Evaluation of the mesoscale effect of photocatalytic pavements and vegetation on air quality

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Introduction

In the last decade, new strategies have been developed to reduce air pollution levels without changing emissions. In this work we analyze and compare the impact of two of them: the use of photocatalytic materials on the streets of cities, and the introduction of trees in the urban canyons. Differently than previous studies that focused mainly on the microscale, here we focus on the mesoscale. So, the scientific question that motivates the work is:

what could be the effect on urban air quality of these strategies if they are applied not only in few streets, but over the entire city?

The methodology adopted is based on numerical simulations carried on with the mesoscale model WRF, with the multilayer urban parameterization BEP-BEM. Since we do not want to study a specific city, but search for a general tendency, idealized simulations are performed over cities with different population density (e. g. different urban structure), with an approach similar to Martilli (2014). A short description of the model and the urban parameterization is presented in section 2. An essential information for this study is the deposition velocity over the photocatalytic materials, and over vegetation.

The Model: WRF+BEP+BEM.

WRF (Weather Research and Forecasting model) : prognostic, non-hydrostatic atmospheric model

BEP (Building Effect Parameterization , Martilli et al. 2002), urban parameterization implemented in WRF. Features: multilayer scheme, accounts for the impact of buildings on drag, temperature and TKE equations. Effect of shadowing and radiation trapping in the street canyon are considered (the solar radiation reaching the street level is computed). In addition the Building Energy Model (BEM, Salamanca et al. 2010) computes the exchanges of heat between the interior and the exterior of the buildings, including the effect of air conditioning.

Instead of using a complex photochemical model, the pollution is represented by resolving advection and diffusion of a passive tracer that represents the mass concentration of Nitrogen (N), in all its forms (NO, NO_2, N_2O_5, etc.). Regardless the number of reactions that the emitted nitrogen undergoes in the atmosphere, in fact, this quantity is conserved.

Effect of Photocatalytic pavements.

In the LIFE MINOx-STREET project different photocatalytic materials have been tested, involving both laboratorory as large-scale tests in order to assess their physical and mechanical properties, on the one hand, and NO_x depolluting capacity, on the other. Surface deposition velocities were then inferred from laboratory data. The most performing product has also been implemented in ambient conditions and the mentioned value has been supported by field measurements under certain climate-weather conditions associated to high NOx pollution levels (M. Palacios et al., 2015). To represent the effect of the pavements in WRF, a sink term for the N tracer is introduced at the surface for all the urban grid points, and applied only when the solar radiation reaches the ground (solar radiation is necessary to trigger the photocatalytic reactions). This term is estimated as:

$$S = -v_{dep\_PHOT}\frac{1}{V_{cell}\Delta z}[N_{NO}]$$

Here V_{cell} is the fraction of air in the lowest grid cell (e. g. without the volume of the buildings), Δz is the depth of the lowest grid cell (3 m in this case), and $[N_{NO}]$ is the fraction of N that is NO. Since the passive tracer simulated represents the total mass of N, it is necessary to estimate which fraction of the tracer is NO. To do this, it is assumed that close to the emissions, the mass of N is in a large majority shared between NO and NO_2, and that the photo stationary state applies, something reasonable if VOC emissions are not very high (Sanchez et al. 2015, this conference), given that , the fraction of is $\frac{[NO]}{[NO_X]} = \frac{J_{NO}}{k[O_3]+J_{NO}}$

where J_{NO} and k are reaction constants. A constant ozone equal to 20 ppb, considered representative of the situation very close to the emissions, is used.

Effect of Vegetation.

Vegetation, intended as trees in the streets, affects the pollutant concentration in two ways: by modifying the flow – and so the dispersion – and by capturing the pollutants through deposition on the leaves. To represent the impact on the flow, following Krayenhoff et al. (2015), one extra term is added in the equation of momentum to account for the drag induced by the leaves as: $Drag_{veg} = -L_D C_{DV}\langle\overline{U}\rangle\langle\overline{u}\rangle$

Where *LAD* is the leaf area density, and C_{DV} is the drag coefficient of the leaves, taken equal to 0.2. Another extra term is added in the TKE equation to represent the enhanced dissipation due to the leaves, like:

$$Diss_{veg} = -\beta_d L_D C_{DV}\langle\overline{tke}\rangle\langle\overline{U}\rangle$$

Where β_d =6.5. The interactions between radiation and vegetation are neglected.

