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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INTRODUCTION

Air quality assessment in urban areas through a computational fluid dynamics (CFD) model is in continuous development because of 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.

The impact of using increasingly detailed boundary conditions 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.

CASE STUDY

The urban hot-spot selected is located in a 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 at 18 m above ground level (AGL) and two sonic anemometers close to a main road at 8 and 6 m (yellow and blue points in Fig. 1, respectively). The concentration of pollutants is recorded at the air quality monitoring station (red point in Fig. 1) belonging to the Madrid Council and is located in the center of the research area. More detail in Borge et al. (2016).

Figure 1. Research area from Google Earth.

MODELLING APPROACH

WRF

The meteorological mesoscale model used is a model particularly adapted to simulate the urban atmosphere (Chen et al, 2011). The resolution of the nested domains are 48, 16, 4, 1 and 500mThe presence of the canopy in the lowest numerical levels is taken into account by adding a drag and heat fluxes form urban surfaces and building interiors (BEP-BEM, Martilli et al. (2002) and Salamanca et al. (2010)).

CMAQ

The chemistry-transport model used is Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006)

Microscale traffic emission model

Detailed traffic emissions with a resolution of 5 m x 5 m in 300 m x 300 m around the square are obtained from a microscale traffic model (Quassdorff et al., 2016)

Inlet vertical profiles of:
- Meteorological variables
- Background of NO, NO_2 and O_3

Surface heat flux at ground

Daily pattern of detailed traffic emission

CFD MODEL

CFD model based on the Reynolds-averaged Navier-Stokes (RANS) equations with the realizable turbulence k-ε closure

- Computational domain: 1300 m x 1300 m x 270 m
- Polyhedral irregular mesh: Grid resolution of 5 m from boundaries to 2 m within the central region of 400 m x 400. The grid size is 1 m close to the ground and buildings
- Unsteady CFD-RANS simulation from 06UTC to 18UTC of 1st July, 2015
- The buoyancy terms are included with the Boussinesq's approximation
- The NOx-O_3 photostationary state mechanism is implemented
- The inlet turbulent dissipation rate (ε) is computed as, $\varepsilon_{in} = C_\mu{}^{3/4}\, k_{in}{}^{\frac{3}{2}}/(\kappa z)$
- The boundary conditions are changing every 1h
- Detailed traffic emissions in 300 m x 300 m around the square and moreover they are uniformly extended to the entire domain.
- The daily pattern of traffic emission is considered and the emission scenario is changing every hour.
- The emitted ratio NO_2-to-NOx is 0.3 based on the Madrid inventories (Borge et al., 2014)

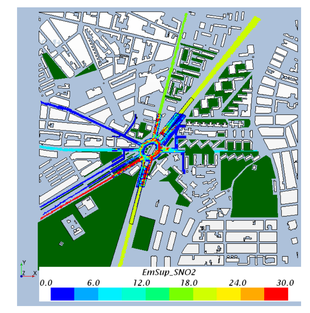

Figure 2. Computational domain of the CFD simulation

METEOROLOGICAL VARIABLES

At 18 m AGL :

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 45° 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.

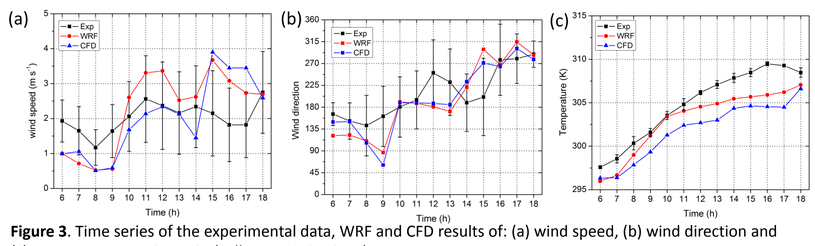

Figure 3. Time series of the experimental data, WRF and CFD results of: (a) wind speed, (b) wind direction and (c) temperature at 18 m AGL (yellow point in Fig. 1).

At 8 m AGL:

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.

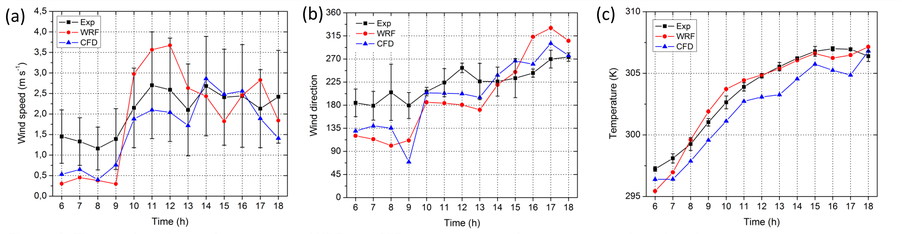

Figure 4. Time series of experimental data, WRF and CFD results of: (a) wind speed, (b) wind direction and (c) temperature at 8 m AGL (blue point in Fig. 1)

