CFD Modelling of Reactive Pollutants Dispersion and Effect of Photocatalytic Pavements in a Real Urban Area

B. Sanchez(1), JL Santiago(1), A. Martilli(1), M. Palacios(2), M. Pujadas(2), L. Nuñez(2), M. German(2), J. Fernandez-Pampillon(3) and J.D. Iglesias (4)

(1) Atmospheric Pollution Modelling, Air Pollution Division, CIEMAT, Madrid, Spain
(2) Atmospheric Pollution Characterization and POC, Air Pollution Division, CIEMAT, Madrid, Spain
(3) National University of Distance Education (UNED), Madrid, Spain
(4) Alcobendas City Council, Madrid, Spain

Outline

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2. **Experimental Campaign**
3. **CFD Model Description and Set-Up**
4. **Results**
   - Evaluation of the chemical effects on pollutants dispersion with experimental data
   - Analysis of the Photocatalytic Effect
5. **Conclusions**

1. Introduction

- Exhaust gases are the main source of NO and NO_2 emissions in an urban area

Worsen of Urban Air Quality

- An accurate understanding of urban air quality requires considering the coupled behavior between dispersion of reactive pollutants and atmospheric dynamics.
- Usually, NO and NO_2 are modeled as passive tracer at microscale.

Which is the impact on NO and NO_2 concentrations by including chemical reactions in a CFD model in a real urban zone?

- The behavior of the photocatalytic materials has been studied extensively in controlled laboratory conditions and they are being considered as a possible solution to reduce NOx concentrations in urban areas.

Which is the efficiency of this material in real urban areas?

- Within the framework of LIFE MINOx-STREET Project, the efficiency of photocatalytic materials is being researched in real urban scenarios.

Main Objective: CFD Modelling of NO and NO_2 dispersion applying different chemical approaches including the NO deposition effect by photocatalytic pavement in a real urban area

1. Evaluation of the chemical effects on NO and NO_2 dispersion

Comparison with experimental measurements

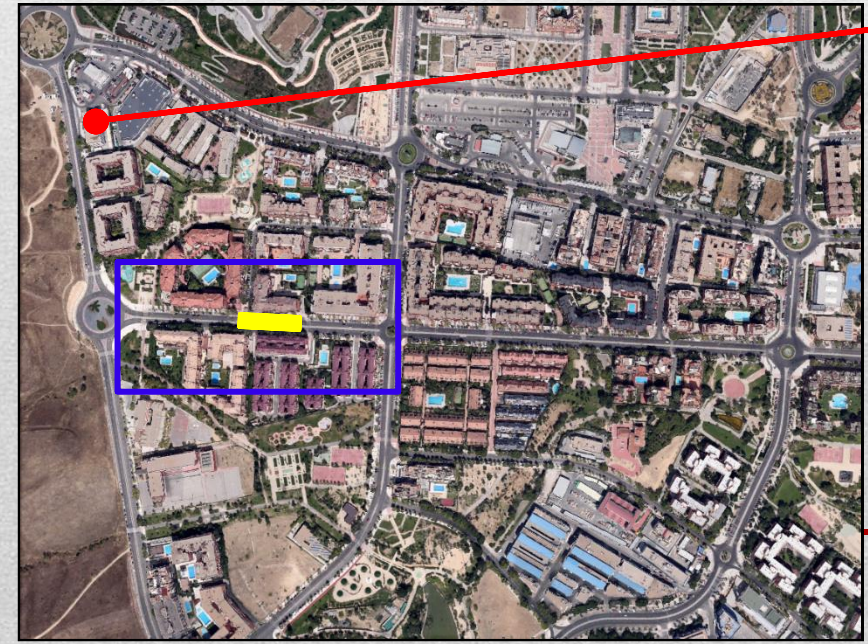
2. Analysis of the photocatalytic effect on NO concentration

2. Experimental Campaign

- Location: North of Madrid
- 25th September - 25th October → The maximum effectiveness of NO deposition by Photocatalytic Materials is obtained under specific meteorological conditions

$R > 400\ Wm^{-2}$
$RH < 65\ \%$
$U < 5\ m\ s^{-1}$

29th September, 2015 → 12.00-13.00 UTC



- Background Measurements (●) → h = 20 m, d = 300 m

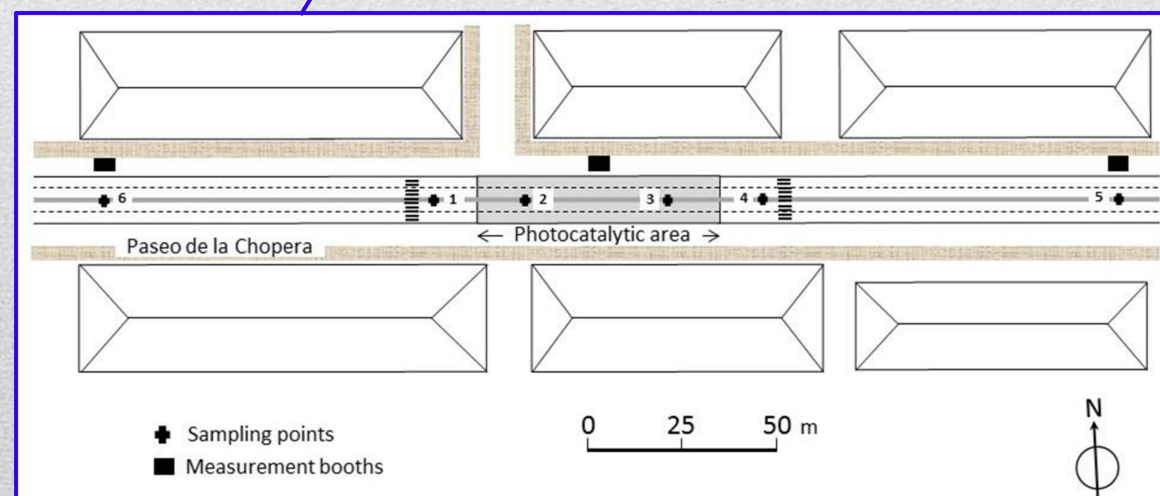
  - Wind speed and direction
  - Pollutants concentration: NO, NO_2 and O_3

In the research area:

- Photocatalytic area
  - L= 60 m
  - NO deposition: $V_d = 0.5\ cm\ s^{-1}$

Laboratory Tests

- Measurements Points
  - 6 sampling points: NO and NO_2
  - h=1m



More details in the poster session of this conference (Pujadas et al. (ID. 090))

3. CFD Model Description and Simulations Set-Up

Numerical simulations are based on the Reynolds averaged Navier-Stokes equations (RANS) with the k-ε turbulence model (STARCCM+ v9.04.011-R8)

