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MODELLING REACTIVE POLLUTANTS DISPERSION IN AN URBAN HOT-SPOT IN SUMMER CONDITIONS USING A CFD MODEL COUPLED WITH METEOROLOGICAL MESOSCALE AND CHEMISTRY-TRANSPORT MODELS

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Abstract: Air quality assessment requires detailed studies about urban air pollution. In a city, the interaction between atmosphere and urban morphology induces complex flow pattern which leads to irregular spatial distributions of pollutants in the streets. In addition, the influence of chemical reactions and the atmospheric variability make difficult to reproduce the reactive pollutants dispersion at microscale, especially in summer conditions. In this season, the thermal effects acquire greater importance than in winter since that considerably modify the air flow and therefore, the pollutants dispersion in the streets. Furthermore, the chemical constants are linked with the air temperature and solar radiation, hence, the inclusion of chemical mechanism to model the NO and NO_2 dispersion in an urban hot-spot becomes necessary. The aim of this work is to simulate reactive pollutants dispersion during several hours in summer conditions in an urban hot-spot using a computational fluid dynamics (CFD) model. To achieve this purpose, the vertical profiles resulted from a meteorological mesoscale simulation (WRF) are used as inputs in the CFD simulation. Besides, in relation to the background concentration of pollutants, the outputs of a chemistry-transport simulation (CMAQ) are also imposed as inlet condition at microscale. Additionally, detailed traffic emissions of NO and NO_2 are implemented into the CFD simulation based on the results of a microscale traffic emission model. Lastly, focusing on studying the NO_2 dispersion, the photostationary state mechanism is implemented in the CFD simulation. Thus, the time series of meteorological variables and pollutants concentration resulting from the CFD simulation are thoroughly evaluated against measurements at several points from an experimental campaign carried out in the research area (in the framework of TECNAIRE project). Regarding the air quality assessment, the deviation of NO_2 concentration including chemical reactions in the CFD simulation is quantified in comparison with a non-reactive pollutant. In this way, the improvements included in the CFD modelling and the conclusions obtained from this analysis provide information on how to simulate reactive pollutant dispersion in an urban hot-spot in summer conditions.

Key words: *CFD-RANS model, reactive pollutants, mesoscale models, WRF, CMAQ*

1. INTRODUCTION

Air quality assessment in urban areas through a CFD model is in continuous development owing to its high resolution to solve the air flow and pollutants dispersion in the real geometry of a city. One of the main sources of uncertainties are the boundary conditions used in the simulation. In that regard, the use of outputs from a mesoscale model can provide more complete information about the atmospheric conditions and improve the input data of the microscale simulation. Kwak et al. (2015) developed an integrated system of mesoscale models with the weather research and forecasting (WRF) model and the community multiscale air quality (CMAQ) model providing the time-dependent boundary conditions to the CFD simulation. They have shown that the use of a CFD model improves the accuracy for the NO_2 and O_3 concentration at street level compared to the outputs of CMAQ, because the spatial heterogeneity is better reproduced.

The impact of the use of boundary conditions increasingly detailed in the CFD simulations is tackled in this study. For that, an unsteady CFD simulation from 06 to 18UTC over an urban hot-spot in summer conditions is performed coupling the outputs from WRF and CMAQ simulations in that area. The time series of meteorological variables and turbulent parameters are validated at several points with experimental data. And as for the pollutants concentration, the deviation produced by the chemical reactions is also analyzed and evaluated with the air quality monitoring station.

2. CASE STUDY

The urban hot-spot selected is located in a large square of Madrid (Spain) which consists of a heavily trafficked roundabout crossed by a main exit road through a tunnel. The meteorological deployment is composed of an anemometer at a building's roof (18m above ground level) and two sonic anemometers close to a main road at a height of 8 and 6 m (yellow and blue points in Fig.1a, respectively). The concentration of pollutants is recorded at the air quality monitoring station that belongs to the Madrid Council and is located in the research area. More detail can be found in Borge et al. (2016).

