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CFD MODELLING OF PARTICLE MATTER DISPERSION IN A REAL HOT-SPOT

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Abstract: Urban air quality is one of the main environmental concerns. The interaction between atmosphere and buildings induces complex flows within the streets and squares. This fact joint with the traffic emissions produce a heterogeneous distribution of pollutants with strong gradients of concentration. The main objective of this work is to obtain high resolution maps of particle matter concentration using a Computational Fluid Dynamic (CFD) model so as to analyze air quality and population exposure. This study is focused on a heavily trafficked roundabout in Madrid (Fernandez Ladreda square). To achieve this objective, CFD modelling coupled with detailed emissions of PM_{10} and $PM_{2.5}$ and outputs from WRF meteorological mesoscale model is performed. Emissions from vehicle exhaust, particle resuspension, pavement abrasion and brake and tire wear are considered with a horizontal resolution of 5 m x 5 m. The effects of urban vegetation are also modelled. Modelling results are evaluated for several periods of summer and winter by using data from experimental campaigns carried out in this zone in the framework of the TECNAIRE research project.

Key words: *Coupling mesoscale-microscale models, CFD modelling, detailed traffic emissions***.**

INTRODUCTION

Urban air quality is one of the most important environmental challenges and the largest environmental health risk in Europe due to the high percentage of population that lives in cities and the high pollution levels there. The complex flow patterns within the urban canopy joint to the irregular traffic emissions along the city induce a heterogenous pollutant distribution within streets and squares. In order to capture these strong concentration gradients, high spatial resolution is needed. In this way, Computational Fluid Dynamics (CFD) models which are able to solve explicitly the complex air flow and dispersion induced by urban obstacles seem to be an adequate tool to study this issue. This study is focused on particle matter dispersion in a real urban hot-spot in Madrid (Spain). CFD modelling coupled with mesoscale model outputs and detailed emissions of PM_{10} and $PM_{2.5}$ is used to obtain high resolution maps of particle matter concentration. The comparison of modelling results (meteorology and concentration) against data from experimental campaigns carried out in this zone in the framework of the TECNAIRE research project (Borge et al., 2016) allowed us to analyze how to improve some aspects of CFD modelling.

DESCRIPTION OF THE STUDY AREA AND EXPERIMENTAL CAMPAIGNS

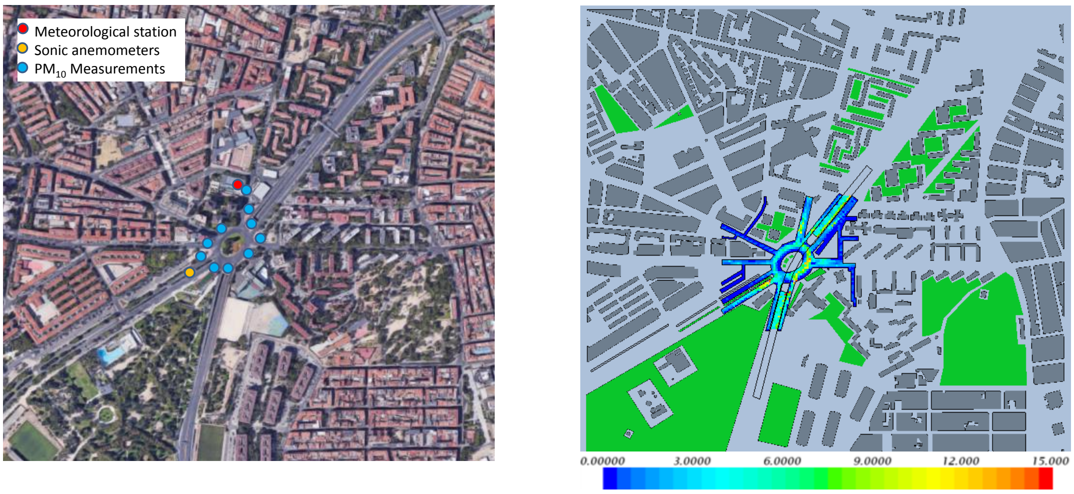
The area of study is located in the south-west of Madrid city in a heavily trafficked roundabout (Fernandez Ladreda square) with a main road crossing under it through a tunnel (Figure 1). This location, which presents high levels of pollution, is complex in terms of urban morphology (buildings and vegetation), intense road traffic, interaction of emissions sources and presence of pedestrian (Borge et al., 2016; Sanchez et al., 2017a).

Meteorological monitoring

Two experimental campaigns were carried out in this zone during winter and summer 2015. This study is focused on two days (25th February and 6th July) which are simulated by CFD model from 6 to 18 UTC. Atmosphere conditions were monitored in three points (Figure 1a): a) wind speed and direction were recorded by a meteorological station in the roof of a building (*Iberdrola* building) at 18 m above ground level (AGL), approximately and, b) micrometeorological parameters were measured by two sonic anemometers at 6 and 8 m AGL. The point at *Iberdrola* building was taken as representative of general meteorological conditions.