- Domain: 1.5 km x 1 km
  - Building height ~ 20m

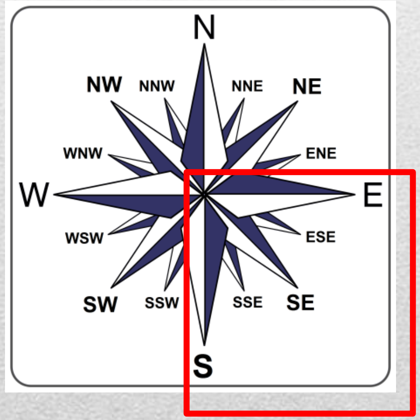
- Polyhedral Mesh
  - Out ~ 6 m
  - In ~ 2m with refine regions (<1 m)

→ $2.3 \cdot 10^6$ grid cells

CFD Model Description and Set-Up

- Unsteady state simulations
- Inlet boundary conditions from experimental data (●)
  - At roof of the building (h=20 m)
  - d=300 m
  - $\Delta t = 5min$

- Meteorological conditions → Neutral atmospheric conditions



$$u_{in}(z) = \frac{u_*}{\kappa} \ln\left(\frac{z}{z_0}\right)$$

$$k_{in} = \frac{{u_*}^2}{{C_\mu}^{1/2}}$$

$$\varepsilon_{in}(z) = \frac{{C_\mu}^{3/4} {k_{in}}^{3/2}}{\kappa\, z}$$

u_*: Friction Velocity
C_μ: Constant (0.9)
z_0: Roughness length
κ: von Karman constant (0.4)

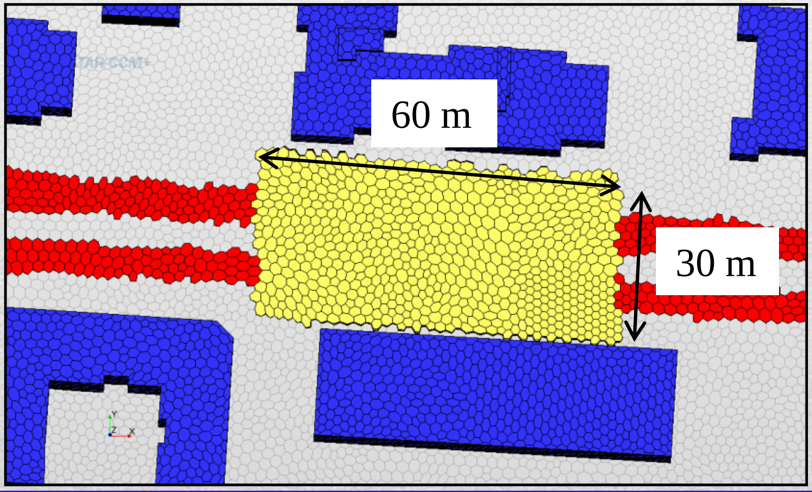
- Background concentration: NO, NO_2 and O_3 ➜

	Values range
NO	[5.06 – 6.98] ppb
NO_2	[9.16 – 11.99] ppb
O_3	[39.60 – 46.63] ppb

- Chemical approaches
  - Non-Reactive pollutants
  - Photostationary Steady State (PSS):

$$\begin{cases} \mathrm{NO_2} + h\nu \longrightarrow \mathrm{NO} + \mathrm{O} \\ \mathrm{O} + \mathrm{O_2} + \mathrm{M} \longrightarrow O_3 + \mathrm{M} \\ \mathrm{O_3} + \mathrm{NO} \longrightarrow \mathrm{NO_2} + O_2 \end{cases}$$

- Photocatalytic effect

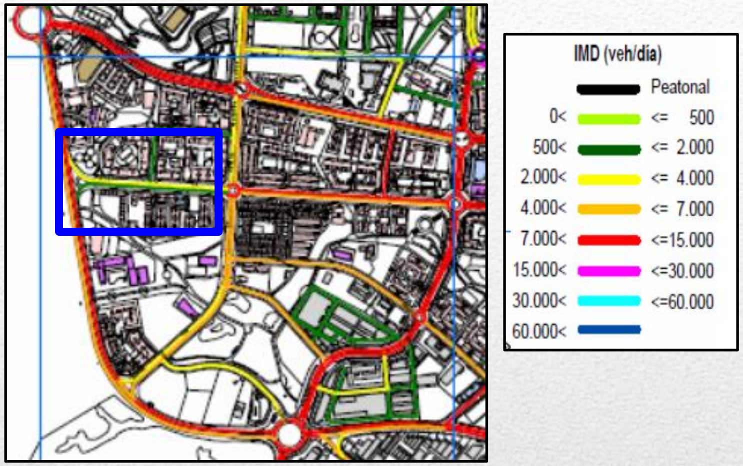


- Sink of NO: $dep_{\mathrm{NO}} = -[\mathrm{NO}] \cdot \mathrm{V_d}$
- $\mathrm{V}_{\mathrm{d},exp} = 0.5\ \mathrm{cm}\ s^{-1}$ ← Laboratory Tests

NO Transport Equation

$$\frac{\partial NO}{\partial t} + U_i \frac{\partial NO}{\partial x_j} = D \frac{\partial^2 NO}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\left(K_c \frac{\partial C_i}{\partial x_j}\right) + [\Delta\, NO]_{Chem} + S_{em} + depNO$$

- NOx Emission



- Emission Factor (EF):

Vehicle type	NOx (g/km)
Bus	3,46
Motorbike	0,13
Vehicle	0,44
Light vehicle	0,81
Heavy vehicle	1,86

  - $\mathrm{NO} + \mathrm{NO_2} = \mathrm{NO_x}$
  - Volumetric emission ratio (*): $\frac{\mathrm{NO}}{\mathrm{NO_2}} = 10$

- Within the studied area:
  - No. of vehicles
  - Vehicle type

The emission changes every 5 min

$$S_{NOx} = EF_{type\_veh} \cdot N_{veh}$$

- Outside the studied area:

$$S_{NOx}(out) = TN_{veh,RS} \frac{DTI_{out}}{DTI_{RS}} EF_{veh}$$

$TN_{veh,RA}$: Total number of vehicles in the research street
DTI_{RS}: DTI in the research street