3. MODELING APPROACH

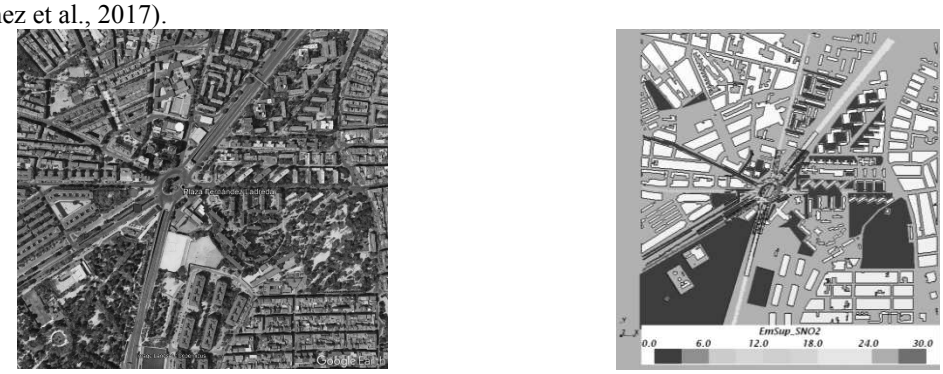
The modelling system consists of coupling the outputs from the mesoscale simulations into the CFD simulation so as to model the reactive pollutants dispersion in the streets over time in summer conditions.

3.1. Mesoscale Models Description

The mesoscale simulations are carried out during the experimental campaign from 29th June to 20th July 2015. The meteorological mesoscale model (WRF) used is a model particularly adapted to simulate the urban atmosphere (Chen et al, 2011). The five nested domains are 48, 16, 4, 1 and 0.5 km. In the lowest levels, it takes into account the strong gradients of mean variables, the turbulent fluxes and even the heat in buildings and its exchange with air in order to obtain a high understanding of the physical processes in urban roughness sublayer (BEP-BEM, Martilli et al. (2002) and Salamanca et al. (2010)). In regard to the pollutants concentration, the chemistry-transport model used is Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006).

3.2. CFD Simulation Setup

The CFD model used is based on the Reynolds-averaged Navier-Stokes equations (RANS) with the realizable k-ε turbulence closure. In addition, the buoyancy terms are included with the Boussinesq's approximation. The size of the computational domain over the research area is approximately 1300 m x 1300 m x 270 m. The polyhedral irregular mesh used has a base resolution of 5 m. Besides, the grid size applied within the central region of 400 m x 400 m is 2 m and even 1 m close to the ground and buildings (Sanchez et al., 2017).



(a) (b)

Figure 1. (a) Research area from Google Earth. At the yellow and blue points are the meteorological stations and at the red point is air quality monitoring station (b) Computational domain of the CFD simulation.

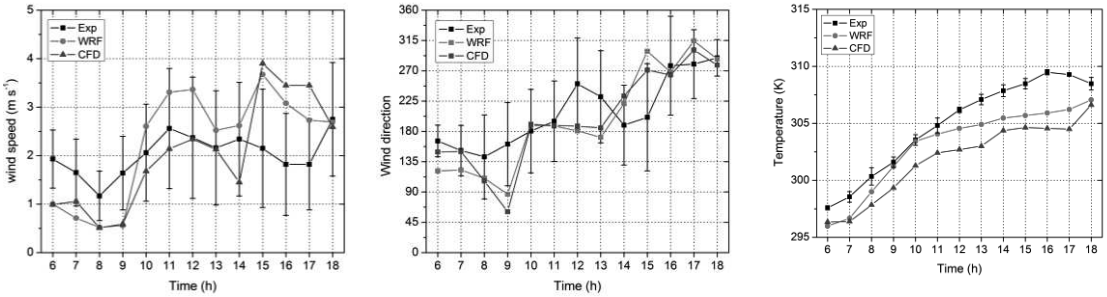
The CFD simulation is performed in unsteady conditions and covers from 06UTC to 18UTC of 1st July, 2015. The vertical profiles of horizontal wind components, air temperature and turbulent kinetic energy (k) derived from WRF for a grid cell corresponding to the CFD domain, are imposed at inlet in the microscale simulation. The boundary conditions for the turbulent dissipation rate (ε) are computed as, $\varepsilon_{in}=C_{\mu}^{3/4}\, k_{in}^{3/2}/(\kappa z)$. The surface heat flux derived from WRF is established at ground of the CFD domain since in summer conditions the thermal effects are important and considerably modify the flow pattern and therefore, the pollutants dispersion. The boundary conditions for pollutants are also obtained from the CMAQ simulation for the corresponding grid cell, and used as inputs for the CFD simulation. All boundary conditions are changing every 1 h. On the other hand, the detailed traffic emissions in an area of 300 m x 300 m centered on the square are obtained from a microscale traffic emission model (Quaassdorff et al., 2016) with a resolution of 5 m x 5 m; and they are uniformly extended to the rest of

the domain. The daily pattern of traffic emission is considered and the emission scenario is changing every hour. The emitted ratio NO_2-to-NO_x is 0.3 based on the Madrid emission inventories (Borge et al., 2014). Lastly, the chemical interactions between the primary emitted pollutants NO and NO_2 are considered in the CFD simulation through the photostationary state.

