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CFD MODELLING OF EFFECTS ON NO_X CONCENTRATION OF PHOTOCATALYTIC MATERIALS APPLIED TO A SIDEWALK PAVEMENT AND A BRICK WALL IN A REAL STREET CANYON

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Abstract: Nowadays, urban air pollution is an important environmental problem and it is mostly dominated by traffic emissions of reactive pollutants like nitrogen oxides (NOx). Currently, photocatalytic materials are being researched as a possible solution to reduce NOx concentrations in urban areas. These materials are activated in the presence of sunlight and act as a sink of NO concentration in air. However, even if the behavior of the photocatalytic materials has been studied extensively in controlled laboratory conditions, the efficiency in real urban areas is still matter of debate. Within the framework of LIFE-MINOx STREET project, the efficiency of these materials applied on different surfaces is analyzed in outdoor conditions. In this study, the effects on NO concentration of a photocatalytic material applied over a brick wall and sidewalk pavements of a real street canyon are studied using a Computational Fluid Dynamic (CFD) model. To achieve this purpose, the reactive pollutant dispersion is modelled taking into account the chemical reactions using the photostationary state. The NO deposition is modelled by means of a sink of NO in the transport equation using a deposition velocity for each material according to laboratory experiments. Finally, the reduction of NO due to the photocatalytic material is analyzed in several scenarios and its reduction effect is also evaluated. Therefore, the decrease of NO concentration due to photocatalytic material is studied comparing the simulations with and without deposition on this material under the same meteorological conditions. The simulation results are evaluated against field measurements carried out in the real street canyon (see poster Pujadas et al. (2017))

Key words: *Photocatalytic material, air pollution abatement, CFD model*

1. INTRODUCTION

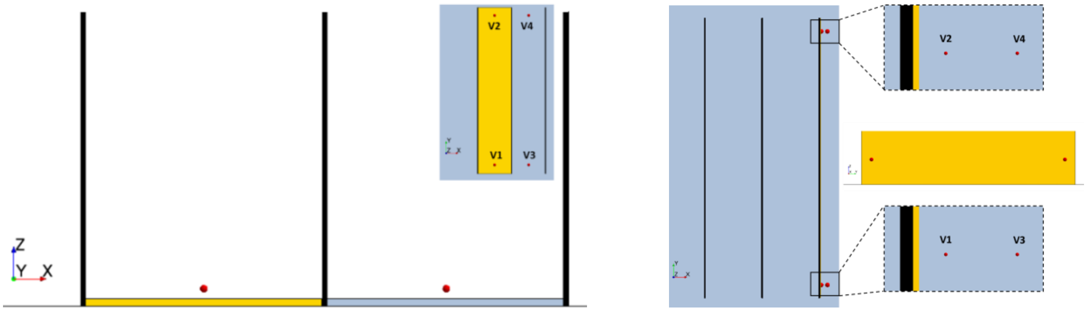
In the last decade, photocatalytic materials are being studied as a possible solution to reduce nitrogen oxides (NOx) concentrations in urban areas. Photocatalytic TiO_2 materials are activated in the presence of sunlight and act as a sink for the NOx concentration in urban air. While the behavior of the photocatalytic materials has been studied extensively in controlled conditions in laboratory, the study of its efficiency in real urban areas is still a huge challenge.

In the framework of the LIFE MINOx-STREET project, two full-scale street-canyons are created to study the depolluting effect of photocatalytic materials applied to several surfaces in outdoor conditions. These two consecutive street canyons were built in an urban area to experimentally study the deposition effect by comparing one street with each other, where just in one street the photocatalytic material is applied (see Pujadas et al., 2017, poster H18-168). The continuous variation of the wind direction hinders to quantify the NO reduction of the photoactive street concerning the other. With the purpose of complementing the experimental results, the NO deposition effect derived from these materials is simulated for several wind directions in the street canyon by a computational fluid dynamics (CFD) model. In addition, the NO sink over several photocatalytic surfaces is evaluated over time changing the atmospheric conditions.