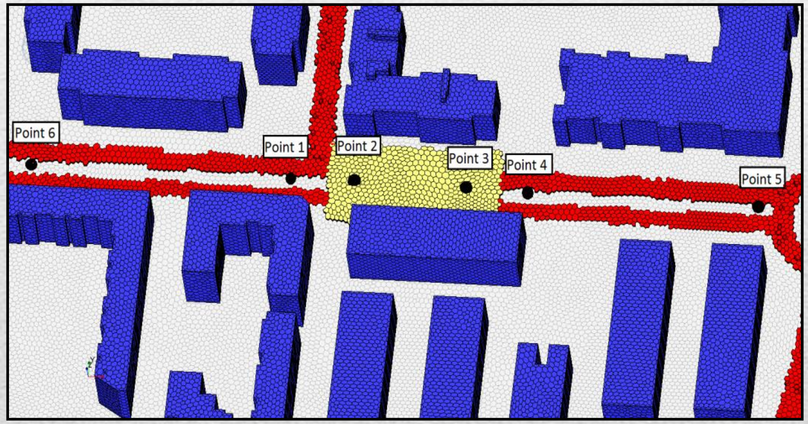
(*) Baker et al., 2004

4. Results

1. Evaluation of the simulated chemical approaches

Differences in the simulated concentration of NO and NO_2 regarded as:

- Non-reactive pollutants
- Photostationary Steady State



1.1. Spatial distribution concentration

1.2. Time series at measurements points

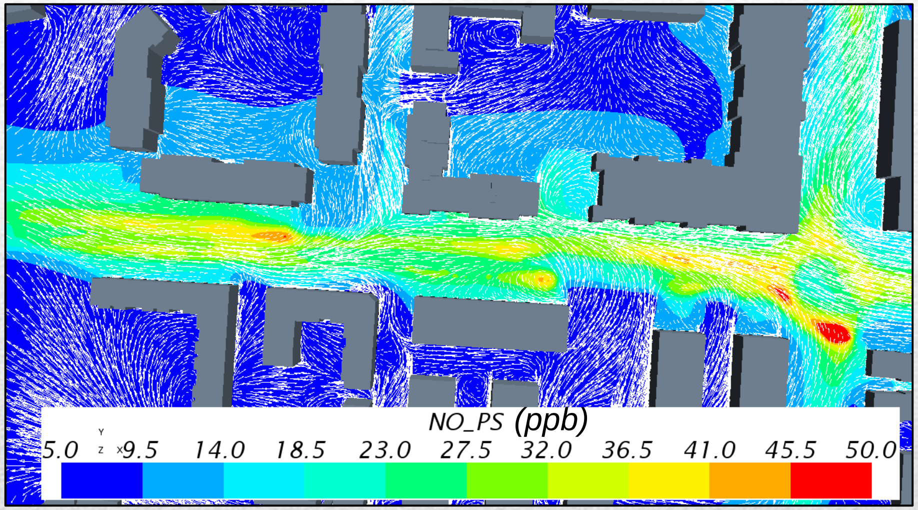
1.3. Evaluation of the time average concentration using experimental data

2. Study of the photocatalytic effect using simulation results in a real urban scenario

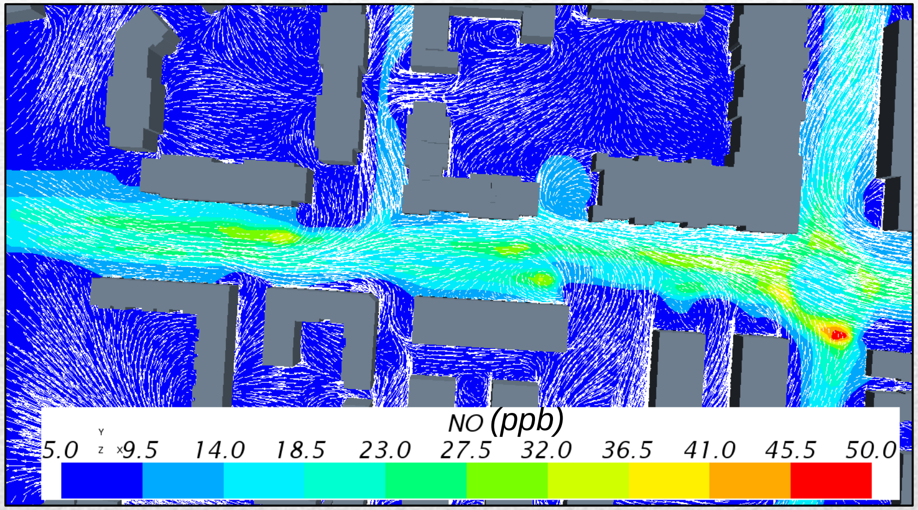
4.1. Evaluation of the simulated chemical approaches

