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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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.

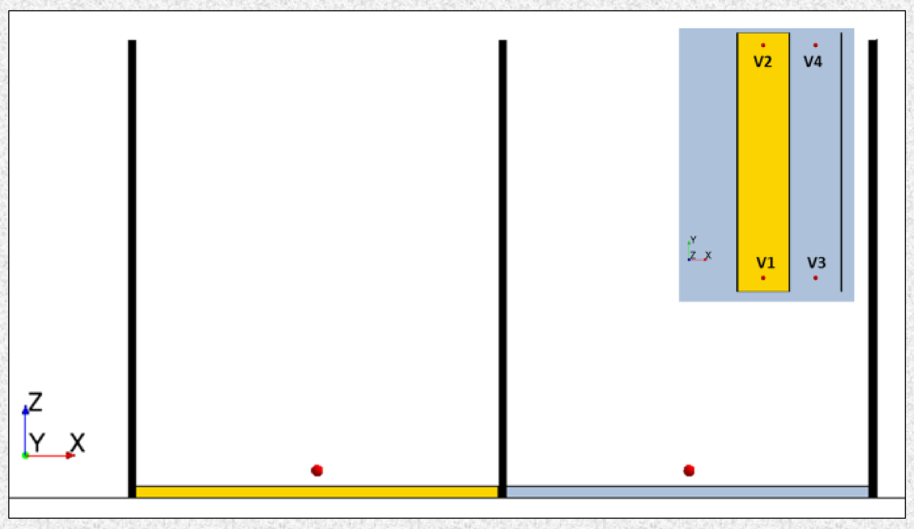
In the framework of the LIFE MINOx-STREET project, two full-scale street-canyons are created to study the depolluting effect of photocatalytic materials applied to several surfaces in outdoor conditions. These two consecutive street canyons were built in an urban area to experimentally study the deposition 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 objective of this work is to simulate the NO deposition effect induced by the photocatalytic materials for specific wind directions in the full-scale street-canyon through a Computational Fluid Dynamics (CFD) model.

LOCATION AND EXPERIMENTAL DATA

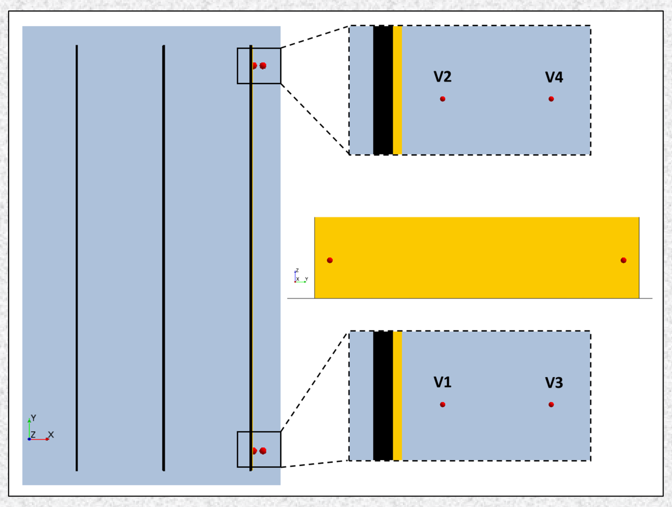
- Reference point out of the street-canyons (SC) at 3m:
  Wind speed and direction, temperature NO, NO_2 and O_3
- Measurement points in the SC: V1, V2, V3 and V4 → **NO and NO_2**
- Yellow area represent the photocatalytic surface

Sidewalk Pavement

- All points at 0.3 m above ground level (AGL)