2. CASE DESCRIPTION

2.1. Location and experimental data

The experimental system consists of two consecutive street-canyons formed by three walls of 0.1mx20mx5m separated 4 m from each other. The photocatalytic effect is evaluated in sidewalk and facade separately in two experimental campaigns. In both campaigns one reference point out of the street canyons registered the meteorological data and the background concentration of NO, NO_2 and O_3. For the sidewalk case, the left street is covered by the photocatalytic material (yellow area, Fig. 1a). And as far as the facade, the photocatalytic material is implemented on the right face of the right street canyon (yellow area, Fig. 1b). In regard to the NO and NO_2 concentration measured within the street canyon, the experimental deployment consists of four lines at 0.3 m (V1, V2, V3 and V4) which registers the NO and NO_2 concentration. The placement of these air sampling points for each experimental campaign is shown in Fig 1. More details about the experimental campaigns in Pujadas et al. (2017).

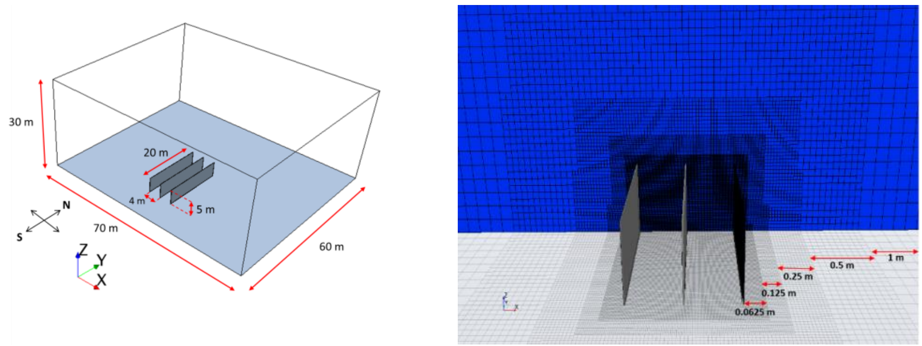


(a) (b)

Figure 1. Overview of the experimental deployment of: (a) The sidewalk case, where V1, V2, V3 and V4 are located at 0.3 m above ground and (b) the facade case, where V1 and V2 are at 0.08 m and V3 and V4 at 0.4 m from wall, all of them at 2.5 m above ground. The yellow area represents the photoactive coating.

2.2. CFD Model Description

The CFD model used is based on the Reynolds-averaged Navier-Stokes equations with the k-ε realizable turbulence closure. The domain size is 70mx60mx30m and the streets canyons (20mx5mx0.1m) are located at 10 m from the inlet. The trimmer mesh used increases progressively its size from 0.1 m around the streets canyons to 2 m in the boundaries. The total mesh has 6 million of grid points.

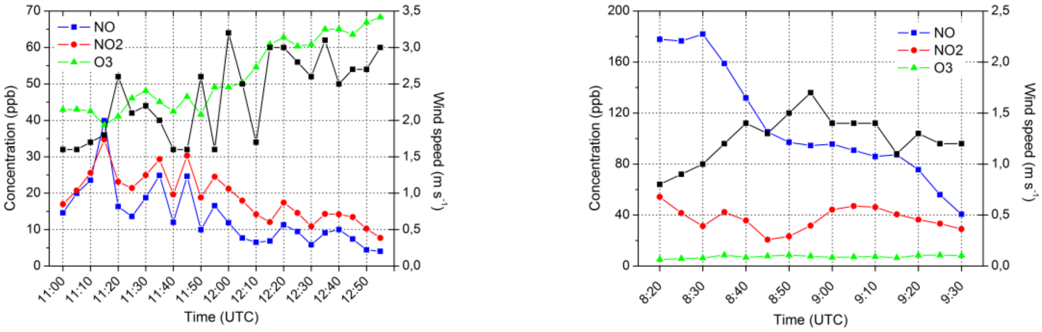


(a) (b)

Figure 2. (a) Computational domain and (b) the trimmer mesh used.

The two simulations, one for each experimental campaign, are performed in unsteady conditions with 1s of time step. Neutral atmospheric conditions are assumed for the three wind directions selected: S, SE and SW. Apart from the wind direction which is constant in time, the inlet conditions are changing every 5 min based on the experimental data at the reference point.

The vertical profiles of wind speed, turbulent kinetic energy and turbulent dissipation rate are imposed at inlet assuming neutral atmospheric conditions by the logarithmic equations, and NO, NO_2 and O_3 concentrations are spatially uniform at the inlet (Fig. 3). The chemical reactions are modeled by the NO_x-O_3 photostationary state (Sanchez et al., 2016), and the chemical rate constants are computed in based on the zenith angle and the air temperature. The NO deposition due to the photocatalytic material is modeled as a NO sink by means of $F_{dep}= -V_d \cdot NO$. From the laboratory tests, the deposition velocity (V_d) of the photocatalytic material applied to the sidewalk is $10.1 \cdot 10^{-3}$ m s^{-1} and for the facade is $3.57 \cdot 10^{-3}$ m s^{-1}.



