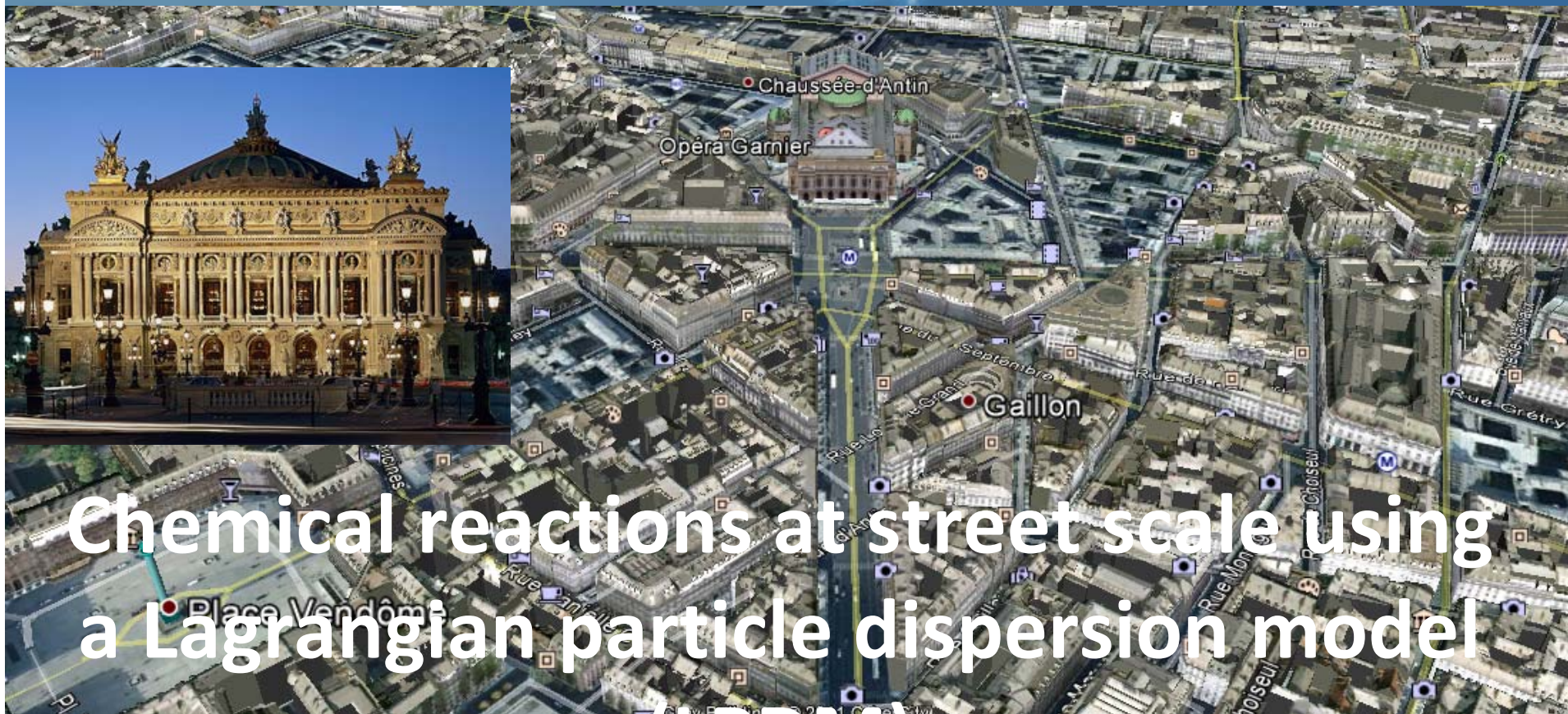


ARIA Technologies

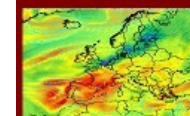


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15th International Conference on
Harmonisation Within
Atmospheric
Dispersion Modelling for
Regulatory Purposes
HARMO 15