Facade

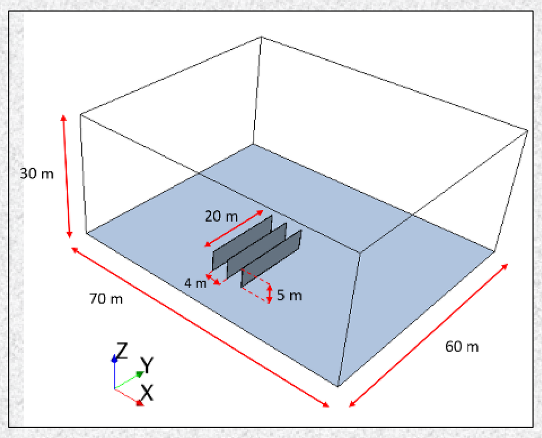


From wall:
- V1 and V2 at 0.08 m
- V3 and V4 at 0.40 m

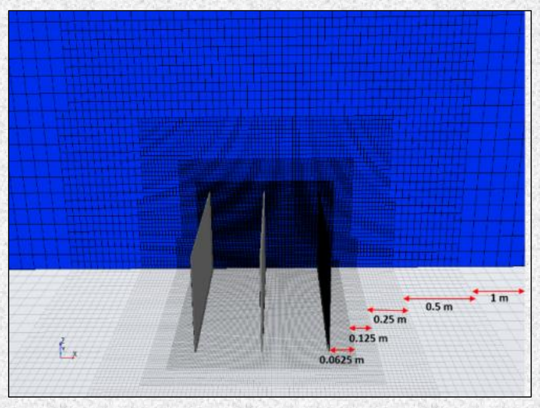
More detail about the experimental campaign in poster H18-168.

CFD MODEL DESCRIPTION

Geometry and Mesh



- Domain: 70 m x 60 m x 30 m
- SC size: 0.1 m x 20 m x 5 m
- Width: 4

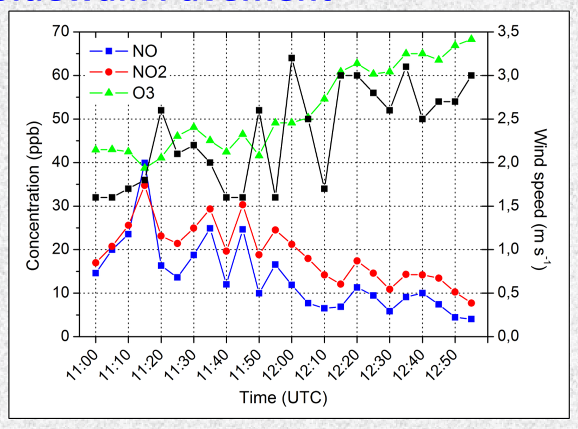


- Trimmer mesh
- Grid resolution: From 0.0625 to 2 m
- Total grid points: $6 \cdot 10^6$

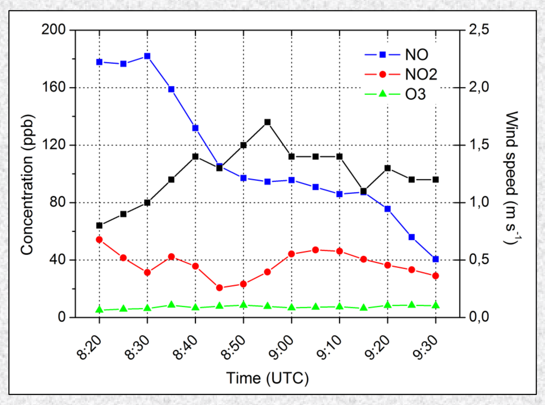
Simulation setup

- CFD-RANS model: Unsteady simulations
- Neutral atmospheric conditions
- $NOx\text{-}O_3$ photostationary state (Sanchez et al., 2016)
- Deposition Flux: $F_{dep} = -NO \cdot V_d$
- Inlet conditions from reference point
- Deposition velocity for the material applied on:
  - Sidewalk pavement: $10.1 \cdot 10^{-3}$ m s^{-1}
  - Facade: $3.57 \cdot 10^{-3}$ m s^{-1}

Sidewalk Pavement



Facade

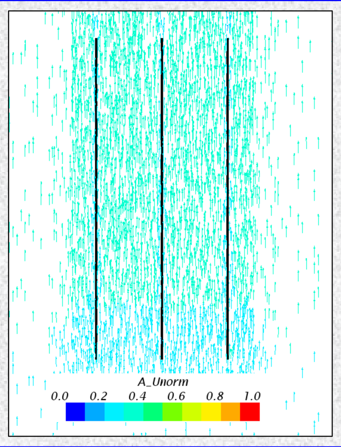


FLOW PATTERN

The flow pattern of the normalized wind speed for the cases S and SE

South wind direction

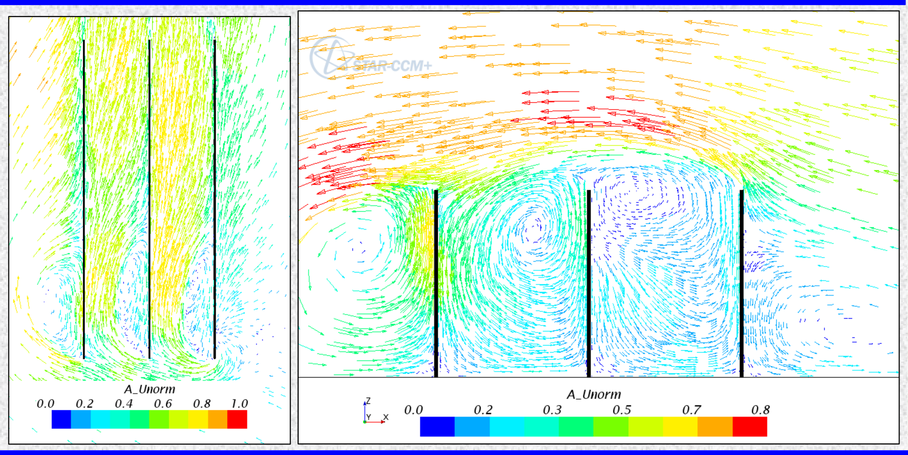
In the S case, the wind blows parallel to the street-canyon and both streets can be considered equivalent.