The deposition on the leaves is estimated by introducing a sink term in the conservation equation of the tracer equal to: $S = -v_{dep\_VEG}L_D[N_{NO_2}]$

Here $[N_{NO2}]$ is the fraction of N that is NO_2, because this is the species that is most captured by the leaves. To estimate the value of the deposition velocity only the canopy resistance is considered because the model already computes the concentration at the level of the leaves (no need for aerodynamic resistance). Following Hirabayashi et al. (2012), the canopy resistance is the result of three resistances:

$$\frac{1}{R_C} = \frac{1}{r_s + r_m} + \frac{1}{r_t}$$

r_m is the mesophyll resistance, equal to 100 s m^{-1} for NO_2, r_t is the cuticular resistance equal to 20000 s m^{-1} for NO2, while r_s is the stomatal resistance which depends on the PAR (photosyntetically active radiation) estimated from Baldocchi et al. (1987) typical values for a tree like the Oak are chosen. Note that when there is no solar radiation, only cuticular resistance is active. Since the deposition is for NO_2, the sink is:

$$S = -v_{dep\_VEG}L_D\frac{k[O_3]}{k[O_3]+J_{NO}}[N]$$

Scenarios.

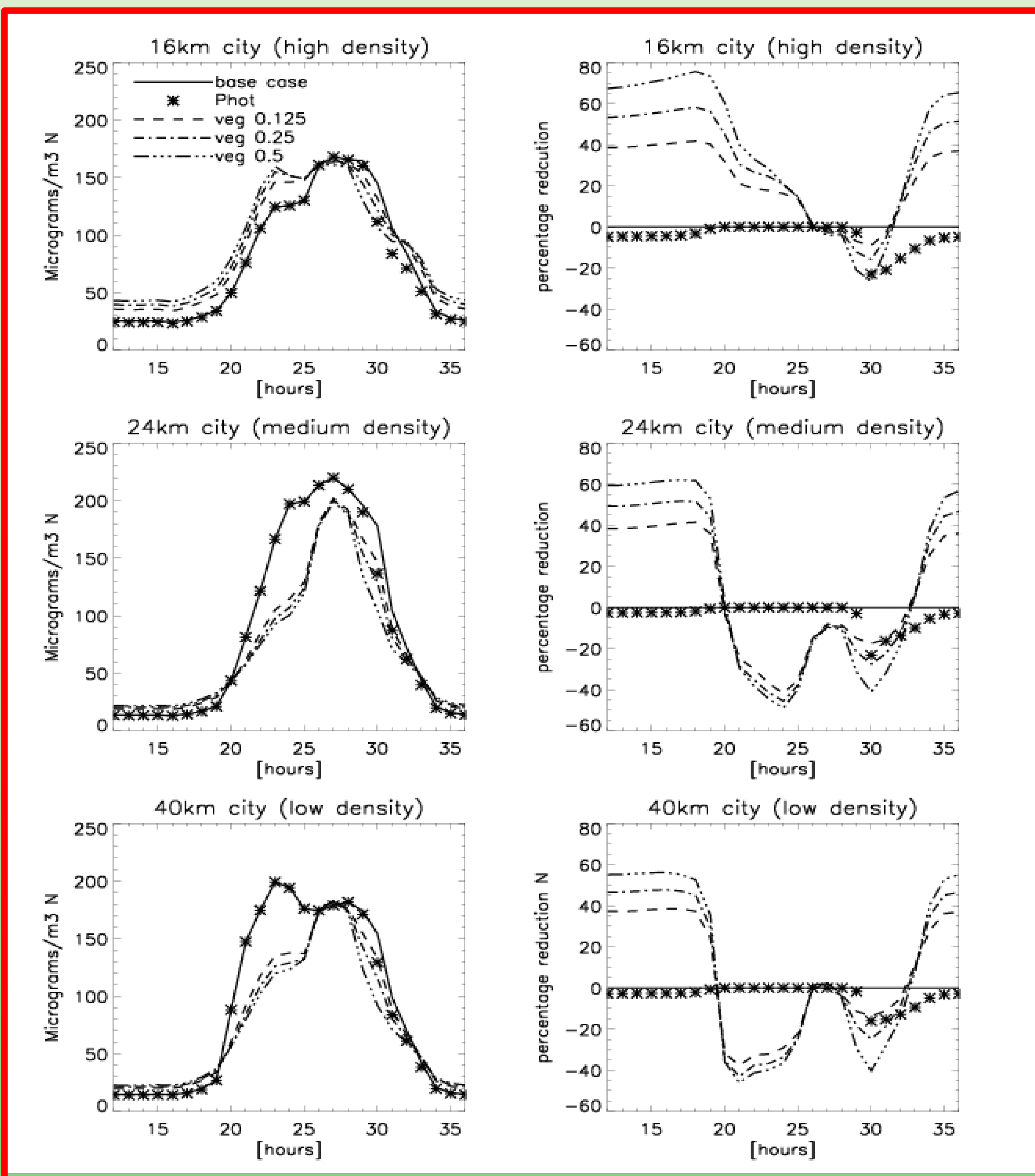
The urban scenarios considered are a subsection of those used by Martilli (2014). The domain is flat, and the cities are located in the middle. All the cities have 10 millions of inhabitants, but their density changes, which causes a change in city size and morphology, as illustrated in Table 1 below.