- **Spatial distribution at h=1 m → t=60 min**

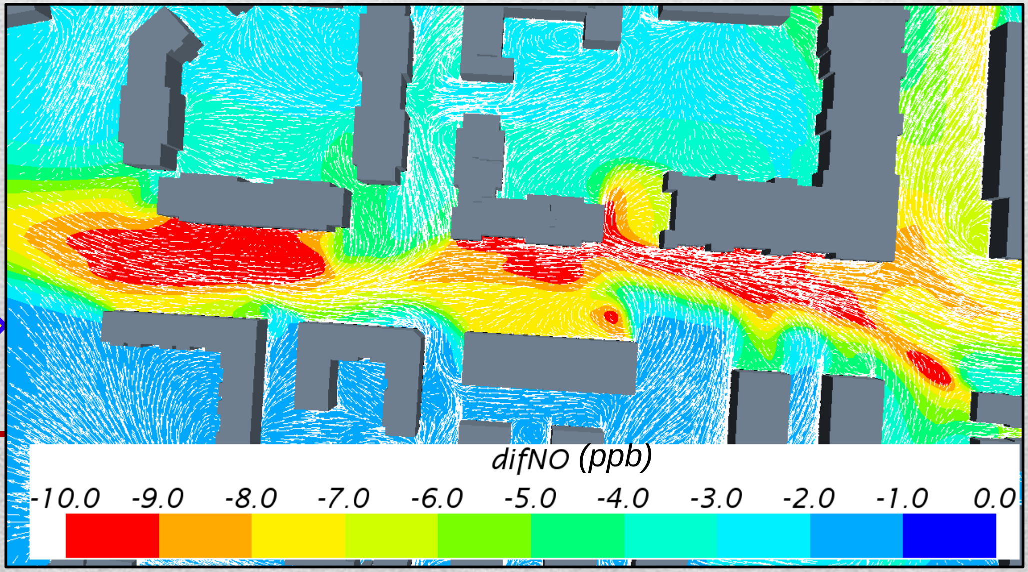
NO tracer



NO reactive

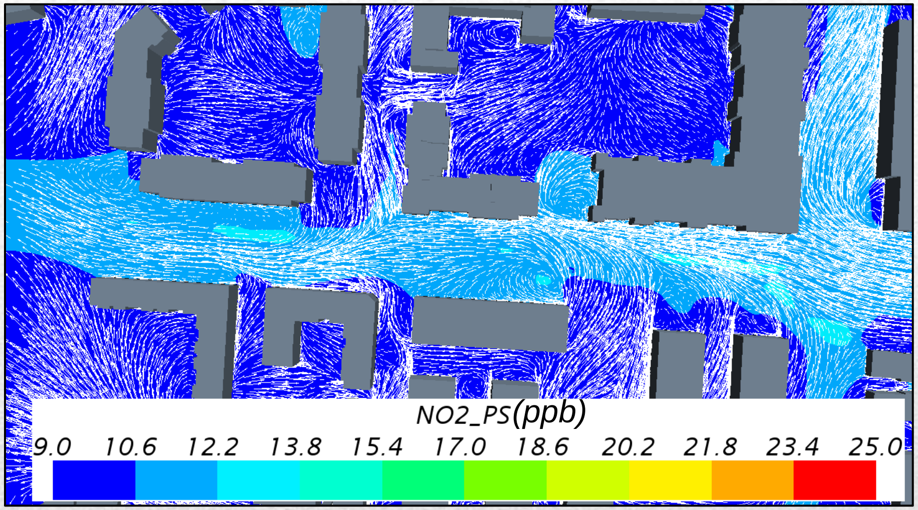


$$\boldsymbol{difNO = NO_{reactive} - NO_{tracer}}$$

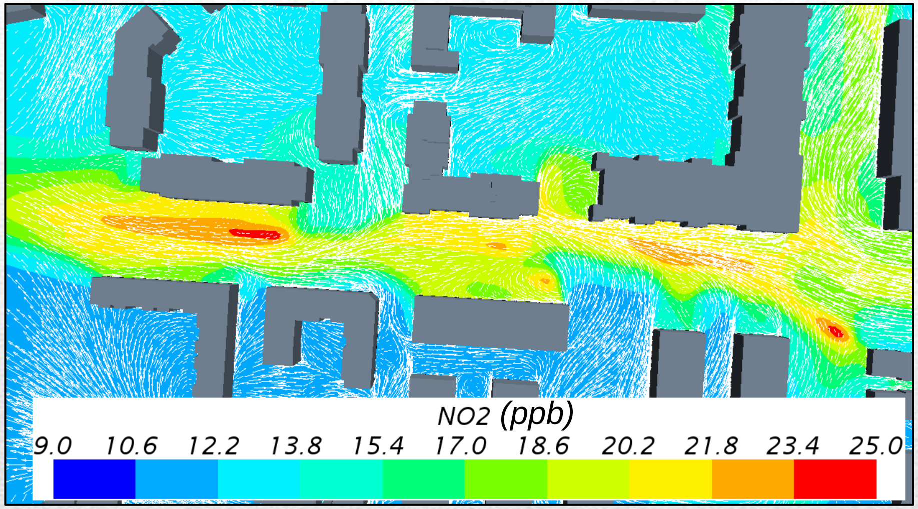


- Spatial distribution at h=1m → t = 60 min

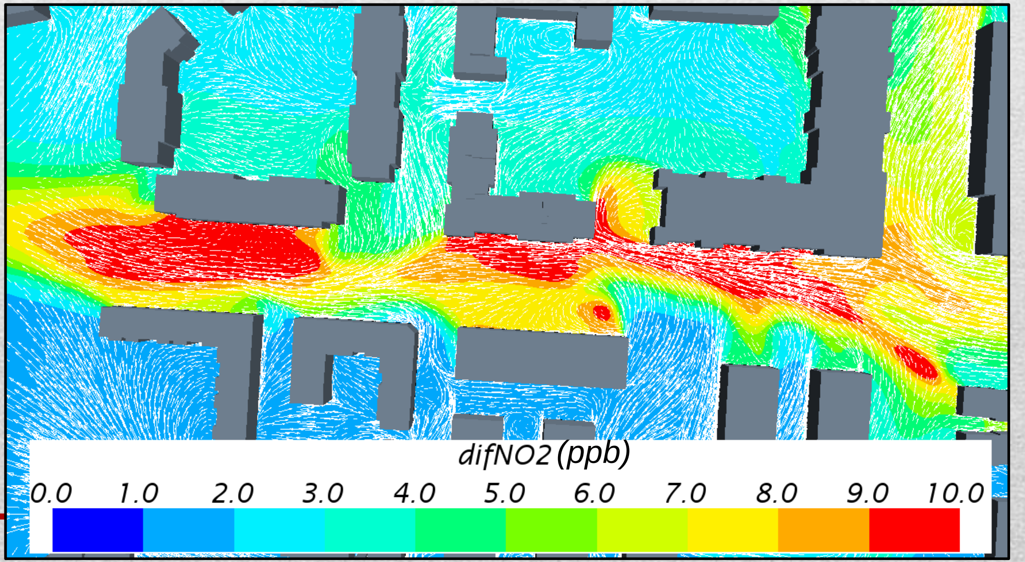
NO$_2$ tracer



NO$_2$ reactive



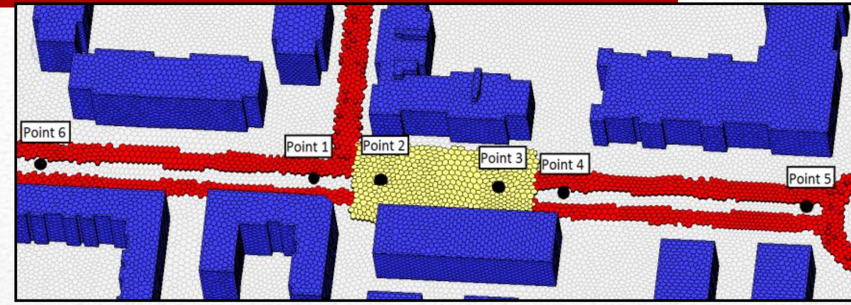
$$difNO_2 = NO_{2,reactive} - NO_{2,tracer}$$