South-East wind direction

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.

The flow pattern for South-West is symmetric to the SE.

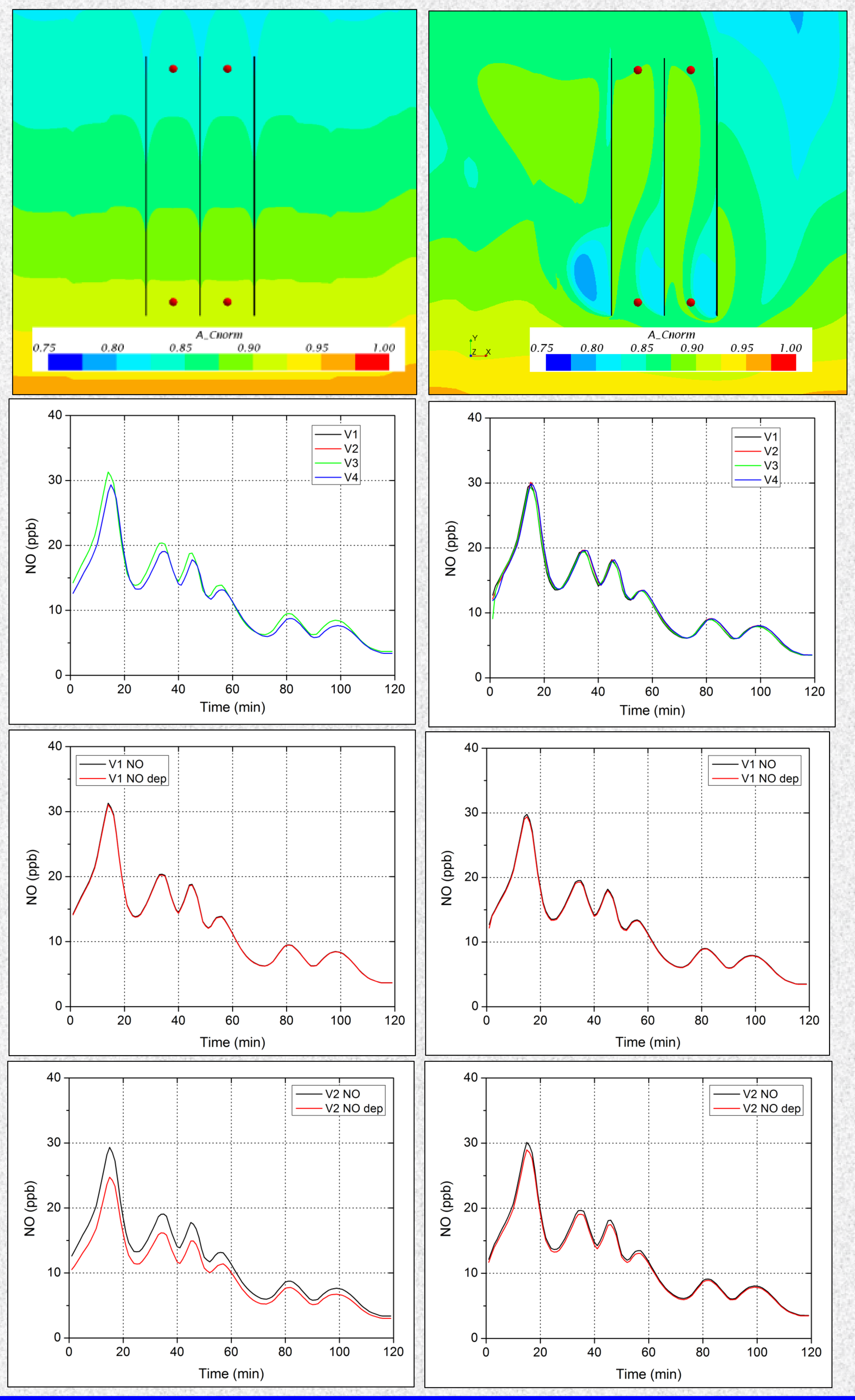


SIDEWALK PAVEMENT

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, SE or SW during that time in the CFD simulation. Two simulations are performed for each wind direction, with and without NO deposition, NO and NO_{dep} respectively, over the photocatalytic surface.