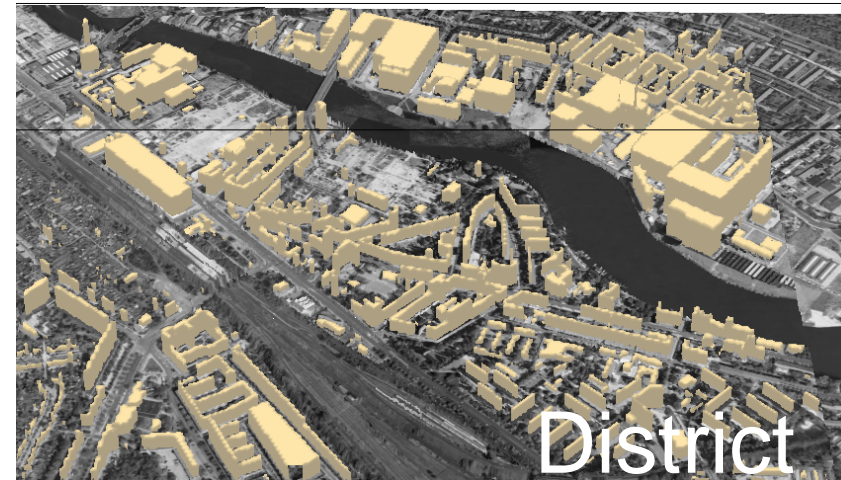
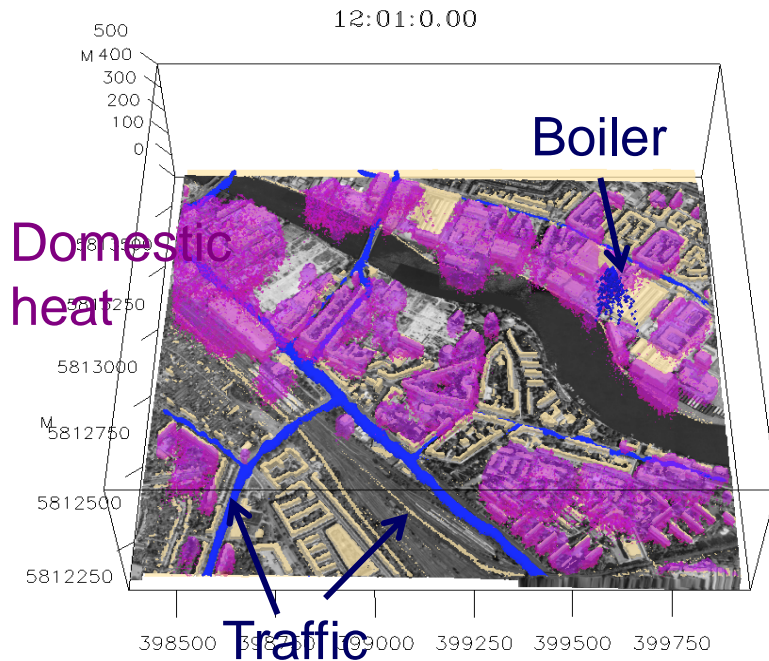
6-9 May 2013
Madrid, Spain

First
Announcement

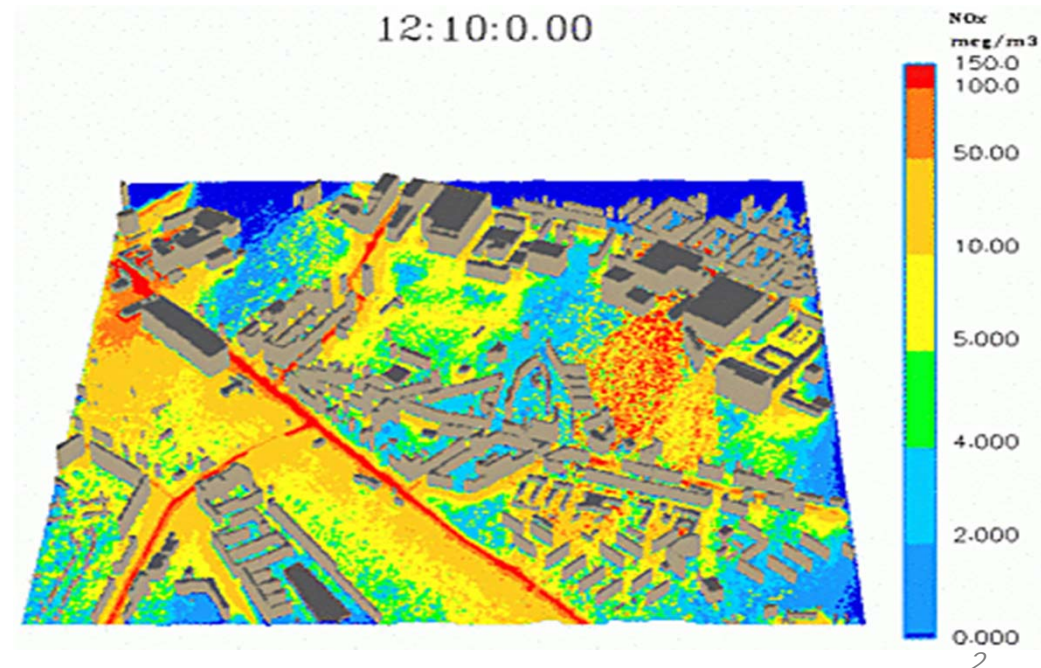
CONTEXT : Urban air quality



NO_x emissions



Are NO₂ concentrations compliant with UE Standards ?



Goals of the study



- **Chemical reaction formulation for LPDM at street level.**
- **Are the segregation terms significant?**
- **Sensitivity to the NO/NO₂ ratio in the emission source.**
- **Sensitivity to the city level background.**
- **What are the relevant reactions at street scale applied to traffic pollution for operational use?**

Chemical reactions

- The model describes emission of NO_x from traffic inside a constant background of ozone, Bo_3
- Each particle released from the source carries an initial mass of NO (m_{NO}), NO_2 (m_{NO_2}) and a deficit from the Ozone background ($m_{\text{def}_{\text{O}_3}}$) [Alessandrini et. al. (2009) see also H14-188]
- $\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$ ($k=0.31$) [$1/(\text{ppm}\cdot\text{s})$]
- $\text{NO}_2 + \text{O}_2 + h\nu \rightarrow \text{NO} + \text{O}_3$ ($J=0.0145e^{-0.4/\cos Q}$) [$1/\text{s}$]