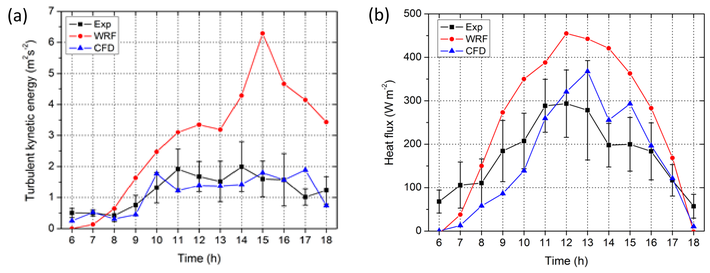

Figure 5 Time series of WRF and CFD results against to the experimental data of: (a) HF and (b) k

The turbulent parameters such as the turbulent kinetic energy (k) and the heat flux (HF) are also analyzed at 8 m (Fig. 5). In regard to the HF, either WRF or CFD reveal precise outcomes with a NMSE 0.26 and 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.

POLLUTANTS DISPERSION

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_R (modelling as reactive pollutant) and O_3 reveals a good agreement with a correlation coefficient of 0.89 and 0.95 respectively

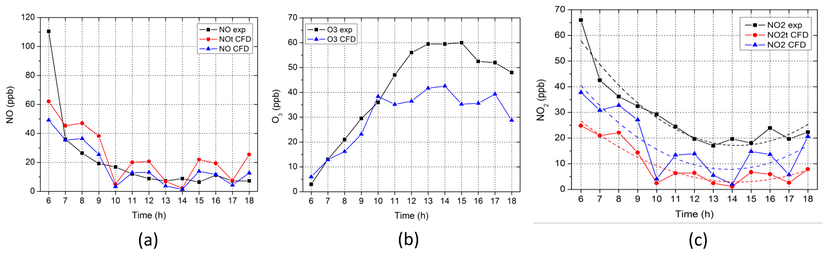

Figure 6. Time series of: (a) NO, (b) O_3 (ppb) and (c) NO_2 concentrations in ppb registered at air quality monitoring station (black) and the CFD results by simulating the pollutants as inert species (red) and reactive compounds (blue)

The evolution of NO_2 simulated, either NO_{2R} or NO_{2T}, show sharp variations 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. 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. 6c). 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.

The ratio NO-to-NO_2 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-NOx shows little variations over time but always around the ratio NO_2-to-NOx imposed into the emissions (0.3). In contrast, the NO_{2R}-to-NOx is closer to the value computed from experimental data.
This slight difference on NO_2 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.

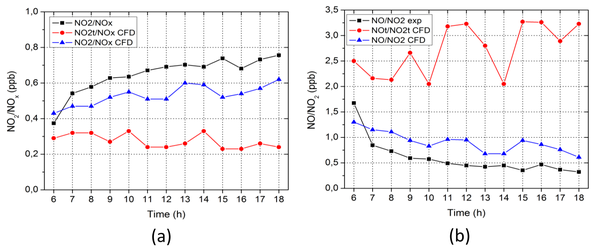

Figure 7. Time series of: (a) NO-to-NO_2 and (b) NO_2-to-NO_x registered at air quality monitoring station (black) and the CFD results by simulating the pollutants as inert species (red) and reactive compounds (blue)

Figure 8 shows the distribution of NO2, 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.

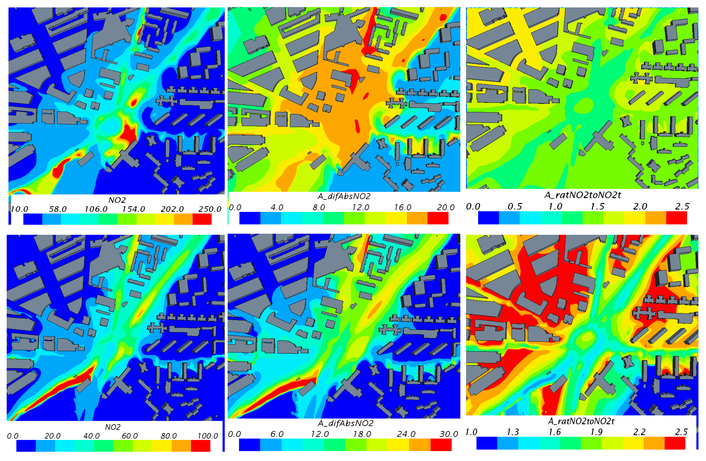

Figure 8. (*left to right*) The spatial distribution of NO_{2t} concentration (ppb), NO_{2R}-NO_{2T} and the ratio NO_{2R}-to-NO_{2T} at (above) 06UTC and (bellow) 12UTC.

The chemical deviation from tracer is higher at 12 than 06 UTC

The 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.

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.

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 at least be included the photostationary 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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