$$\delta NO_{dep}\,(\%) = \frac{(NO_{dep} - NO)}{NO} \cdot 100$$

South wind direction **South-East wind direction**

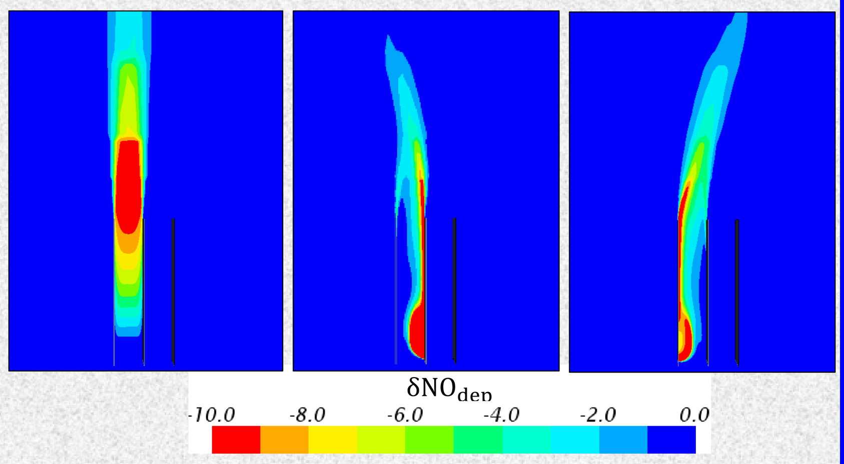


- Slight differences in the measurements points
- For SE direction: the maximum reduction are around 2 % in V1 and 4 % in V2
- For SW direction: the maximum reduction are around 5 % in V1 and 7 % in V2
- For S direction:
  - At V1: Insignificant difference of NO from NO_{dep}
  - At V2: the maximum reduction is 17.5%
  - In average: δNO_{dep} is 0.6 % in V1 and 14 % in V2

Horizontal section of δNO_{dep} for S, SE and SW

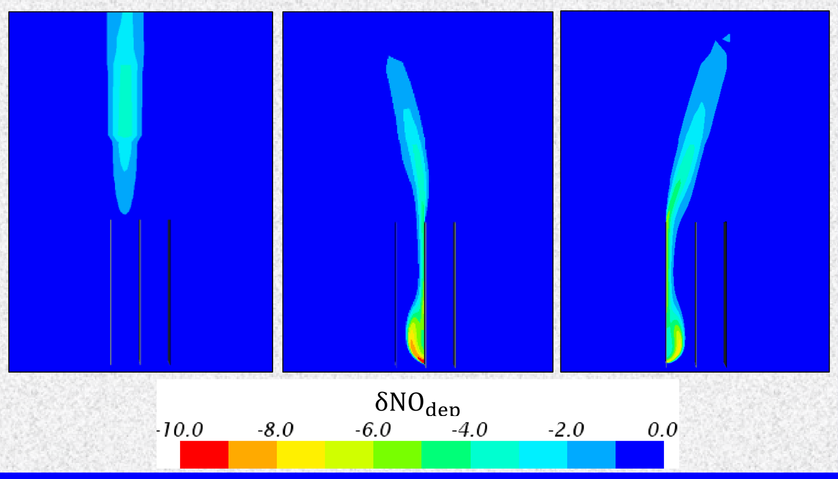
At the time of the maximum difference:

At **0.5 m** AGL: For S: The area affected by the NO deposition covers the major part of the photocative street and it leaves a trail out of it. In contrast for SE, the maximum area of difference is located in the vortex created in the street, as in the case of SW direction.



At **1.5 m** AGL: In regard to the vertical effect, the photocatalytic effect is reduced below 9% as well as the area affected.