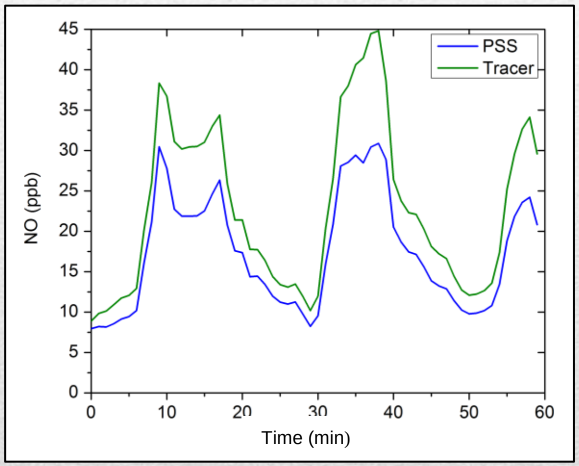
- **Time series of simulated NO**

Differences Tracer and Reactive → Location

Differences Tracer and Reactive → Atmospheric conditions



Point 1



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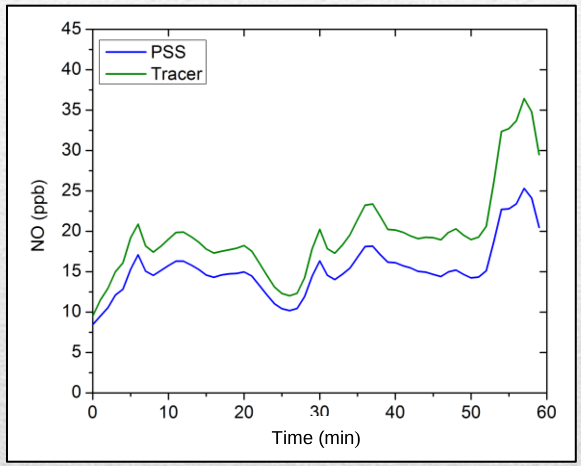

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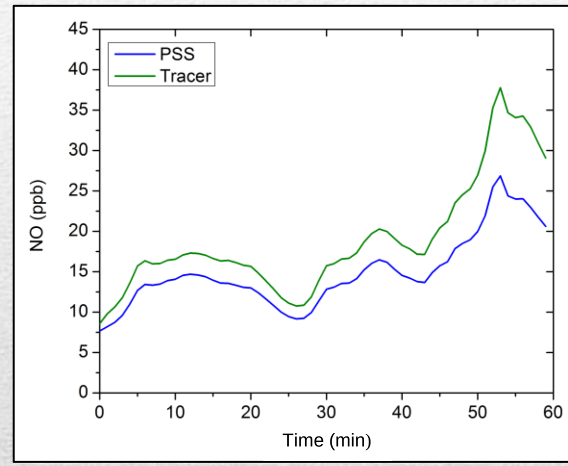

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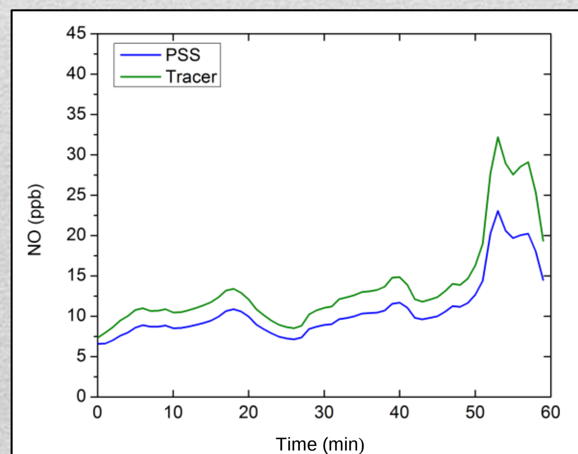

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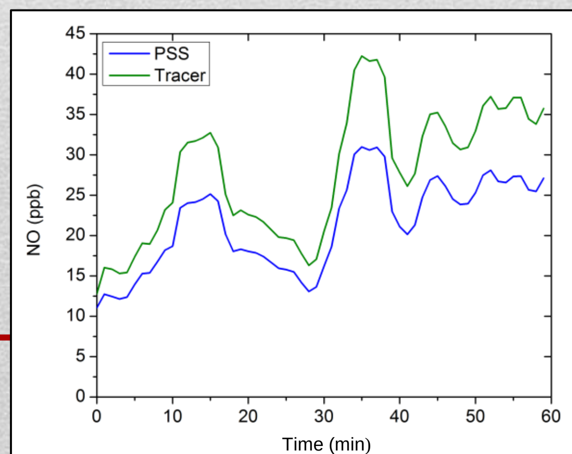
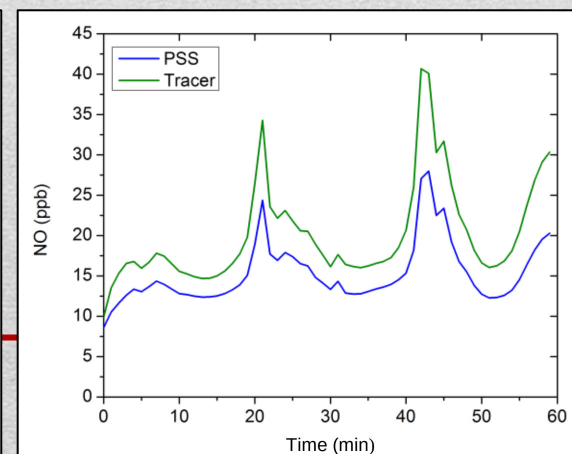
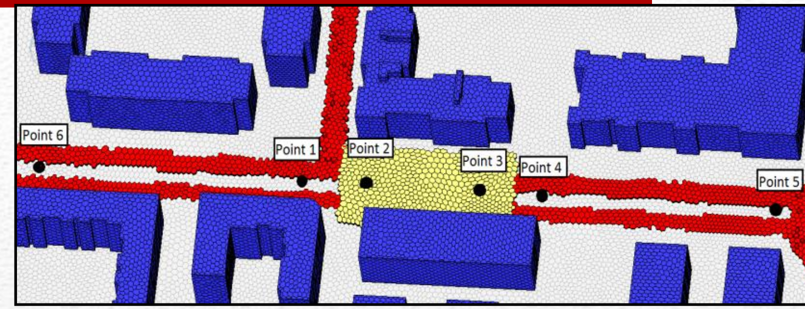