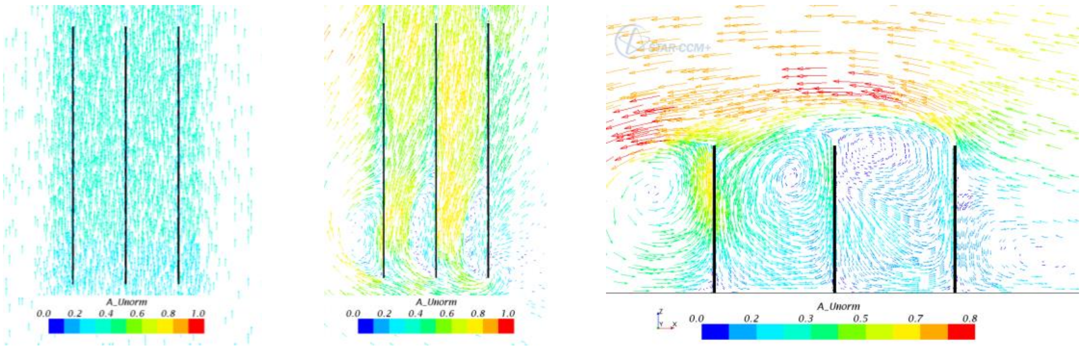
(a) (b)

Figure 3. Time series of wind speed, NO, NO_2 and O_3 concentration for (a) the sidewalk case and (b) the facade case.

3. EFFECTS OF PHOTOCATALYTIC MATERIALS IN A REAL STREET CANYON

3.1. Flow Pattern

To analyze the influence of the wind direction on the analysis of the NO deposition, three wind directions are studied: S, SE and SW (not shown). Figure 4 depicts the flow pattern of the normalized wind speed for the cases S and SE. In the S case, the wind blows parallel to the street-canyon and both streets can be considered equivalent, in contrast in the SE case the non-parallel wind induces eddies in the street that change the pattern from one street to the other.

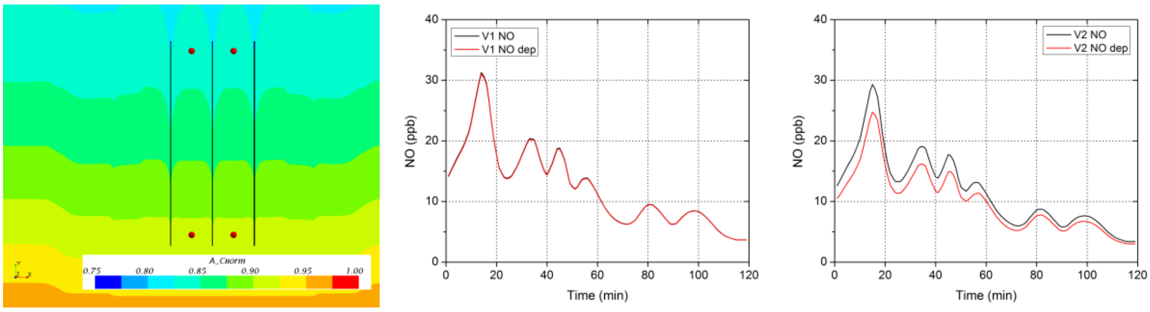


(a) (b) (c)

Figure 4. Horizontal section of the flow pattern at 3 m for the wind direction: (a) South and (b) South-East. (c) Vertical section at the middle of the street-canyon for the South-East case.