The rate of change of particle's content

$$\frac{dm_{NO}}{dt} = -\frac{dm_{NO_2}}{dt} = -\frac{dm_{defO_3}}{dt} = -k(B_{O_3}m_{NO} - \langle C_{NO} \rangle m_{defO_3}) + Jm_{NO_2}$$

Concentration

- **Summation in cell divided by the cell volume gives the average reaction rate equation**

$$\begin{aligned} \frac{d\langle C_{NO} \rangle}{dt} &= -\frac{d\langle C_{NO_2} \rangle}{dt} = -k\langle C_{NO} \rangle (B_{O_3} - \langle C_{defO_3} \rangle) + J\langle C_{NO_2} \rangle = \\ &= -k\langle C_{NO} \rangle \langle C_{O_3} \rangle + J\langle C_{NO_2} \rangle \end{aligned}$$

Traffic induced turbulence

- The moving vehicle induces a turbulence which effect the pollutant dispersion near the source. This turbulence is modeled as an injected TKE with emission rate \dot{Q}_{TKE} which should be modeled or measured.

Simple Model

- N - the number of vehicles per second
- \dot{Q} - the NO_x emission rate

$$N = \frac{\dot{Q}}{0.2}$$



- The emitted amount of NO_x by a single vehicle $\sim 0.2\text{g/s}$
- V - the average velocity of the vehicle ($\sim 10\text{m/s}$)
- The amount of TKE per vehicle $\sim (\alpha V)^2$ $\alpha \approx 0.1$

$$\dot{Q}_{TKE} \sim N(\alpha V)^2 = 5 K \dot{Q}$$

The segregation term



Definition

- $A+B \rightarrow C \quad dA/dt=dB/dt=kAB$
- $d\langle A \rangle/dt=d\langle B \rangle/dt=k\langle AB \rangle=k(\langle A \rangle\langle B \rangle + \langle A'B' \rangle)$

The Conditional Concentration

- The segregation term can be considered as a correction in the reaction equation by the conditional concentration

$$\frac{dm_{NO}}{dt} = -\frac{dm_{NO_2}}{dt} = -\frac{dm_{defO_3}}{dt} = -k(B_{O_3}m_{NO} - C_{NO}^C m_{defO_3}) + Jm_{NO_2}$$

The conditional concentration

- The conditional concentration is the average concentration for particles along their trajectories
- The time evolution of conditional concentration is given by:

$$\frac{dC_{NO}^c}{dt} = -\frac{C_{NO}^c - \langle C_{NO} \rangle}{T_{mix}}$$

- The mixing time T_{mix} is proportional to the Lagrangian time scale ($T_{mix} = 0.6 T_L$)

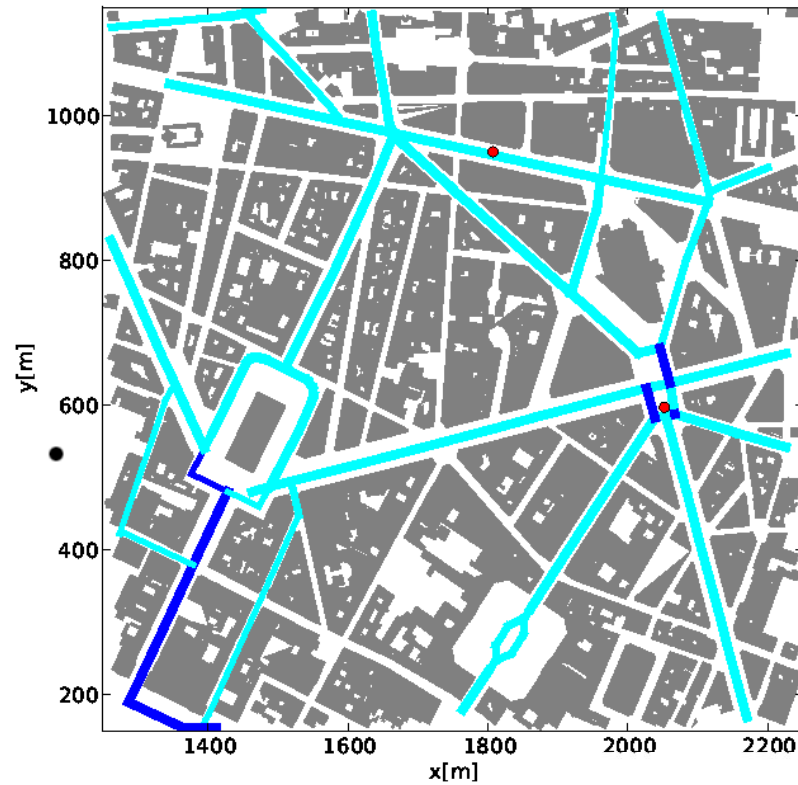
Including the segregation term has a negligible influence on the results at street scale