Point 6

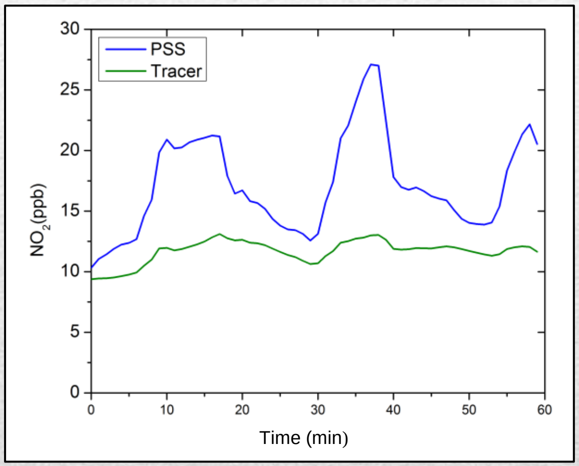


Results | Evaluation of the chemical approaches

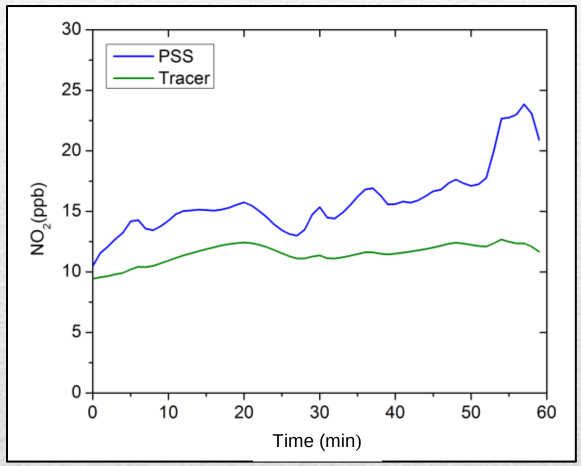


- **Time evolution of NO_2**

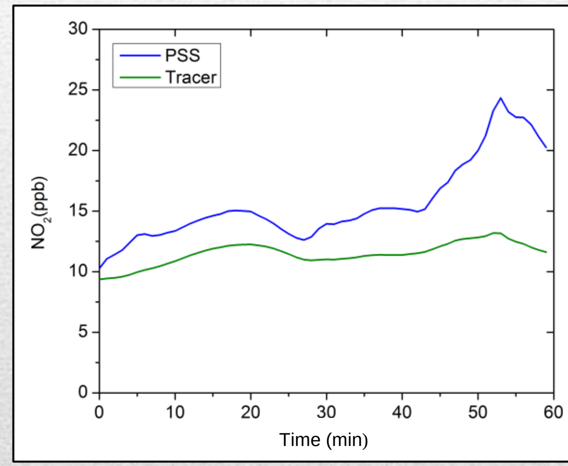
Point 1



Point 2



Point 3



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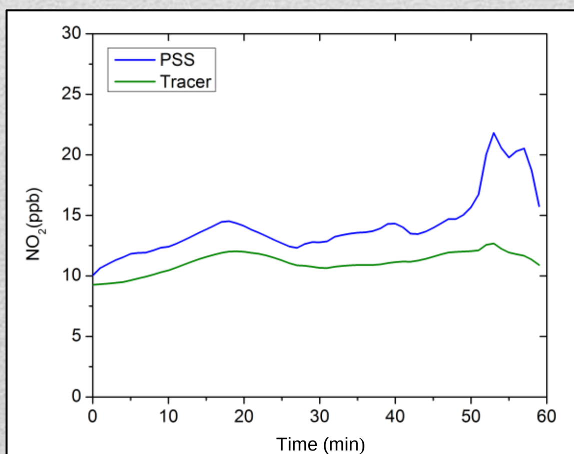

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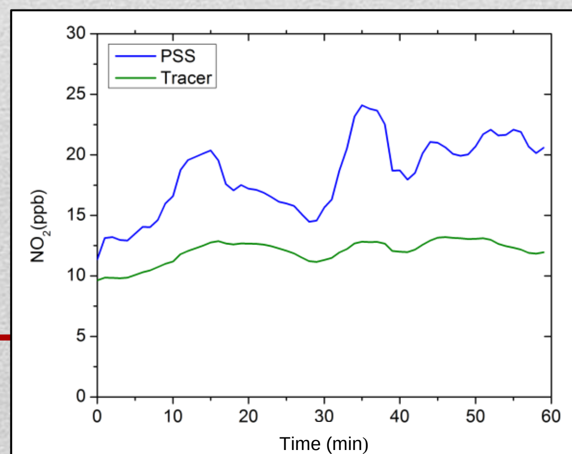

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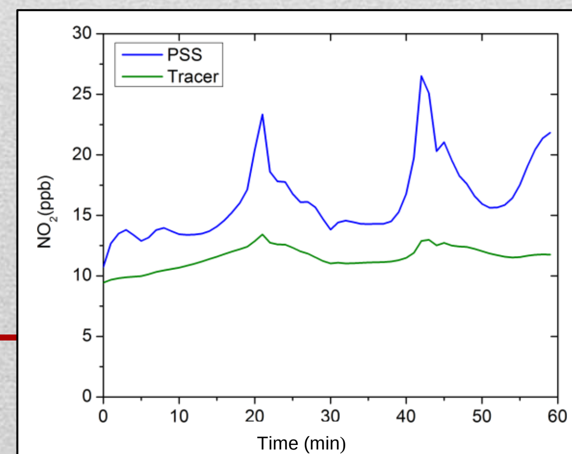
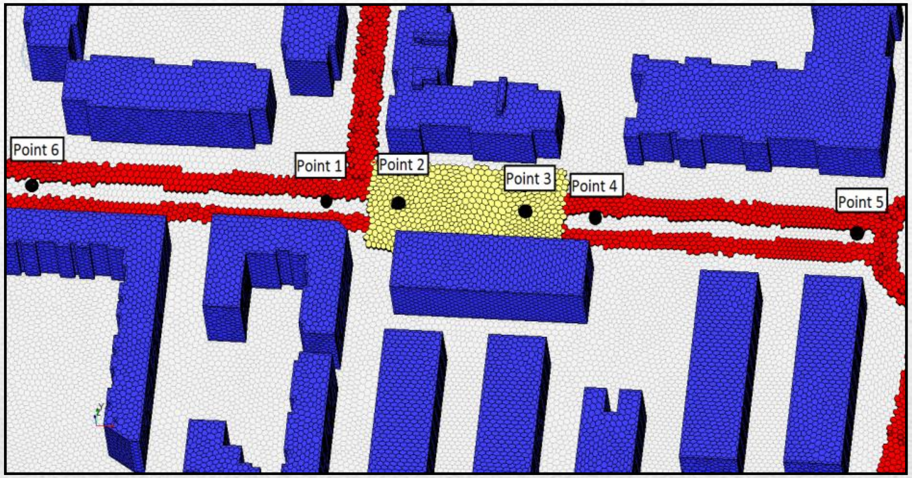
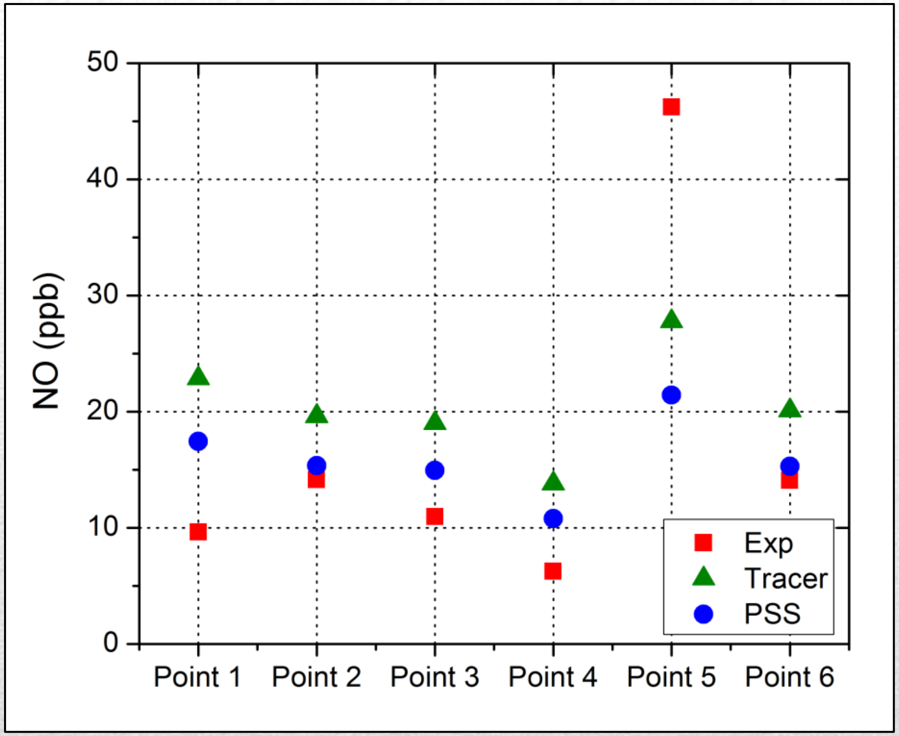


