] [8]. As a consequence, both wind intensity and direction change during the day and this makes the choice of the input data for the CFD a non-trivial issue.

During the considered IOP, a three-axial ultrasonic anemometer placed outside W8 measured wind velocity and direction at 4 Hz and provided the input data for the unsteady CFD simulation. Moreover, concentration in number (#/cm^3) of particulate matter (0.3–10 μm) was also measured, both outside and inside the classroom, using an optical particle sizer (OPS 330, TSI).

2.2. CFD simulations

The CFD software ANSYS Fluent 18.2 was employed to simulate both airflow and concentration of PM within the classroom. The numerical grid used for the simulations consisted of a three-dimensional structured mesh. The grid resolution (7.5 cm) was chosen after a sensitivity analysis as the best compromise between accuracy and computational costs (the resulting number of grid nodes was about $1.2 \cdot 10^6$).

Two kinds of numerical simulations were performed: steady and unsteady. In the first case, the flow field was computed using the Reynolds-averaged Navier−Stokes (RANS) equations along with the Re-Normalization Group (RNG) k-ε balance equations for the closure (see e.g. [9]). The latter shows better results in the case of confined environments, especially for turbulent incompressible flows [10]. With steady RANS, a statistically steady description of turbulent flow is carried out and the calculated airflow assumes the meaning of time averaging of the actual turbulent field. In the second case, the flow was computed using an unsteady RANS (URANS) approach, where the time-varying mean flow structures are resolved [11]. Note that in both approaches only the statistics of the turbulence is simulated.

Regarding the PM dispersion, it was calculated for the unsteady case by means of the Fluent Discrete Phase Model (DPM), implemented in ANSYS Fluent [12].

3. **Results and discussions**

3.1. Steady CFD simulations

Three RANS simulations were firstly conducted varying window and door opening configurations in order to investigate the role played by the boundary conditions in the flow pattern. For all the three case studies, an entering velocity equal to 0.3 ms^{-1} was imposed at the windows (perpendicular to them), while the outflow condition was set at the doors. The chosen wind velocity can be considered as representative of the value observed during the whole field campaign. The different settings used for the simulations are listed in Table 1.

Table 1. Steady simulation settings

Steady case	Inlet location	Velocity inlet	Outlet location	Pressure outlet
A	W8	0.3 ms^{-1}	D1	Atmospheric
B	W2	0.3 ms^{-1}	D2	Atmospheric
C	W2, W4, W8	0.3 ms^{-1}	D1	Atmospheric

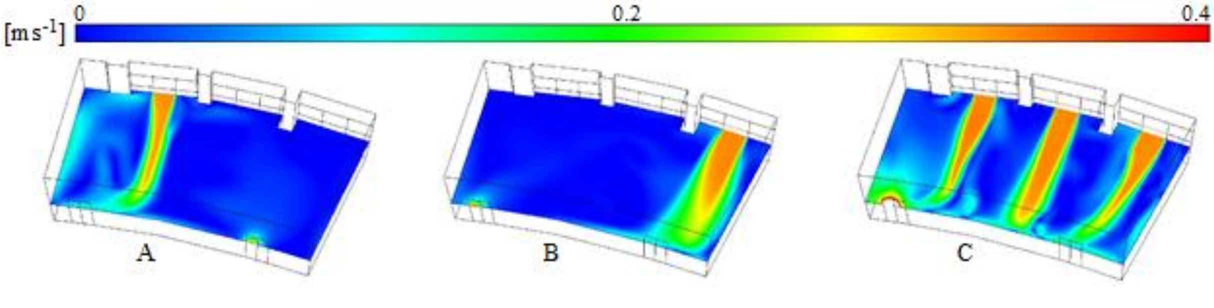

Figure 2. Maps of the mean velocity fields computed along the horizontal planes at 1.5 m above the classroom floor for the three opening configurations (steady case).

The velocity fields simulated along the horizontal plane at 1.5 m above the classroom floor for the three opening configurations are shown in Fig. 2. As expected, the flow pattern changes considerably and this confirms that the geometry and location of the openings in a confined environment influence considerably the indoor air circulation. The air flow is strongly inhomogeneous and vortical structures are present throughout the flow. The main features are the tongues of larger velocity values in correspondence of the windows and nearby the door, where the latter are a result of the mass balance constraint. Obviously, the spatial inhomogeneity of the flow is expected to play a main role in the dispersion mechanisms within the classroom. Similar considerations hold in the case of forced ventilation (not shown), where the airflow is governed by air conditioning apparatus.

3.2. Unsteady CFD simulation

The unsteady CFD simulation refers to a two-hour period (0950–1150 local standard time, IOP#1) and was conducted considering the same door/window opening configuration as in case A (Table 1). As mentioned before, by means of the URANS approach the non-stationary mean-flow structures are resolved, bearing in mind that only the statistics of the turbulence is simulated as for the RANS. The data measured during the field campaign were used to set the boundary conditions at W8. In particular, the wind velocity and direction acquired at 4 Hz by the external anemometer have been averaged over 15 s and provided 480 velocity values imposed at W8. Similarly to the steady case studies, the outflow condition was set at D1.

Figure 3 shows the mean velocity fields calculated by the model along the horizontal plane at 1.5 m above the classroom floor in two different time steps. They depict two characteristic airflow patterns that took place in the classroom during the two hours of simulation. The two maps differ profoundly and this fact is a signature of the variability of the meteorological conditions. As already mentioned in Sect. 2.1, the wind came from NE night time and for the first hours of day (i.e. nearly perpendicular to the windows, see Fig. 1), and from S from late morning onwards. As a result, the air entered the room from the window in the early morning (Fig. 3a), while it flew in the opposite direction later (i.e. out from the window, Fig. 3b). It is evident from the figure how such a wind rotation affected considerably the air circulation in the classroom.