4. RESULTS

4.1. Meteorological variables

Some meteorological variables from modelling outputs are validated against the experimental data. The results in the WRF cell and in the specific point corresponding to the location of the measurement point of the CFD domain are compared with the experimental data. Thus, the WRF results are also analyzed in order to show the accuracy of inputs in the CFD simulation. Figure 2 shows the time series of wind speed and direction and temperature at **18 m** above ground level (AGL).

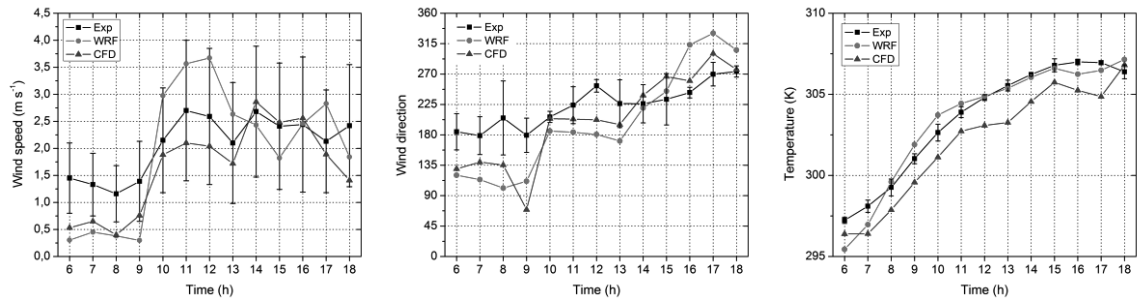


(a) (b) (c)

Figure 2. Time series of the experimental data, WRF and CFD results of: (a) wind speed, (b) wind direction and (c) temperature at 18 m (yellow point in Fig. 1).

In general, the modelling results fit quite well to the measurement within its error range. As for the hourly mean wind direction, either the mesoscale or the microscale results reproduce the wind behavior along the day. Note that experimental wind direction is constantly varying during each hour being these variations greater than 45º in some cases. Even so, the wind speed simulated exhibits a good agreement to the experimental data with the NMSE equal to 0.15 and 0.22 and a FB of 0.10 and 0.006 respectively from WRF and CFD results. The slightly underestimation of temperature by both models is obtained for all hours. In the microscale case, part of this error is due to the fact that the surface heating of buildings is not taken into account and it is only imposed at ground.

Figure 3 shows the same variables but at **8 m** AGL (blue point in Fig. 1). Similarly, at this point, the evolution of wind direction and temperature is captured over time by the models. For the wind speed the statistical parameters NMSE, FB and the correlation coefficient are 0.13, -0.05 and 0.87 for the WRF results and 0.08, -0.24 and 0.91 for the CFD outputs. It represents a small deviation from the experimental data with a slight underestimation, which entails in a high correlation coefficient.

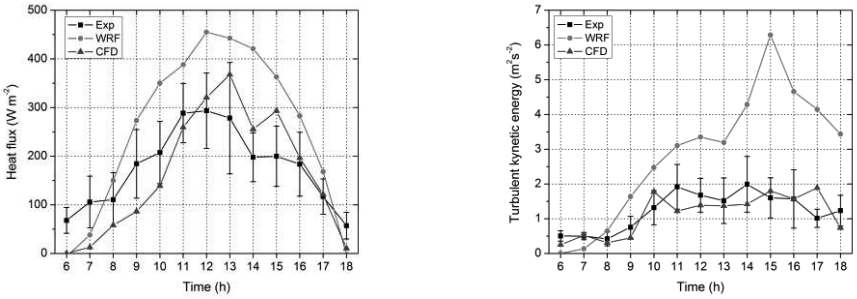


(a) (b) (c)

Figure 3. Time series of experimental data, WRF and CFD results of: (a) wind speed, (b) wind direction and (c) temperature at 8 m (blue point in Fig. 1)