- Comparison of the time average concentration with experimental measurements

  - **NO**





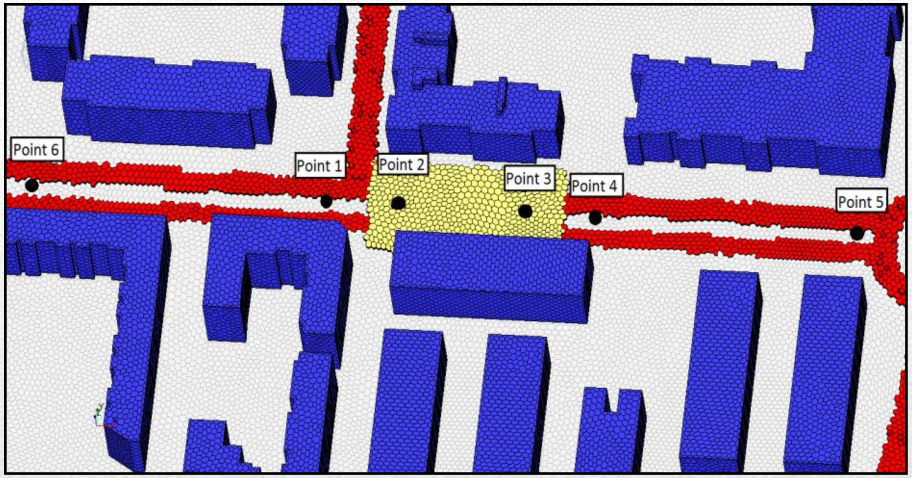
- Including a chemical scheme

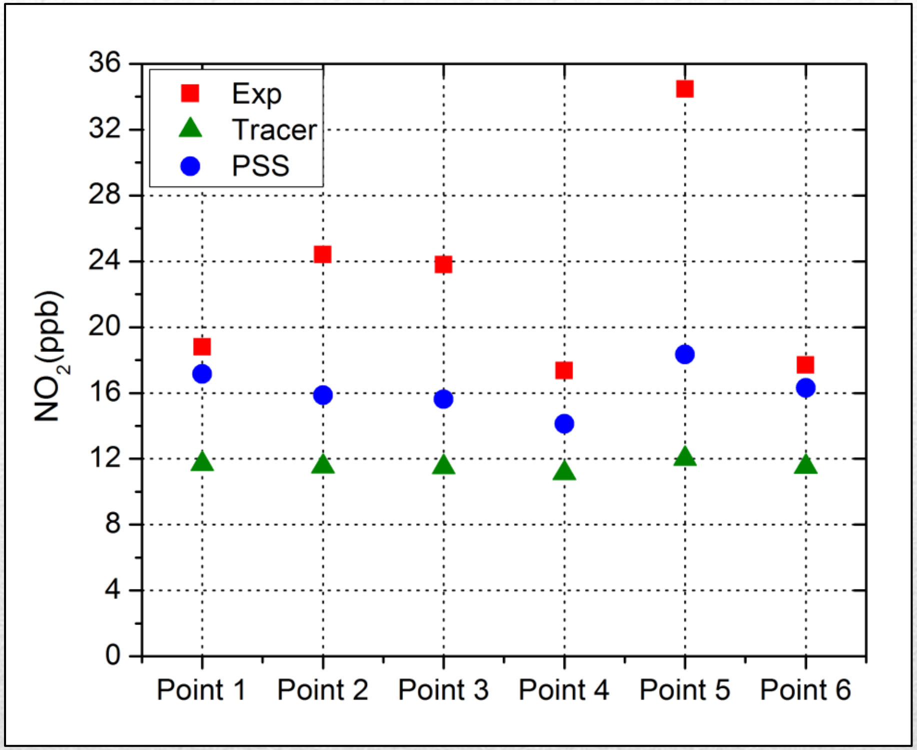
↓

Better fit of NO concentration

	Tracer	PSS	Acceptance Criteria (Goricsan et al., 2011 and Chang et al., 2005)
NMSE	0.30	0.39	NMSE<1.5
FB	-0.20	0.06	-0.3 < FB <0.3
FAC2	66.6%	83.3%	

- **NO_2**





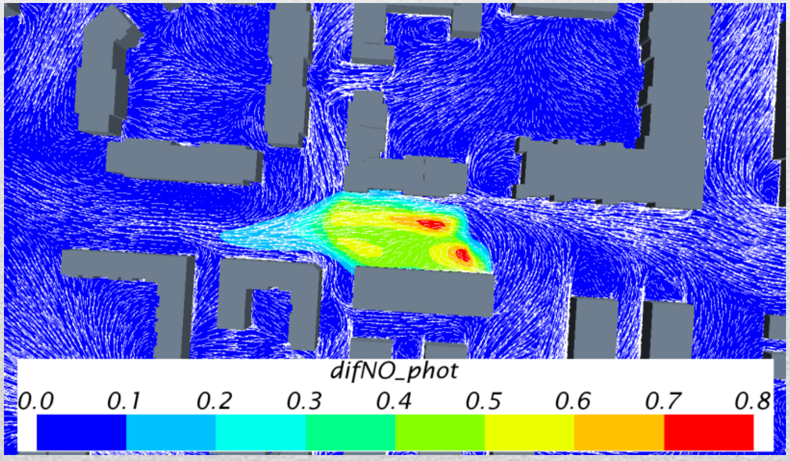
- Underestimation of the NO_2 concentration
- Better results using the photostationary steady state