Model input data

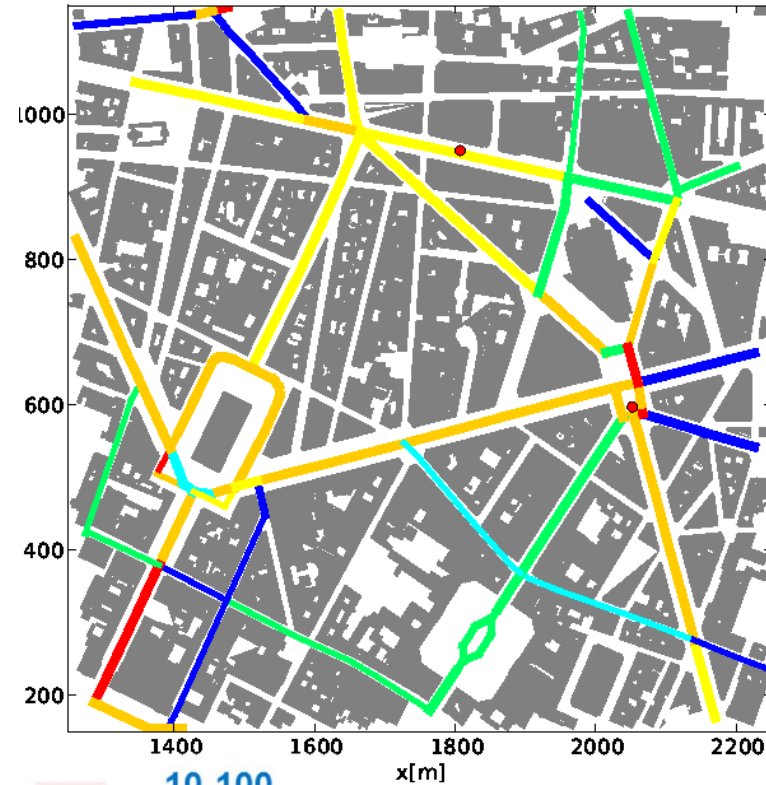


Traffic emission data (NO_x)

At 3:00



At 15:00



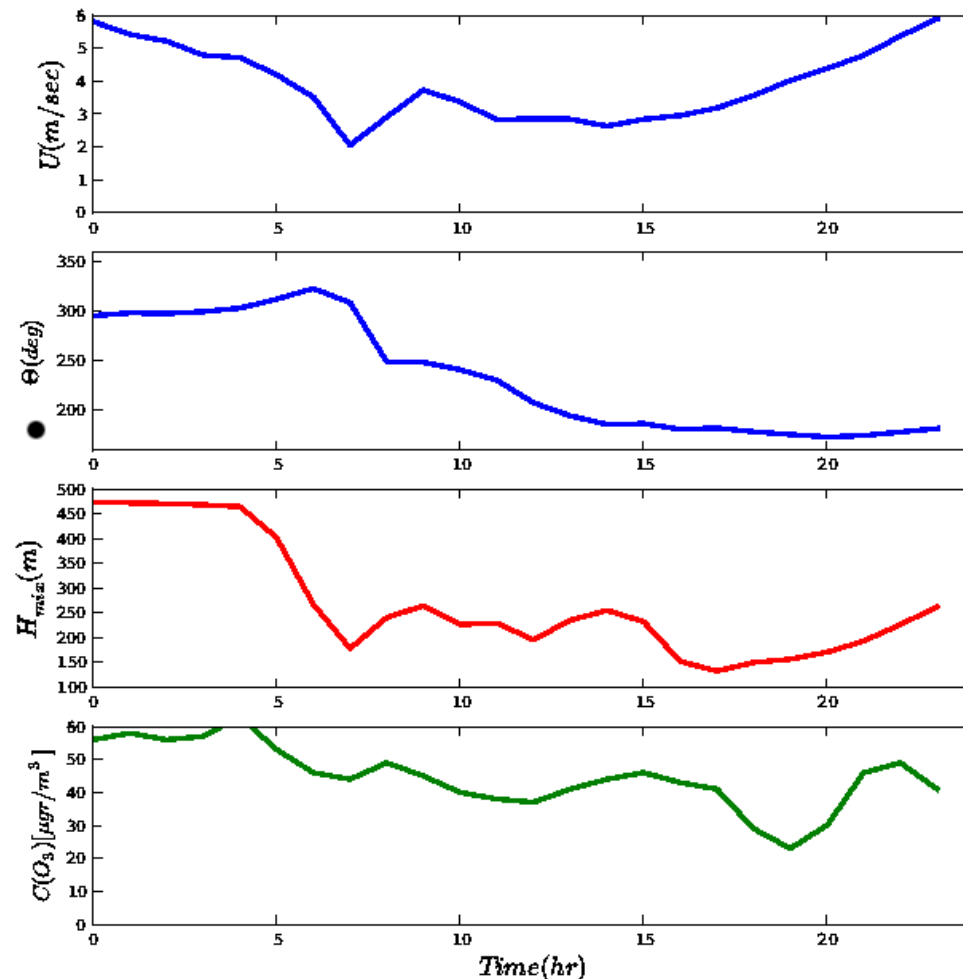
$$\dot{Q} \left[\frac{\mu\text{g}}{\text{m.s}} \right]$$

- 10-100
- 100-200
- 200-300
- 300-400
- 400-900
- >900

Model input data



Meteorological (MM5) and O₃ data Date : 25.02.2011



- Wind speed
z= 54m
(U_{max}=6m/s)
- Wind direction
- Mixing Height
H_{max}=500m
- Ozone
Background
Eiffel Tower
(~300m)
[O₃max]= 60μg/m³