Particulate matter concentration

PM_{10} and $PM_{2.5}$ concentration data were recorded from a Grimm instrument located close to sonics anemometers. In addition, a portable TSI DustTrak^{TM} DRX instrument was moved around the square measuring PM_{10} concentration at several points at a height of approximately 1.5 m.



a) **b)**

Figure 1. Area of study. a) Real geometry. b) Numerical domain with PM_{10} exhaust emissions in µg m^{-2} s^{-1}. Location of vegetation is represented in green.

METHODOLOGY

The main objective is to simulate particulate matter dispersion by means of CFD modelling. In order to improve the uncertainties of CFD modelling, accurate boundary conditions and emissions are required. Meteorological conditions are reproduced coupling mesoscale model outputs to CFD model and emissions implemented in CFD model are taken from traffic and emissions micro-simulation models (see details in next section). Hourly inlet wind direction is taken from meteorological station (*Iberdrola* building) instead of mesoscale model outputs, however the fluctuations of wind direction during each hour are not considered.

MODEL DESCRIPTIONS AND SET-UPS

Meteorological mesoscale model (WRF)

Madrid urban atmosphere at mesoscale was simulated by means of WRF (Weather Research and Forecasting) model (Chen et al., 2001). For winter campaign, four nested domains were simulated with the finest domain with a horizontal resolution of 1 km x 1 km. In vertical, the resolution of the lowest levels are 5 m (see details in Sanchez et al., 2017a). A multilayer urban scheme was used to simulate urban areas (BEP-BEM, Martilli et al. (2002) and Salamanca et al. (2010)). Similar configuration was used to simulate meteorological conditions of summer campaign but with a resolution of the finest domain of 500 m x 500 m.

Traffic emission model

Hourly emissions with resolution of 5 m x 5 m are computed by means of a combination of traffic and emissions micro-simulation models (Quaassdorff et al., 2016). In this study, $PM_{2.5}$ and PM_{10} emissions from vehicle exhaust, particle resuspension, pavement abrasion and brake and tire wear are considered in a region of 300 m x 300 m around the square (Fig. 1b).

CFD model

The CFD model used is based on Reynolds-Averaged Navier-Stokes (RANS) equations with a Realizable k-ε turbulence closure. In addition, buoyancy terms are taking into account using Bousinesq's approach and an equation for temperature is solved. Transport equations are solved for pollutants dispersion with a low Schmidt number (Sc = 0.3). The software used is STAR-CCM+ from CD-Adapco. The size of numerical domain is 1300 m x 1300 m x 270 m. An irregular mesh is used, where the resolution is 2 m approximately around the square with smaller cells than 1 m close to the ground, buildings and the emissions zone. Further from this area the cell size progresivelly increase to 5 m. The total number of grid points is 8.3 10^6 (Sanchez et la., 2017a). Unsteady CFD simulations are performed from 6UTC to 18UTC of 25th February and 6th July. Hourly vertical profiles of wind, temperature (T) and turbulence kinetic energy (TKE) obtained from WRF model in the mesoscale cell corresponding to microscale domain are used as inlet boundary conditions at each hour in the CFD model. The vertical profile of dissipation rate (ε) is computed from TKE profile as, $\varepsilon_{in} = C_\mu{}^{3/4}\, TKE_{in}{}^{3/2}/(\kappa z)$. A radiation model is not implemented in the CFD model, however in order to analyze the effects of surface heat fluxes at different hours, two scenarios are simulated: 1) considering adiabatic the ground and buildings and 2) imposing at ground the surface heat flux computed at mesoscale in the whole domain by WRF at each hour (Sanchez et al., 2017b). In addition, background concentration of PM_{10} is taken from a background monitoring station close to the domain.

RESULTS

Evaluation of meteorological results

Firstly, wind speed and direction is evaluated at 18m AGL in *Iberdrola* building. This point could be considered as a measurement of the general atmospheric conditions, however for some wind directions it is affected by the sheltering of higher building located in the South.