3.2. Photocatalytic effect over sidewalk pavement

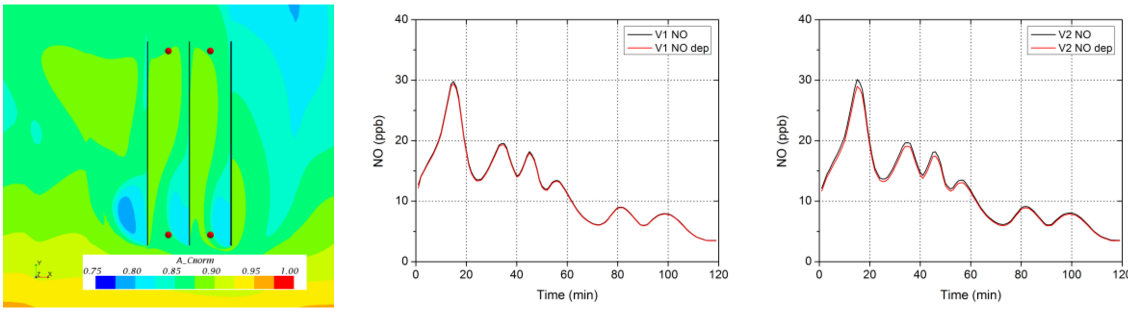
The modelling of the sidewalk surface case is carried out with the boundary conditions recorded from 11UTC to 13UTC on 21th May, 2016. As for the wind direction, due to its large variability and thus the difficulty in quantifying the photocatalytic effect from experimental data, the wind direction is fixed from S or SE during that time in the CFD simulation. Two simulations are performed for each wind direction, with and without NO deposition over the photocatalytic surface. Figure 5a shows the distribution of the normalized concentration (C_N=C/C_{inlet}) for South wind direction where the horizontal gradients are due to the chemical reactions over time. Figure 5.b-c displays the time series of NO concentration with and without deposition (hereafter NO and NO_{dep} respectively) over the photocatalytic coating in the experimental points located on the photoactive street at 0.3 m (V1 and V2). At the beginning of the street, the flow crosses few meters over the photocatalytic surface and for that, the deviation of the NO concentration is barely significant in V1. However, the results in V2 displays a slightly decrease of NO_{dep} respect to the NO and it is variable over time. It is worth mentioning that the deposition effect is also related to the wind speed and the background concentration, thus lower wind speed and greater NO concentration entail larger NO deposition since the residence time close to the photocatalytic coating increases. Assuming that the wind blows from S for 2 h, the maximum value registered is a reduction of 17.5% from NO at V2 and in time average is 0.64% in V1 and 14.24% in V2.



(a) (b) (c)

Figure 5. (a) Horizontal section (z=3m) of the normalized concentration (C_N=C/C_{inlet}). (b-c) NO and NO_{dep} in experimental lines (b) V1 and (c) V2 at 0.3 m above ground.

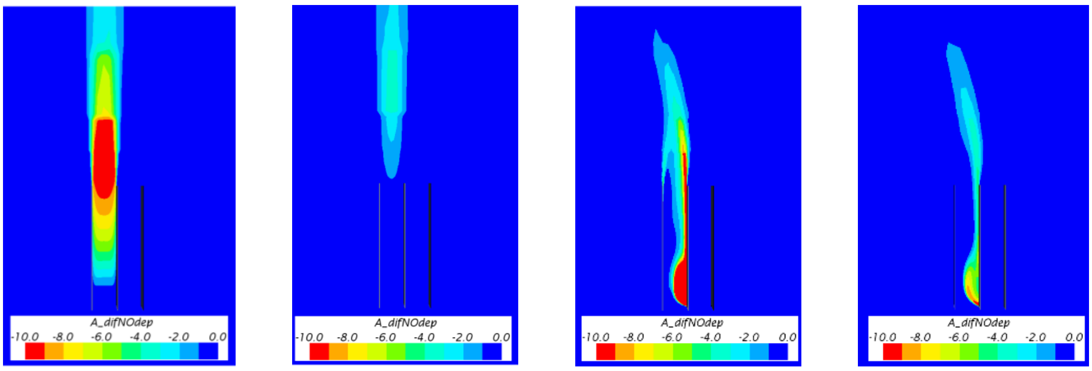
In the SE case, the distribution of pollutants is different in one street from the other (Fig. 6a). Figure 6 b-c shows the slight differences captured at the measurements points due to the change on the flow pattern and consequently, to the eddies formed in the street. Focusing on the deviation of NO_{dep} from NO simulated, there is barely difference in both points registering the maximum values of 1.23% in V1 and 3.14% in V2. For that reason, the variation of wind direction hinders to capture experimentally the NO deposition in outdoors conditions.



(a) (b) (c)

Figure 6. (a) Horizontal section (z=3m) of the normalized concentration (C_N=C/C_{inlet}) without deposition. (b-c) NO and NO_{dep} in experimental lines (b) V1 and (c) V2 at 0.3 m above ground.