Day: 21st of June, latitude 45^o North, simulations starts at 6am, and last for two days. Results between noon of the first day and noon of the second day. Initial and geostrophic wind speed is 5 m/s. Emissions are located at ground level (representing traffic), with a typical daily variation. To facilitate the comparison, the same emission density is kept for the three cities, even if in reality city structure and population density clearly have an impact on emissions. The volume of air (e. g. without the volume of buildings) in the lowest grid cell is considered in the calculation.

For each of the three city types, the following runs have been done: 1) Base Case (no deposition), 2) Phot, with the photocatalytic pavement, 3) Veg, with a layer of vegetation in the whole city between 3 and 6m of altitude above the ground level. For the Veg cases, three different LAD have been considered 0.5, 0.25, and 0.125 m-1.

Population density (and city diameter)

62.5 inh/ha (40 km) Low density	160 inh/ha (24 km) Medium density	390 inh/ha (16 km) High density
H=3m W=60m	H=3m W=8m	H=9m W=18.4m



Time evolution of the spatially averaged concentration of N for the high (top panels), medium (middle panels), and low (bottom panel) density cities. On the left there are the absolute values, and on the right the relative changes compared to the base case. Plots are from noon of the first day to noon of the second day of simulation, and the hours start from midnight of the first day. The meaning of the symbols is explained in the legend.

6. Results.

In the figure the time evolution of the absolute and relative (to the base case) concentrations are represented for all the simulations. The simulations with photocatalytic materials on the ground have the same flow as the base case, since this material does not affect the exchanges of heat and momentum between the atmosphere and the surfaces. Clearly the difference respect to the base case are during the day (since during night time, due to the lack of solar radiation, the pavements are inactive), and can reach maximum impacts between 20% and 30%, during the morning and central hours of the day. However, the time of the maximum impact of the photocatalytic pavement is not when the peak of concentration is modeled (just around sunrise). On the other hand, the presence of the trees modifies the flow. The model suggests that the presence of the trees reduces ventilation in particular during the afternoon hours, and for the case of the dense city (in this case trees are below the top of the buildings) also during the first part of the night. On the other hand, for the medium and low density cities (here the trees are above the buildings), the modification of the flow results in a decrease of the concentration during night. This effect is not due to the deposition on the leaves which is minimum during night (only cuticular, since stomata are closed). It is probably due to the reduction of the wind speed that in this case reduces also the cooling of the surfaces. The atmosphere above the city is, then, less stable and the pollutants are dispersed on a deeper layer. This type of effect is the result of a series of complex interactions between the dynamic and thermodynamic of the vegetation, and need to be confirmed by measurements, or more detailed numerical studies. In any case, the effect is quite large and has an impact on the maxima. Similarly to the case with photocatalytic materials, during the morning and central hours of the day, trees reduce the concentrations by a similar amount – and this is likely due to the deposition.

This behaviour is summarized in Table 1 below. It is clear that the photocalytic materials, at least in the results of these simulations, have no impact on the maximum, while they have a relatively small (3-4%) impact on the daily averages. On the other hand, vegetation reduces the maximum, increases the daily averages for the high density cities, and reduces the averages for the low and medium density cities.

	Maximum (Micrograms/m3 N)			Daily Average (Micrograms/m3 N)		
	High density city (16km)	Medium density city (24 km)	Low density city (40km)	High density city (16km)	Medium density city (24 km)	Low density city (40km)
Base case	168	220	199	81	92	93
Photocatalytic pavements	168	220	199	77	88	90
Vegetation (LAD=0.125)	165	202	183	89	76	80
Vegetation (LAD=0.25)	163	200	183	92	74	77
Vegetation (LAD=0.5)	161	198	183	93	71	75

Conclusions

Photocatalytic pavements have a small impact but always positive (reduction of concentration), while vegetation can have both impacts (negative and positive), and that the modification of the dispersion can be very significant. This is coherent with results from a microscale study with a CFD model (Santiago et al. 2014), that shows that the modification of the dispersion due to the vegetation, in comparison with deposition effects, can have positive or negative impact depending on the position of the vegetation and its density.

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