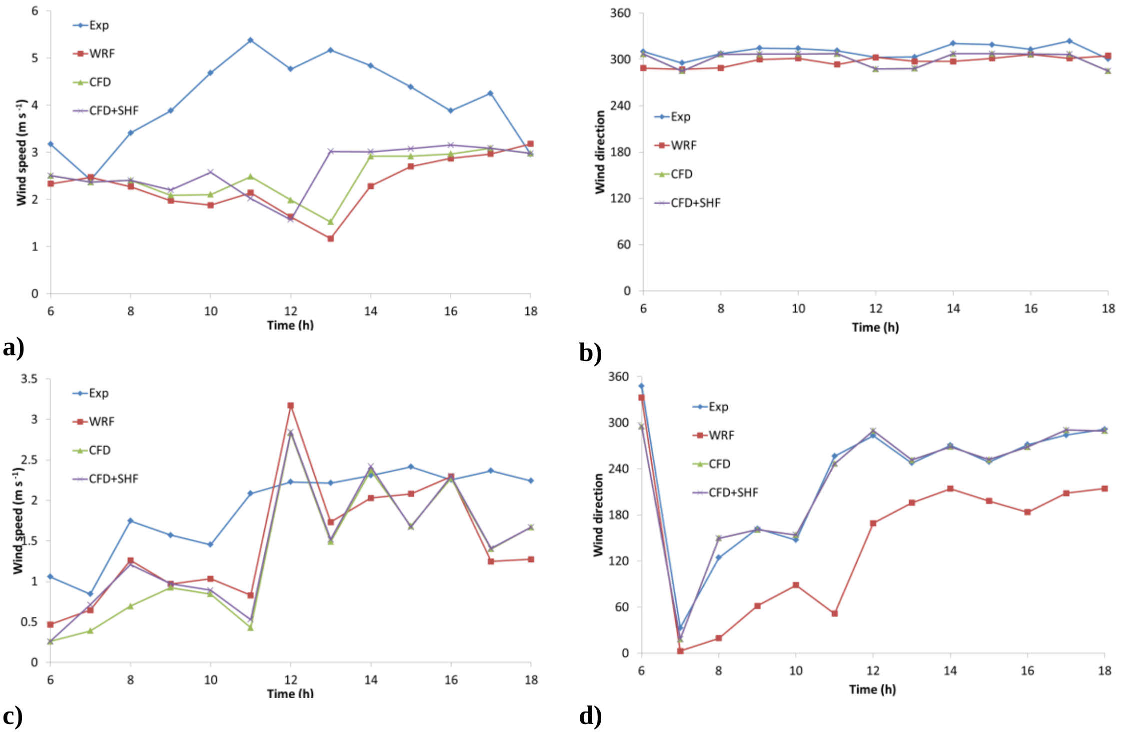


Figure 2. Time series at 18 m AGL of experimental data, WRF and CFD (with and without surface heat fluxes) results of: a) wind speed and b) wind direction for 25th February. c) wind speed and d) wind direction for 6th July.

Figure 2 shows that on 25th February the wind speed is understimated by WRF and CFD model. This indicates that the wind speed imposed at inlet in the microscale domain is lower than actual wind speed and thus the CFD results are influenced by this issue. On 6th July, modelling results are much closer to the experimental data. Hourly mean wind direction is in agreement with experimental data. From Figure 3, we can observe that the CFD results fit better with measurements for 6th July due to more accurate inlet conditions. For the winter day, the inlet wind speed underestimation induces an underestimation of the wind speed and a high underprediction of the TKE measured by the sonic anemometers. In addition, considering the surface heat flux (SHF) at ground improve the CFD results, especially TKE. This could be important for pollutant dispersion at some hours where the TKE computed without SHF is almost 0, for example at 8UTC of 6th July.