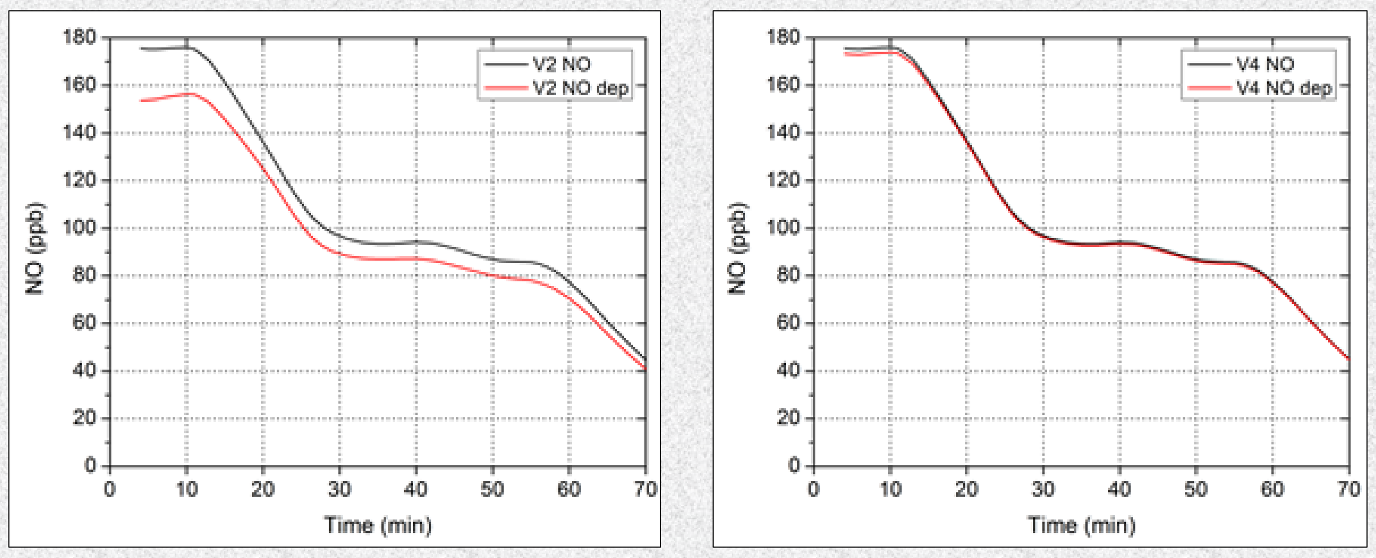
Therefore it displays that its influence is just discernible close to the ground.



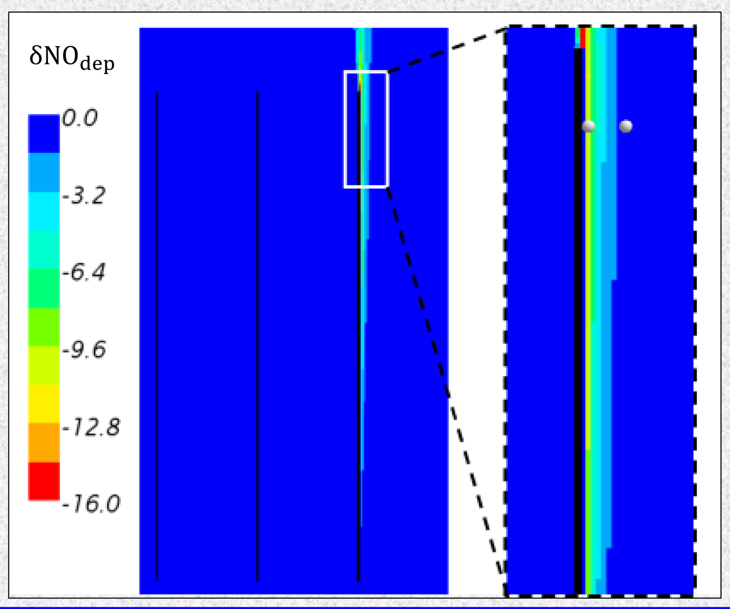
FACADE

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 direction

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.
- 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.
- Horizontal section of δNO_{dep}: The area obtained is confined near to the facade and the values are below 10%
- As for the experimental values, a long period with south component of wind direction is selected. Without deposition, the time average of the ratio NO_{V2}/NO_{V4} is 1 either from the measurements or from modelling. Instead with NO deposition that ratio drops to 0.909 in the experimental case and 0.917 with the modelling results.



CONCLUSIONS

From these results the main conclusions obtained are:

- Lower wind speed and greater NO concentration benefit the NO deposition since the residence time close to the photocatalytic coating increases.
- The NO decrease is found very close to the photocatalytic surface and its effect decreases on moving away from the photoactive coating.

Therefore, 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.

References

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- Sanchez, B., Santiago, J.-L., Martilli, A., Palacios, M., Kirchner, F., 2016. CFD modeling of reactive pollutant dispersion in simplified urban configurations with different chemical mechanisms. Atmos. Chem. Phys. 16 (18).

Acknowledgements

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