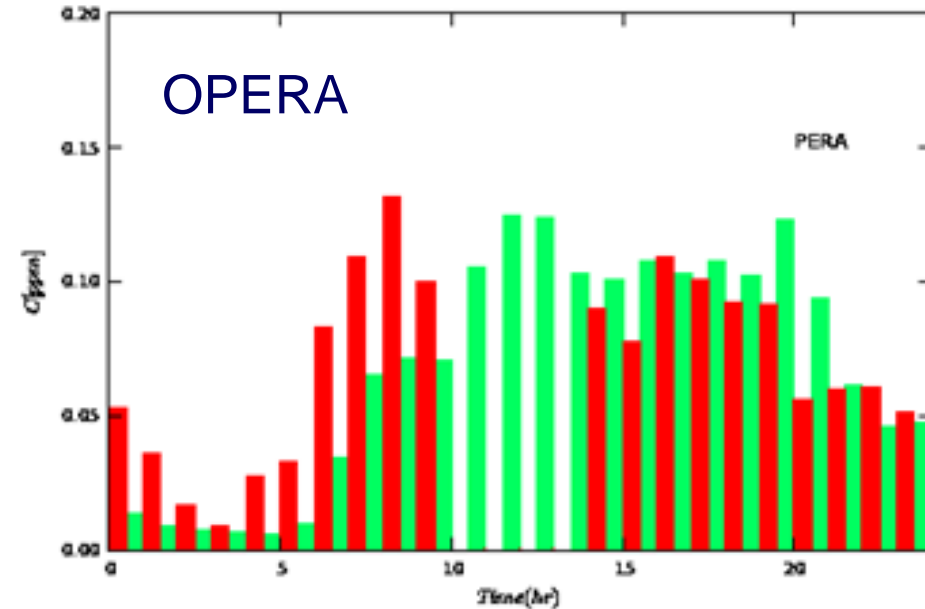
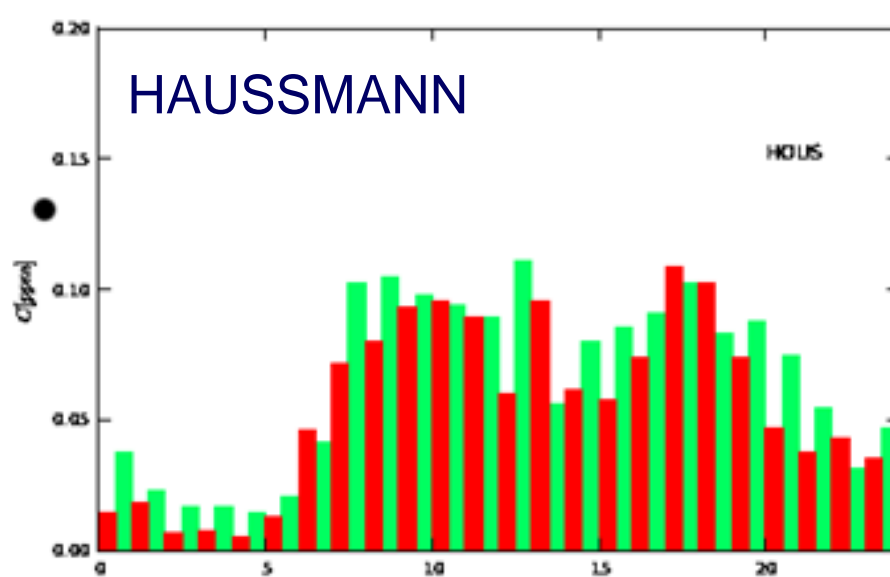
Results