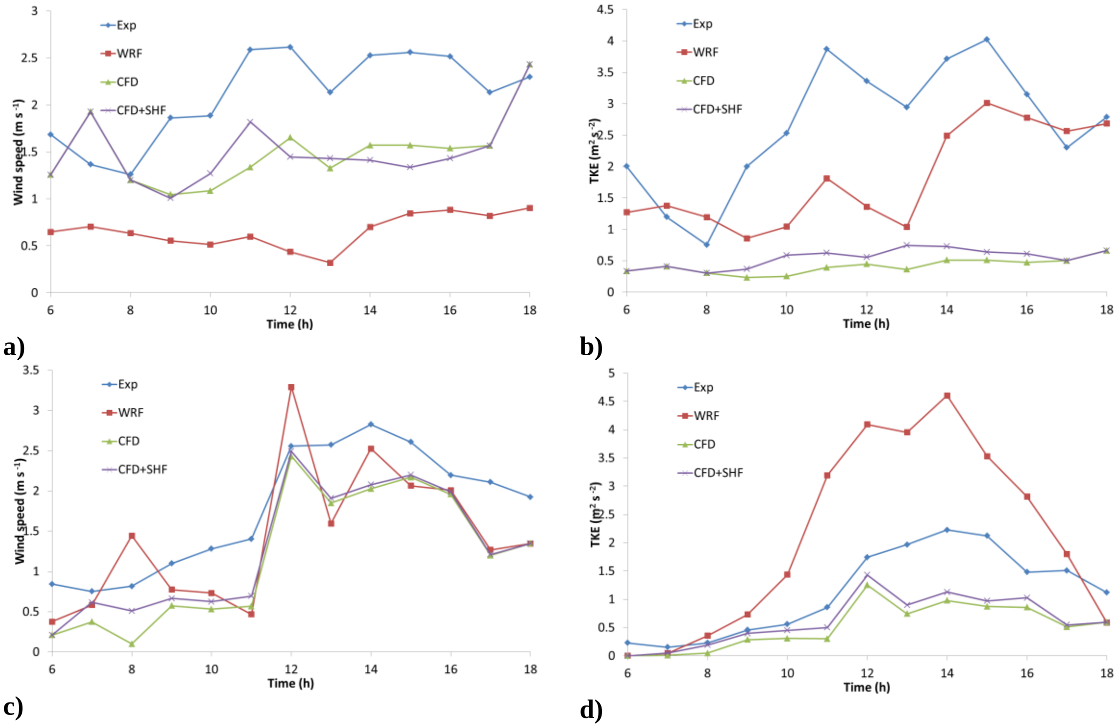


Figure 3. Time series at sonic anemometer located at 6 m AGL of experimental data, WRF and CFD (with and without surface heat fluxes) results of: a) wind speed and b) turbulent kinetic energy for 25th February. c) wind speed and d) turbulent kinetic energy for 6th July.

Evaluation of particulate matter concentrations

In order to illustrate the performance of the CFD simulations of particle matter dispersion, we focus on 7UTC of 6th July, one of the hours where experimental data are available and the meteorology (hourly values of wind speed and turbulence) is well captured by the CFD model. PM_{10} concentration is measured by the portable TSI DustTrak^{TM} at 10 different points during several minutes and by a GRIMM during this hour (see Fig. 4). In the comparison three different CFD modelling approaches are considered (Fig. 5): 1) simulation without surface heat fluxes with Sc = 0.3, 2) simulation with surface heat flux at ground with Sc = 0.3, and 3) simulation with surface heat flux (SHF) at ground with Sc = 0.7. In the previous section, it is observed that meteorological measurements are better reproduced in simulations which take into account SHF. On the other hand, Schmidt number (Sc) is a parameter that according to flow properties and geometries could be in a range from 0.2 to 1.3 depending on the case. The selection of 0.3, which implies a greater diffusion, in this geometry is based on Sanchez et al. (2017a) in order to minimize the error due to processes as heat fluxes or turbulence induced by traffic that were not considered. In Fig. 5 we can observe that modelled concentration is better as SHF is considered in CFD simulation. In this case the dispersion increases by imposing the surface heating at ground providing a better agreement with experimental measurements. The rise of the Sc to 0.7 decrease the dispersion of pollutant and increase the concentration in some points providing a slight overestimation. However, a more detailed analysis about Sc is necesary. Despite it all, the values in some points (8, 9, 10) are underestimated by CFD. This could be due to hourly mean wind direction is imposed at inlet, however the fluctuations of wind direction are significant during this hour.

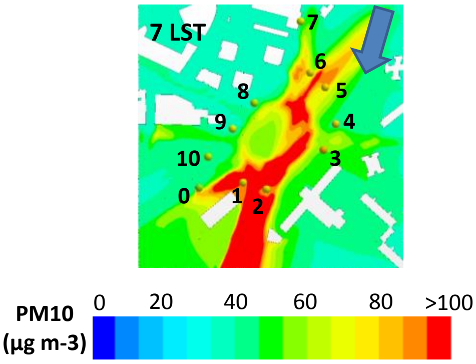


Figure 4. PM_{10} concentration maps at 7UTC at 1.5 m for CFD+SHF with Sc=0.3. The colour of point indicates the experimental value

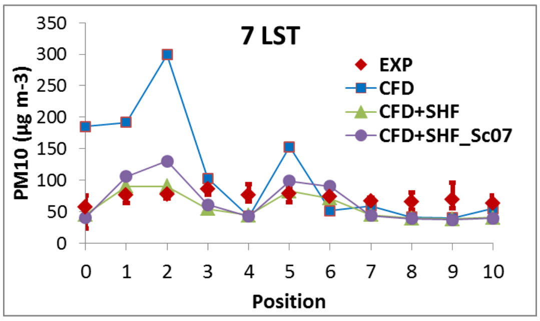


Figure 5. Comparison of experimental PM_{10} concentration at 7UTC in the point measurements with results from CFD with Sc=0.3, CFD+SHF with Sc=0.3, and CFD+SHF with Sc=0.7.. Vertical bars in experimental data indicates the maximum and minimum measured.

CONCLUSIONS AND LESSONS LEARNED

Using WRF outputs as boundary conditions of CFD model including SHF improves microscale results. However, the uncertainties in the inlet boundary conditions affect the performance of CFD simulations. Some parameters as surface heat flux in the meteorology or Schmidt number in the pollutant dispersion should be analyzed in detail for each case depending on processes considered in the model. These are preliminary conclusions and a more extensive study is necesary.

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