	Tracer	PSS	Acceptance Criteria (Goricsan et al., 2011 and Chang et al., 2005)
NMSE	0.55	0.18	NMSE < 1.5
FB	0.65	0.33	-0.3 < FB <0.3
FAC2	50 %	100 %	

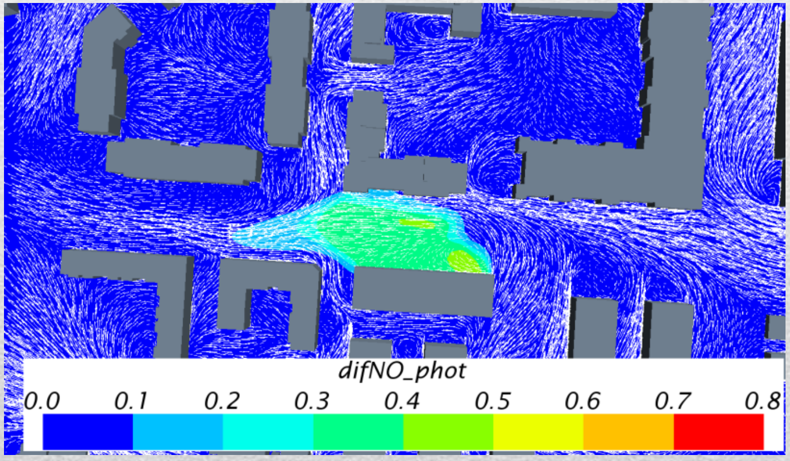
4.2. Analysis of the photocatalytic effect in the real urban scenario

- Photostationary steady state is selected
- 2 CFD simulations with same conditions → With Photocatalytic pavement / Without Photocatalytic pavement
- Spatial distribution at t= 60 min → $\boxed{difNO = NO - NO_{dep}}$

h=1m

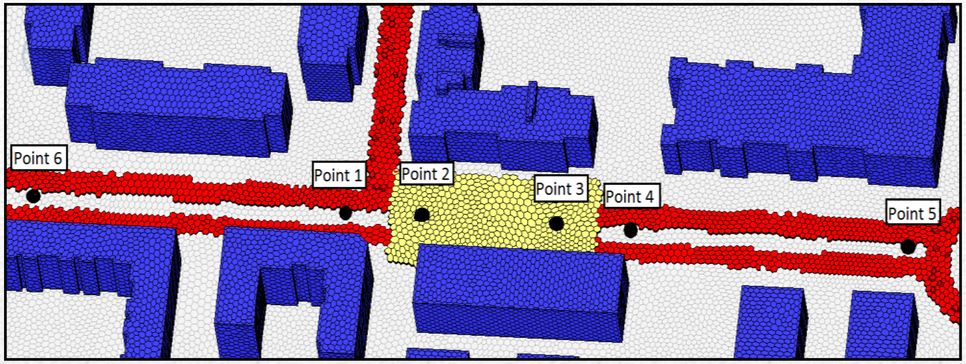


h=3m

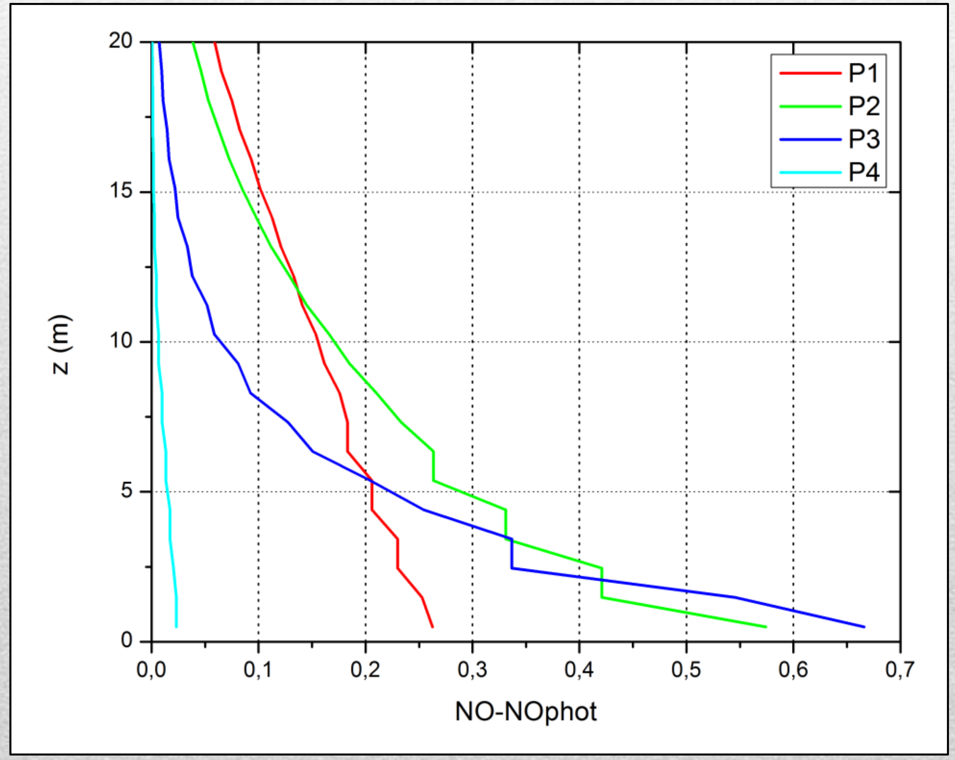


- The photocatalytic effect is negligible and it is only observed over the pavement.
- The reduction in NO concentration at 1 m is slightly higher than at pedestrian level

- **Vertical Profiles of the decrease of NO concentration due to photocatalytic pavement**



   - The maximum value is 0.7 ppb.
   - The maximum differences are found in the points located over the pavement



Conclusions

- The introduction of chemical reactions in the CFD simulations modifies the amount of pollutant concentration so that the NO concentration is reduced and NO_2 concentration is increased.
- NO and NO_2 concentration simulated by both chemical approaches are in agreement with the experimental data.
- Better results of NO and NO_2 concentration are obtained taking into account reactive pollutants using the photostationary steady state.
- The photocatalytic effect is evaluated by means of CFD simulations considering reactive pollutants and the NO deposition due to photocatalytic pavement. The results show a small decrease in NO concentration, even close to the material at ground.
- These results are obtained for a selected photocatalytic material in specific meteorological conditions in a real urban area.

Thank you

HARMO'17

9-12 May 2016 Budapest, Hungary

17th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

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