Reference case

- NO/NO_x ratio = 0.75
- Turbulence parameter $K = 0.5$

Total NO_x Concentration



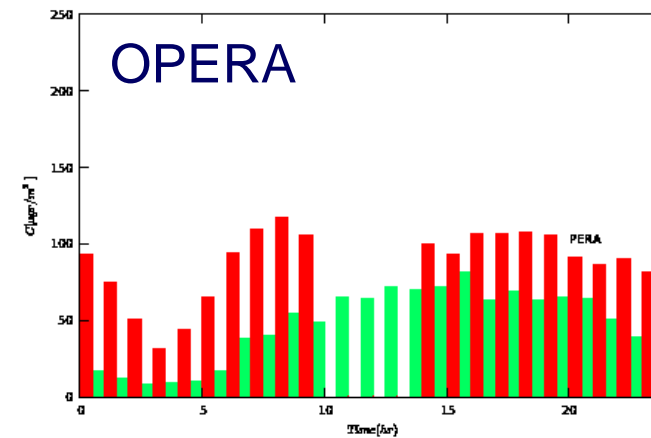
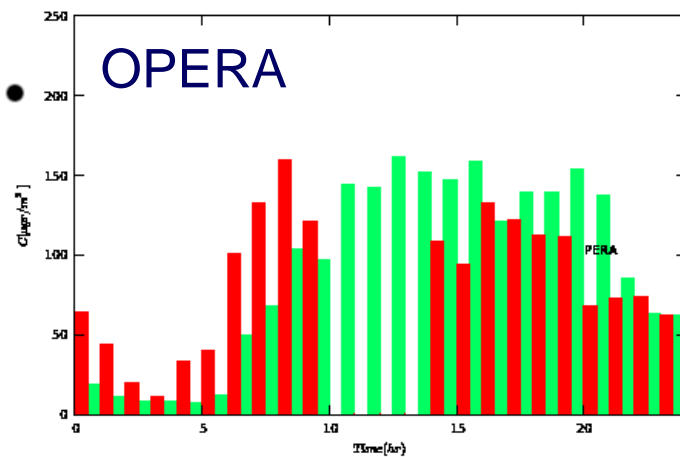
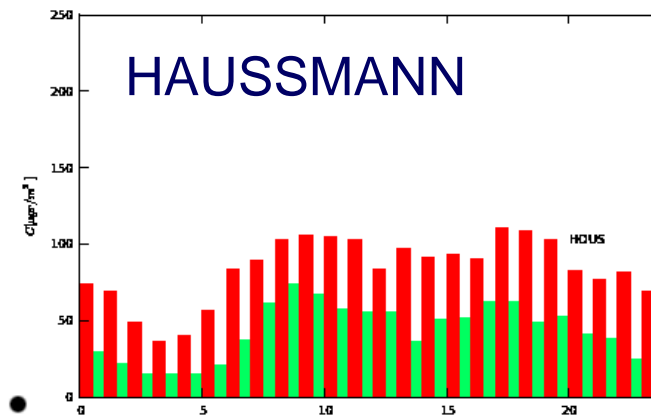
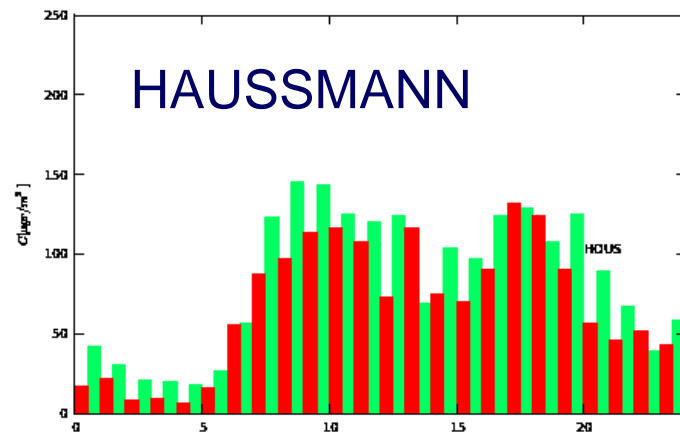
- (red: measured ; green calculated)

Results



NO

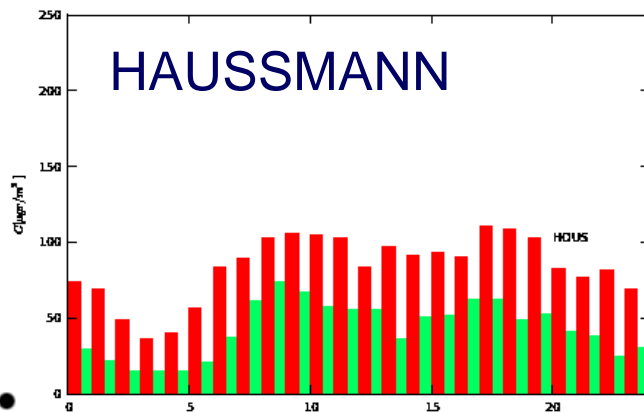
NO₂



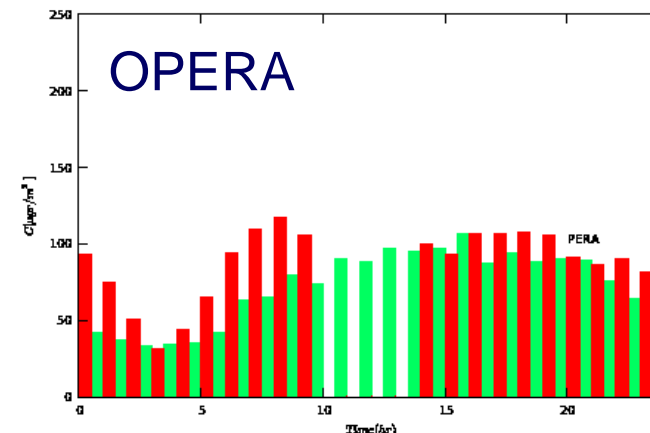
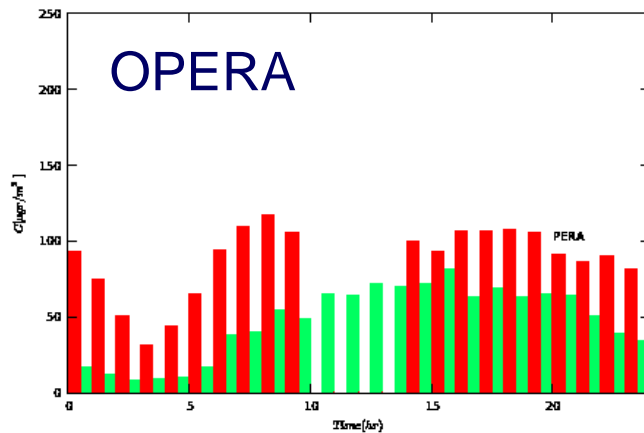
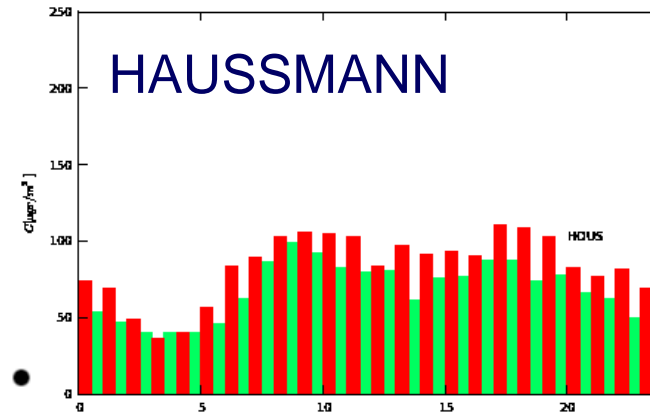
- (red: measured ; green calculated)