To observe the change of the location of the maximum deposition in base to the flow pattern, the map of the deviation δNO_{dep} ((NO_{dep}-NO)/NO·100) for the S and SE wind direction is displayed at several heights (Fig. 7). For S wind direction at 0.5m above ground (Fig. 7a), the area affected by the NO deposition covers the major part of the photoactive street and it leaves a trail out of it. In contrast for SE at 0.5 m (Fig. 7c), the maximum area of difference is located in the vortex created in the street. That variation of the flow produces that the deposition effect at the measurements points is not captured. In regard to the vertical effect, in both cases at 1.5 m, the photocatalytic effect is reduced below 9% as well as the area affected. Therefore it displays that its influence is just discernible close to the ground.

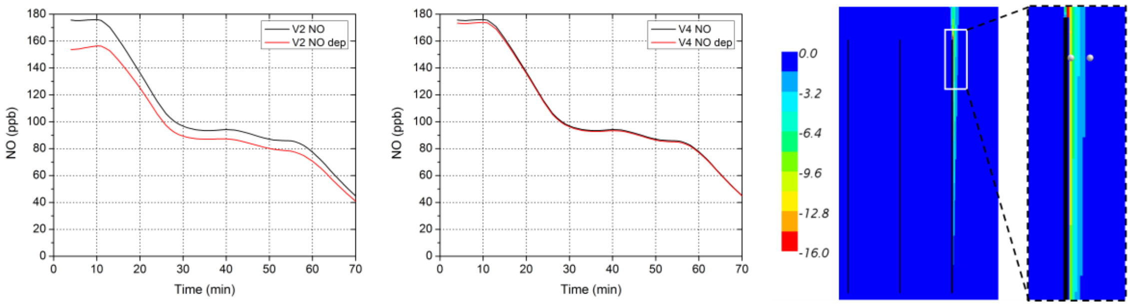


(a) (b) (c) (d)

Figure 7. Horizontal section of δNO_{dep} for S wind at (a) 0.5 m and (b) 1.5m and for SE wind at (c) 0.5 m (d) 1.5m

3.3. Photocatalytic effect over brick wall

The CFD simulation is performed from 0820 to 0930 UTC on 16th November, 2016. In the facade case, the maximum differences by deposition are obtained for the S wind direction. Figure 8 shows the time series of NO and NO_{dep} at V2 and V4. The maxima of δNO_{dep} obtained in V1, V2, V3 and V4 are respectively 0.6%, 12.5%, 0.004% and 1.3%, which corresponds to the first minutes where the NO concentration is high and the wind speed low. These conditions benefit the NO deposition over the photocatalytic coating because of increasing the residence time of NO close to the wall. If we analyzed the time average assuming S wind direction is fixed for 70 min, the average of δNO_{dep} at V2 is 8.6% whereas at V4 is just 0.9%. It concludes that the reduction effect of NO is only registered in points close to the wall. It is proved by a horizontal section of the δNO_{dep} (Fig. 8c) where the area obtained is confined near to the facade and the values are below 10% (Fig. 8d).



(a) (b) (c) (d)

Figure 8. (a-b) Time series of NO and NO_{dep} at (b) V2 and (c) V4. (c) Horizontal section of δNO_{dep} at 2.5 m and (d) zoom in V2 and V4 of δNO_{dep} at 2.5 m.

In regards to the experimental values, there is a long period with south component of wind direction. It is divided in two cases without the photocatalytic effect because there is not solar radiation and the period simulated with enough solar radiation to the photocatalytic process. Without deposition, the time average of the ratio NO_{V2}/NO_{V4} is 1, instead with NO deposition that ratio drops to 0.909 in the experimental case and 0.917 with the modelling results.

CONCLUSIONS

This study focuses on evaluating the NO deposition effect over the photocatalytic material applied on sidewalk pavement and over a brick wall in a full-scale street canyon based on experimental campaigns carried out there. In both experiments, the NO decrease is found very close to the photocatalytic surface and its effect decreases on moving away from the photoactive coating. Despite of the high deposition velocity of the sidewalk pavement the relative differences of reduction are small and very dependent on the wind speed and direction and therefore the turbulence produced in the streets. The main conclusion drawn from these results is that the atmospheric conditions favorable to the NO deposition over the photocatalytic coating are low wind speeds and high pollutants concentrations near to the surface. In any case, to establish a guideline about the atmospheric conditions in which the photocatalytic effect is significant is really complicated since it is closely related to many meteorological variables where the atmospheric turbulence also plays an important role.

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