To further ascertain the validation, the turbulent parameters such as the turbulent kinetic energy (k) and the heat flux (HF) are also analyzed at 8 m (Fig. 4). In regard to the HF, either WRF or CFD reveal precise outcomes with a NMSE 0.26 and 0.0.11 and FB 0.36 and -0.08 respectively. However, the time

series of *k* simulated by the CFD model is improved from the WRF results and its fit to the experimental data is quite accurate. The NMSE is 1.09 and 0.11 and the FB is 0.79 and -0.09 from WRF and CFD outputs respectively. Therefore, the use of boundary conditions in the CFD simulations derived from a mesoscale model provides appropriate results that reproduce the micrometeorology in the research area.

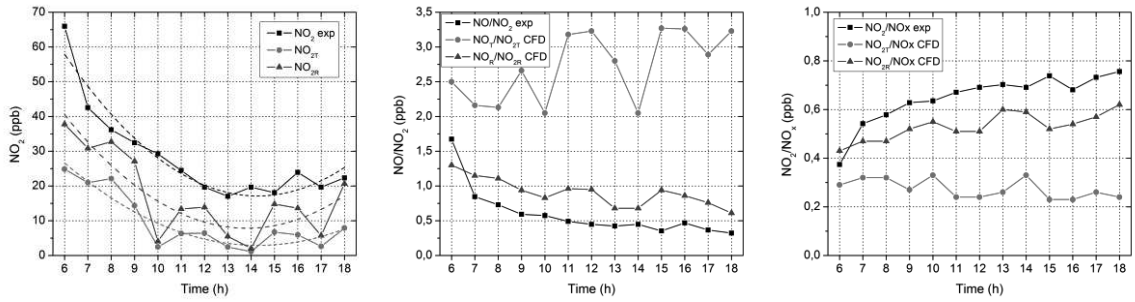


(a) (b)

Figure 4. Time series of WRF and CFD results against to the experimental data of: (a) HF and (b) *k*

4.2. Pollutants concentration

The time series of the concentration of NO, NO_2 and O_3 are analyzed at the air quality monitoring station. The results of NO and O_3 (not shown) reveals a good agreement with a correlation coefficient of 0.89 and 0.95 respectively. Focusing on NO_2, which is simulated as reactive (NO_{2R}) and inert (NO_{2T}) pollutant, the time series of NO_2, the ratios NO-to-NO_2 and the NO_2-to-NO_x is compared with measurements (Fig. 5).



(a) (b) (c)

Figure 5. Time series of: (a) NO_2 concentration (ppb), (b) NO-to-NO_2 and (c) NO_2-to-NO_x registered at air quality monitoring station (black) and the CFD results by simulating the pollutants as inert species (red) and reactive compounds (blue)

The evolution of NO_2 simulated, either NO_{2R} or NO_{2T}, show sharp variations in comparison with the experimental data as well as an underestimation of the measurements. The sharp changes are due to the fact that the wind direction fluctuates over time during 1 h and here, hourly mean values are used to simulate each hour. If these variations were taken into account to simulate the pollutants dispersion, the time series of pollutant would be likely smoothed. With the objective of mitigating that variation and extracting the tendency followed, either the experimental data or the values simulated are adjusted to a polynomial equation (dashed line in Fig. 5.a.). It reveals that the pollutants modelled have the same behavior that the experimental, however the NO_{2R} is higher and closer to the experimental result. In turn, the comparison of the ratio NO-to-NO_2 with that of the air quality station, shows the importance of including chemical reactions in the simulation in order to capture the conversions of NO and NO_2. Besides, the NO_{2T}-to-NO_x shows little variations over time but always around the ratio NO_2-to-NO_x imposed into the emissions (0.3). In contrast, the NO_{2R}-to-NO_x is closer to the value computed from experimental data. This slight difference on NO_2 concentration over time might be related to an underestimation from CMAQ of the background concentration of NO_2 and O_3 or by a deviation in the computation of the chemical constants either by temperature or by solar radiation due to the assumptions considered. Figure 6 shows the distribution of NO_2, NO_{2R}-NO_{2T} and the NO_{2R}/NO_{2T} in order to spatially evaluate the importance of including chemical reactions in summer conditions. At 06UTC, the solar radiation and temperature are lower than at 12UTC and consequently, the chemical constants rate are lower leading to little differences in modelling NO_2 as a tracer instead of a reactive pollutant. For that, the

deviation from tracer is higher at 12 than 06 UTC. In both cases, that difference increases with distance from the traffic emission area because of the high NO emission there. But even at 12UTC the NO_{2R} is up to a factor 1.5 from tracer in this area partly because there is higher available O_3 and the chemical activity is more reactive. It is possible to conclude that modelling NO_2 as reactive pollutant in summer conditions is important to develop the diurnal variation of this pollutant and so to obtain an accurate map of the NO_2 in an urban hot-spot.