NO₂ BACKGROUND INFLUENCE

Without NO₂ background



With NO₂ background



● (red: measured ; green calculated)

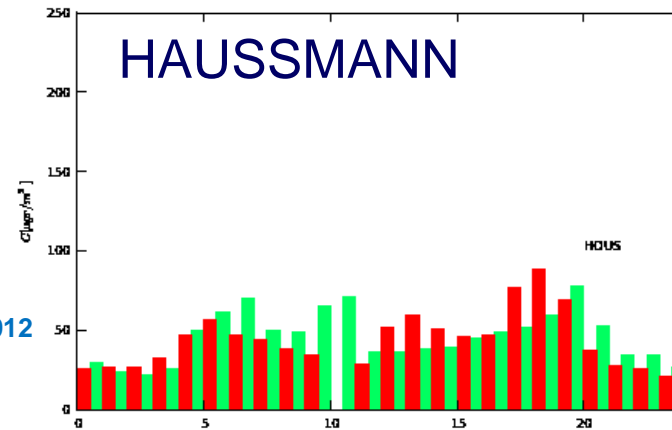
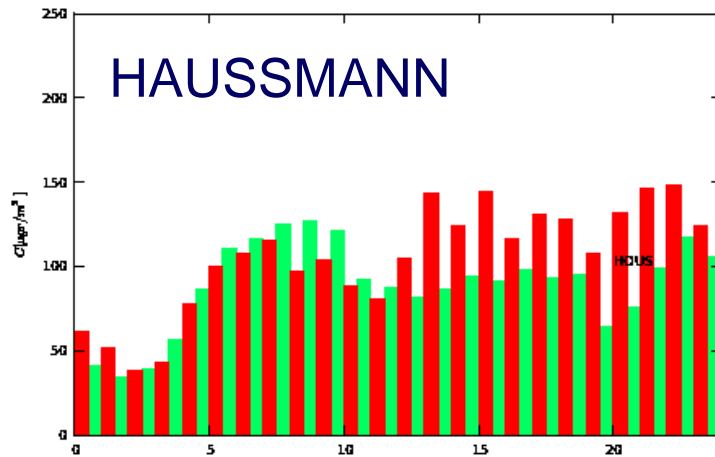
Results



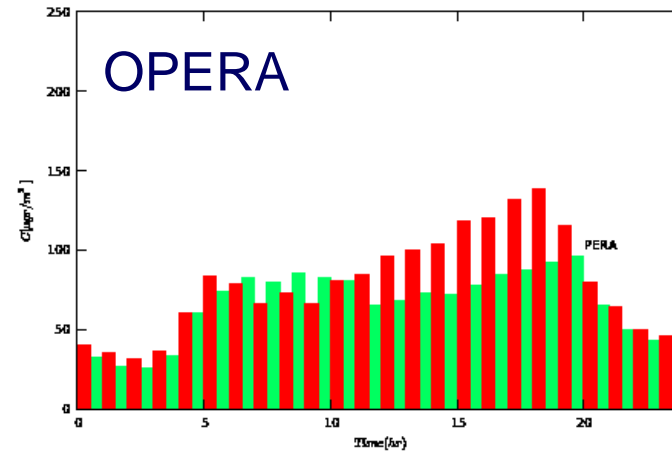
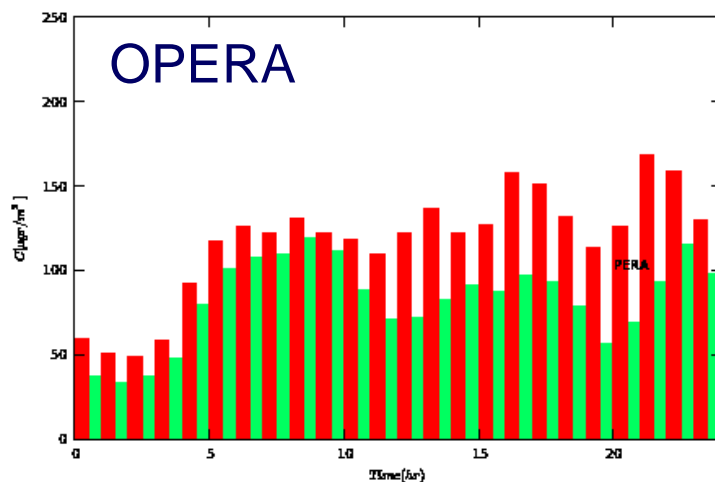
NO₂ predicted concentration