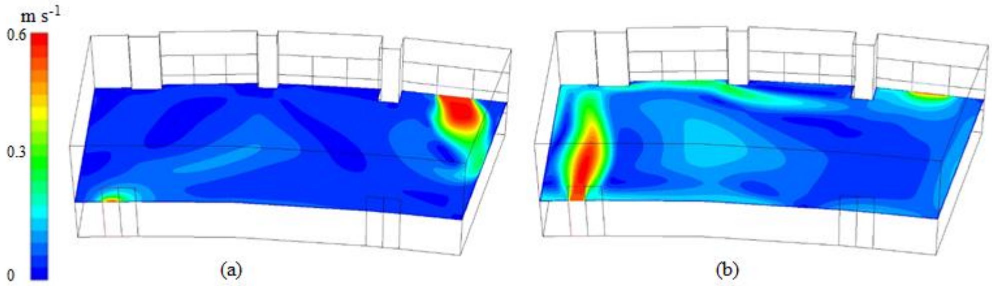

Figure 3. Maps of the mean velocity fields computed along the horizontal planes at 1.5 m above the classroom floor at (a) 900 s and (b) 4500 s (unsteady simulation). In panel (a) the wind enters the window, the opposite occurs in panel (b).

In essence, the results provide further evidence that: i) the boundary conditions influence considerably the indoor velocity pattern; this points out that the knowledge of the external meteorological conditions is of primary importance for a proper simulation of indoor airflows, and ii) when the air enters the door and exits the window the knowledge of the PM concentration in the hallway is expected to be an essential prerequisite in the correct simulation of the concentration field in the classroom. As will be shown below, in fact, the lack of PM data in the hallway during IOP#1 affects the goodness of the simulated PM concentration.

3.3. PM concentration modelling

The DPM model implemented in ANSYS Fluent was used to simulate the time series of the indoor PM concentration at location 3 (see Fig. 1) during the same two-hour period investigated above. The two-way coupling approach available in ANSYS was employed to consider the interaction between the phase “air” and the phase “particle” along with an unsteady particle tracking run with a time step equal to 1 s.

An injection of chemically inert particles simulated the source of PM entering W8. The (unknown) PM source flow rate was derived from the PM concentration and wind velocity measured outside the window. In particular, it was assumed that the particles entered the classroom through the window with the same velocity of the air. A (constant) mass flow rate $Q=5.1\cdot10^{-9}$ kg s^{-1} was calculated and considered representative of the flow rate over the entire window surface for the two hours of simulation. Note that Q must be seen as a rough approximation of the PM flow rate actually present during the analyzed period.

As was shown in Sect. 3.2, the airflow reversed during the two hours, i.e. air entered the classroom from D2 and exited through W8. Since no PM concentrations were measured in the hallway during IOP#1, no PM injection could be set at D1 during the airflow reversal. As a result, an unrealistic “clean air” occurred at D2. This implies that during the flow reversal the simulated PM concentrations lose their significance. In spite of that, they have been calculated also during that period in order to highlight that inconsistency well.

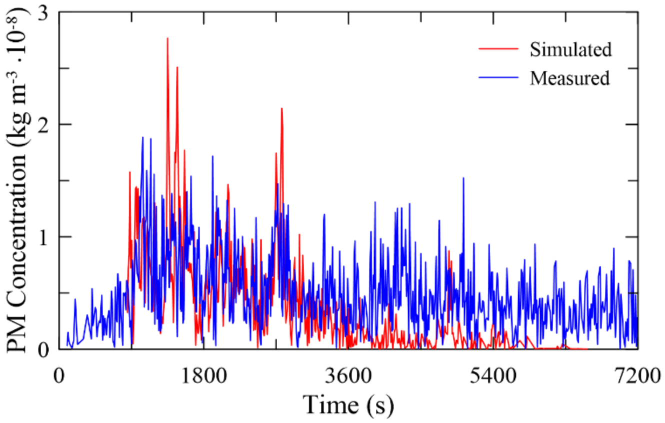

Figure 4. Simulated (red line) and measured (blue line) PM concentrations at control point 3. The origin of the horizontal axis coincides with the start of the simulation (0950 local standard time).

Figure 4 presents the comparison between the time history of the PM concentration measured in the room at control point 3 (see Fig. 1) and the corresponding values simulated numerically. The plot shows a reasonable agreement between the two when the air entered W8 and exited D2 (time $t\lesssim2800$ s, not shown). In particular, the numerical model is capable of catching oscillations with time scales of the order of minutes or even less. This suggest that the setting of the two external forcings, i.e. wind velocity and PM concentration, was reasonable. Conversely, the two concentrations differ substantially during the phase of flow reversal ($t\gtrsim2800$ s), at which the simulated concentration is much smaller than the measured one and tends to zero very quickly as a result of the (unrealistic) progressive emptying of the classroom from the PM. Therefore, any comparison in the concentration during that phase is meaningless. We can only speculate that the results improve when the source flow rate at D2 have been set correctly.

4. Conclusions

In this work, airflow and PM dispersion in a classroom were investigated experimentally and numerically by considering different configurations of the openings (i.e. doors and windows). An unsteady RANS model was used to investigate an Intensive Operating Period lasting two hours during which the micrometeorological conditions varied so that the airflow in the classroom reversed.

The results highlight the influence of room geometry, opening locations and boundary conditions as well as the role played by micrometeorology. Finally, the simulations pointed out the need of using high-frequency input data in order to correctly represent the real forcings that determine the pollutant exchanges and the airflow at the openings.

An extension of the present study will be simulating the PM concentration field also in the case of flow reversal once concentration and air velocity data will be acquired in the hallway.

Acknowledgement

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