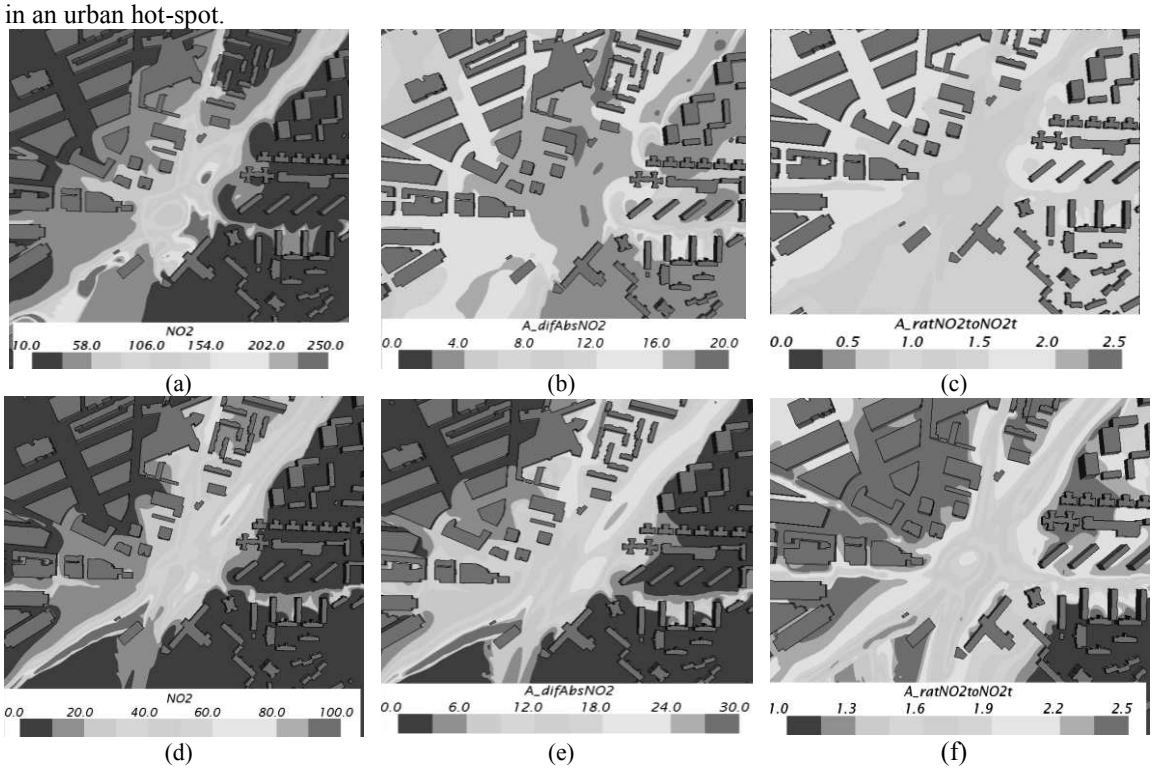


Figure 6. (*left to right*) The spatial distribution of NO_{2R} concentration (ppb), the differences (NO_{2R}-NO_{2T}) of concentration and the ratio NO_{2R}-to-NO_{2T} at (above) 06UTC and (bellow) 12UTC.

5. CONCLUSIONS

- Using the vertical profiles of the atmospheric variables derived from the mesoscale models as boundary conditions for the CFD result in a good agreement of the CFD results with the point experimental data and it allows to obtain a better approximation of atmospheric conditions.
- In summer conditions due to the high air temperature and solar radiation it is important to simulate the NO_2 as reactive pollutant to better represent the concentration in the streets. Although the inclusion of a chemical mechanism increases the computational load, to accurately capture the diurnal variation of NO_2 should be included at least the photochemical scheme.
- The hourly CFD results would improve by changing the boundary conditions every 30 min. It would enhance the pollutants concentration and the meteorological variables representative of every hour.

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