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

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1. 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 first is estimated in the framework of the European project LIFE MINO$_x$-STREET, from a series of laboratory and real scale experiments (section 3). The second (section 4) is deduced from literature information. The set-up of the simulations is presented in section 5, and the results are presented and discussed in section 6. Section 7 is dedicated to conclusions.

2. WRF+BEP+BEM.

The Weather Research and Forecasting model (WRF) is a prognostic, non-hydrostatic atmospheric model that can be used for many applications and among the others the study of the urban atmosphere (Chen et al. 2011). The Building Effect Parameterization (BEP, Martilli et al. 2002), used to represent the interactions between the urban areas and the atmosphere, distributes the impact of the buildings on the momentum (drag), temperature and TKE equations in several numerical layers. For the temperature equation, the heat fluxes from the buildings surfaces are estimated through the calculation of energy balances for roofs, walls, and street, where the 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, NO2, N2O5, etc.). Regardless the number of reactions that the emitted nitrogen undergoes in the atmosphere, in fact, this quantity is conserved.

3. Photocatalytic materials.

A wide variety of photocatalytic products, designed to be applied on different materials, are available on the market. In the LIFE MINOx-STREET project some of them have undergone a strict protocol, 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. For one of the most performing products that can be applied on diverse concrete pavements, and although this parameter varies as a function not only of the photocatalytic product but also of the substrate on which is applied, an average deposition velocity for NO of $v_{dep\_PHOT} = 0.005 ms^{-1}$ was estimated. This photocatalytic products 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:

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

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 NO2, and that the photo stationary state applies, something reasonable if VOC emissions are not very high (Sanchez et al. 2015, this conference):

$$NO_2 + h\nu \xrightarrow{J_{NO_2}} NO + O_3$$
$$O_3 + NO \xrightarrow{k} NO_2 + O_2$$

$$J_{NO_2} = A_j \exp\left(\frac{B_j}{\cos q}\right)$$

$$k = A_k \exp\left(\frac{-B}{T}\right)$$

Where q is the solar zenith angle, and T is the air temperature in Kelvin. A_j, B_j, A_k, and B_k, are constants equal to 1.45 10^{-2} s^{-1}, -0.4, 44.5 10^{-3} ppb^{-1} s^{-1}, and 1400 K respectively. Then it follows:

$$[O_3] = \frac{J_{NO_2}[NO_2]}{k[NO]}$$

Given that $[NO_X] = [NO] + [NO_2]$, the fraction of $[NO]$ is

$$\frac{[NO]}{[NO_X]} = \frac{J_{NO_2}}{k[O_3] + J_{NO_2}}$$

During night, when there is no solar radiation, this fraction is fixed to 0.1. So that the sink of N due to the photocatalytic pavements is:

$$S = -v_{dep\_PHOT} \frac{1}{V_{cell}\Delta z} \frac{J_{NO_2}}{k[O_3] + J_{NO_2}} [N]$$

$[N]$ is the concentration of nitrogen. A constant ozone equal to 20 ppb, considered representative of the situation very close to the emissions, is used.

4. 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 L_D 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:

$$Diss_{veg} = -b_d\, L_D\, C_{DV} \langle \overline{k} \rangle \langle \overline{U} \rangle$$

Where $\langle \overline{k} \rangle$ is the TKE, and b_d is a constant fixed to 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 $[N_{NO_2}]$ is the fraction of N that is NO2, because this is the species that is most captured by the leaves. To estimate the value of the deposition velocity v_{dep_VEG} only the canopy resistance should be 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 NO2, 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). Following Baldocchi et al. (1987) this resistance is estimated as:

$$r_s = r_{s\_\min} + b_{rs} \frac{r_{s\_\min}}{PAR}$$

We chose $r_{s\_\min} = 145.$ s m^{-1}, $b_{rs} = 22$ W m^{-2}, typical values for a tree like the Oak, and PAR is estimated as 43% of the total solar radiation. This parameterization of the stomatal resistance is not very detailed, since it does not account for other paramters like the amount of water I the soil, but it gives resistance values in the correct range. Then, $v_{dep\_VEG} = \frac{1}{R_C}$. Note that when there is no solar radiation, only cuticular resistance is active, and $v_{dep\_VEG} = \frac{1}{r_t} = 0.00005 ms^{-1}$.

Since the deposition is for NO2, the fraction of NO2 compared to NOx is computed as:

$$\frac{[NO_2]}{[NO_X]} = \frac{k[O_3]}{k[O_3] + J_{NO_2}}$$

And the sink is:

$$S = -v_{dep\_VEG} L_D \frac{k[O_3]}{k[O_3] + J_{NO_2}} [N]$$

5. Set-up of the simulations.

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.

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**

Table 1. Parameters of the three cities considered. H is the mean height of the buildings, W is the width of the street. In all the cases, the width of the buildings is 20m, and there is no vegetation fraction (intended as parks) in the city.

The day of simulation is the 21st of June, at latitude 45^o North, the simulations starts at 6am, and last for two days. Results between noon of the first day and noon of the second day are considered. Initial and geostrophic wind speed is 5 m/s, the conditions where highest peak of concentration can be expected. 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}.

6. Results.

In figure 1 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.

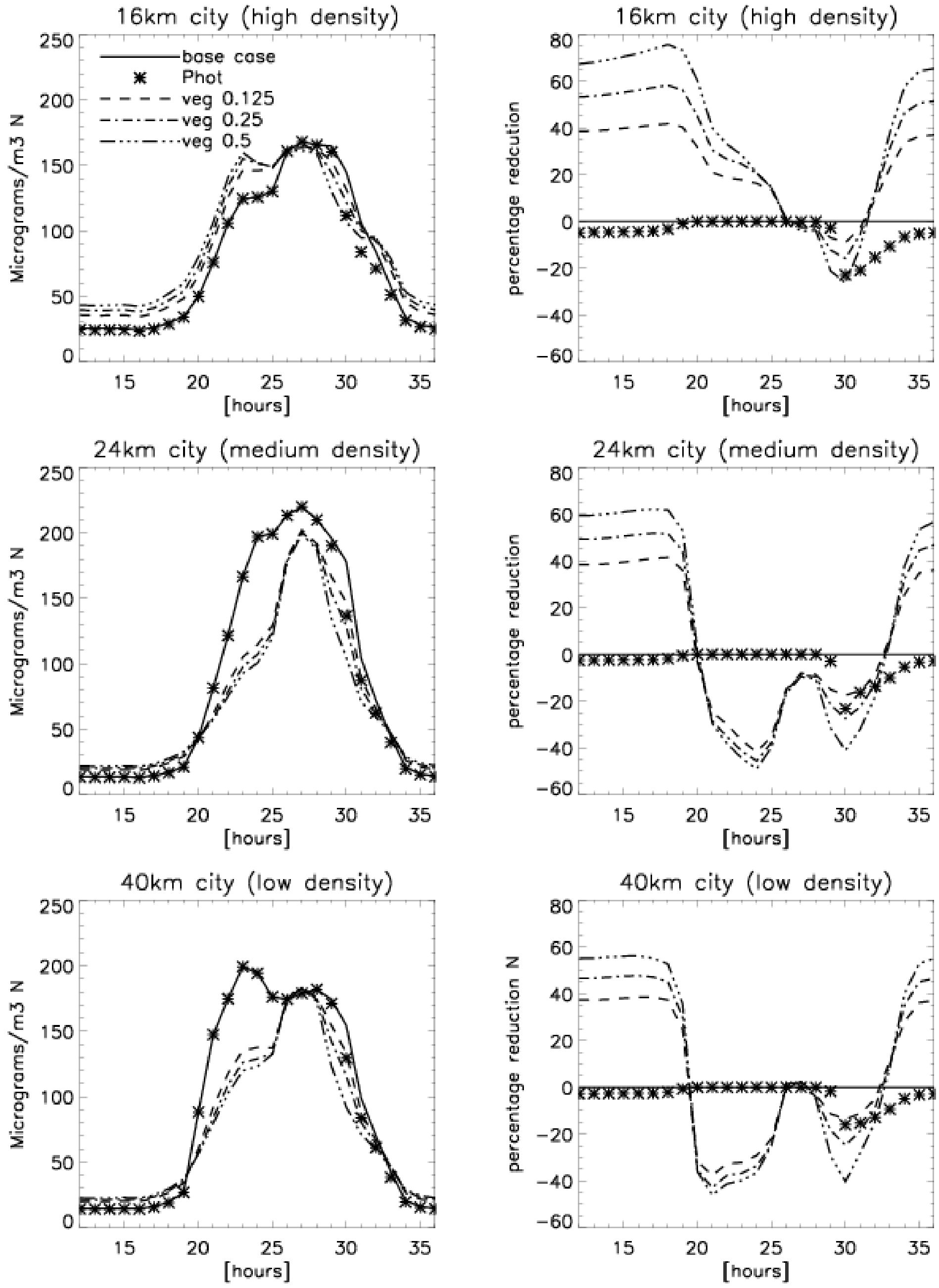

Figure 1 Time evolution of the spatially averaged concentration of N for the high (top panels), medium (middle panels), and low (bottom panel) density cities. On the left there are the absoloute values, and on the right the relative changes compared to the base case. Plots are from noon of the first day to noon of the second day of simulation, and the hours start from midnight of the first day (e. g hour 30 is 6am of the second day). The meaning of the symbols is explained in the legend.

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

Table 1. Maximum and daily averaged values for all the simulations.

7 Conclusions.

A series of idealized 2D simulations have been performed to evaluate the impact on the concentration of N of the use of phtocatalytic pavements and vegetation (street trees) at city wide scale. The main points that can be derived from this study are:

1) The use of photocatalytic pavements at the city scale can result in a decrease of the spatially averaged concentration of N of up to 20-30% during the late morning and central hours of the day. However, these are not the hours of maximum concentration. The impact on the peak, usually attained during the early morning, is very small, and the daily average can be reduced by 3-4%.
2) The inclusion of the trees affects both the flow (e. g. the dispersion) and the deposition. Simulations results seem to indicate that trees can have a negative (e. g. increase of concentration) impact during some hours of the day (in particular afternoon by reducing the ventilation), or a positive impact in different periods, for example during the night (reducing the stability, so increasing the dispersion). These phenomena are the result of complex interactions between different mechanisms (thermal and dynamical), and must be taken with care, since the model is not fully tested for this type of conditions, among the others because lack of experimental data. Moreover, the impact of vegetation on radiation (particularly complex but relrevant, Krayenhoff, et al. 2014) is not considered, and it is left for future work. It is one of the aims of this work to generate the background to motivate new field experiments or detailed numerical simulations with microscale models that can be used to validate and improve the model. On the other hand, in the late morning the impact on concentration, (likely due to the deposition on the leaves) is of similar magnitude than the one produced by the phtocatalytic pavements.
3) As a general conclusion, it can be said that 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.

These findings must be considered as an indication of the relative importance of different mechanisms, and can be used as guidance for future studies. Simulations over real cities and with full chemical mechanisms will be needed to confirm them.

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