24.07.2012

4.09.2012



4.09.2012

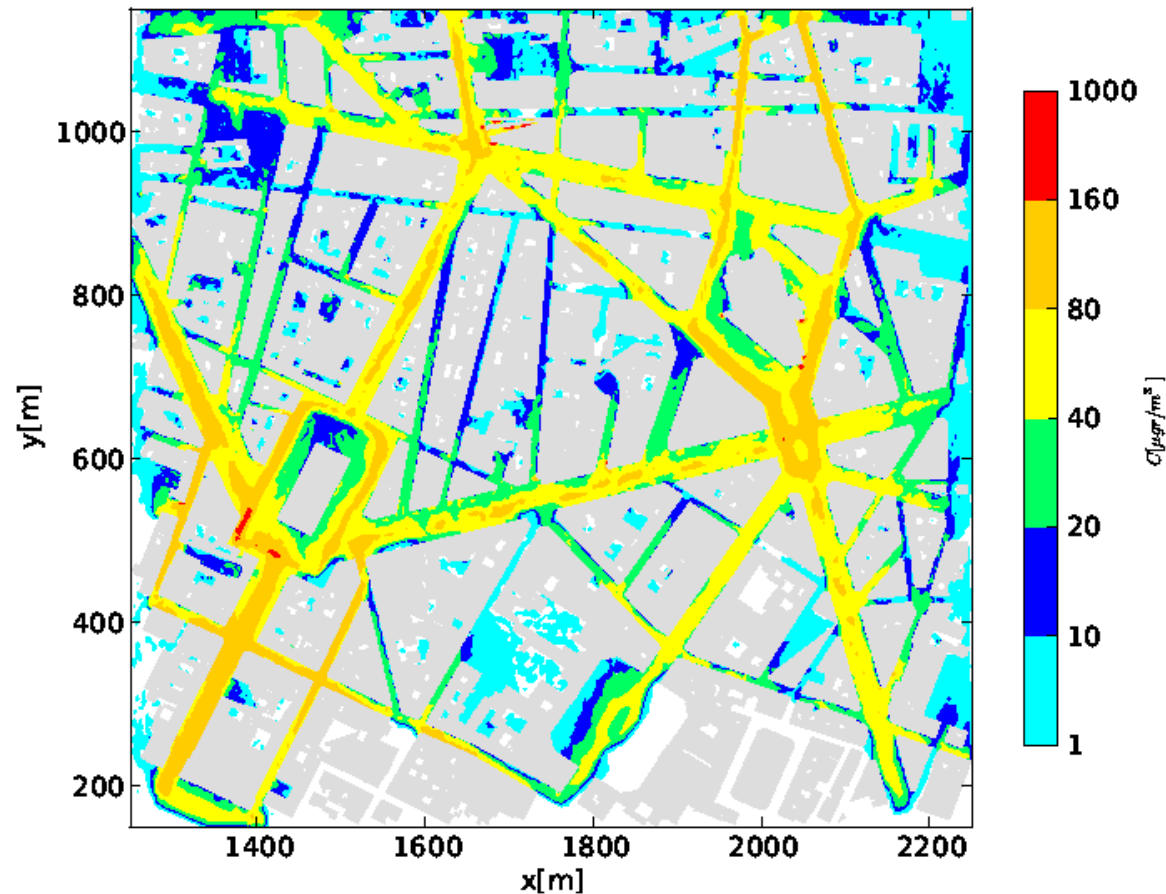


Sensitivity study



■ Ref case : $\text{NO}/\text{NO}_x=0.75$ $K=0.5$ $B_{\text{O}_3}=44$

At 15:00



NO_2

Sensitivity Analysis



Ref : NO/NO_x=0.75 K=0.5 B_{O3}=44

Concentrations at 15:00

	CALCULATED		MEASURED	
	H	O	H	O
NO ₂	(51) 76	(75) 97	75	109
NO	103	146	91	100

[µg / m³]

	NO/NO _x =0.9		K=0.25		B _{O3} =88	
	H	O	H	O	H	O
NO ₂	(30) 55	(42) 66	(65) 90	(80) 105	(63) 89	(90) 115
NO	125	177	128	167	95	135

- Numbers in parenthetic are without NO₂ background

The generic reaction set (GRS)



ROP in GRS

- The GRS equations describes reactions of NO and NO₂ with radical products (RP). $RP + NO \rightarrow NO_2$
- RP are result of photo-dissociation of reactive organic compounds (ROP) $ROP + h\nu \rightarrow RP + ROP$
- The time-scale of RP production from photo-dissociation of ROP is much larger than the transport time over domain of 1x1 Km → **ROP emitted in the area will not affect the results**

If RP are known in the background, the whole set of the GRS should be solved and the result depends on the amount of RP background concentration.

CONCLUSION



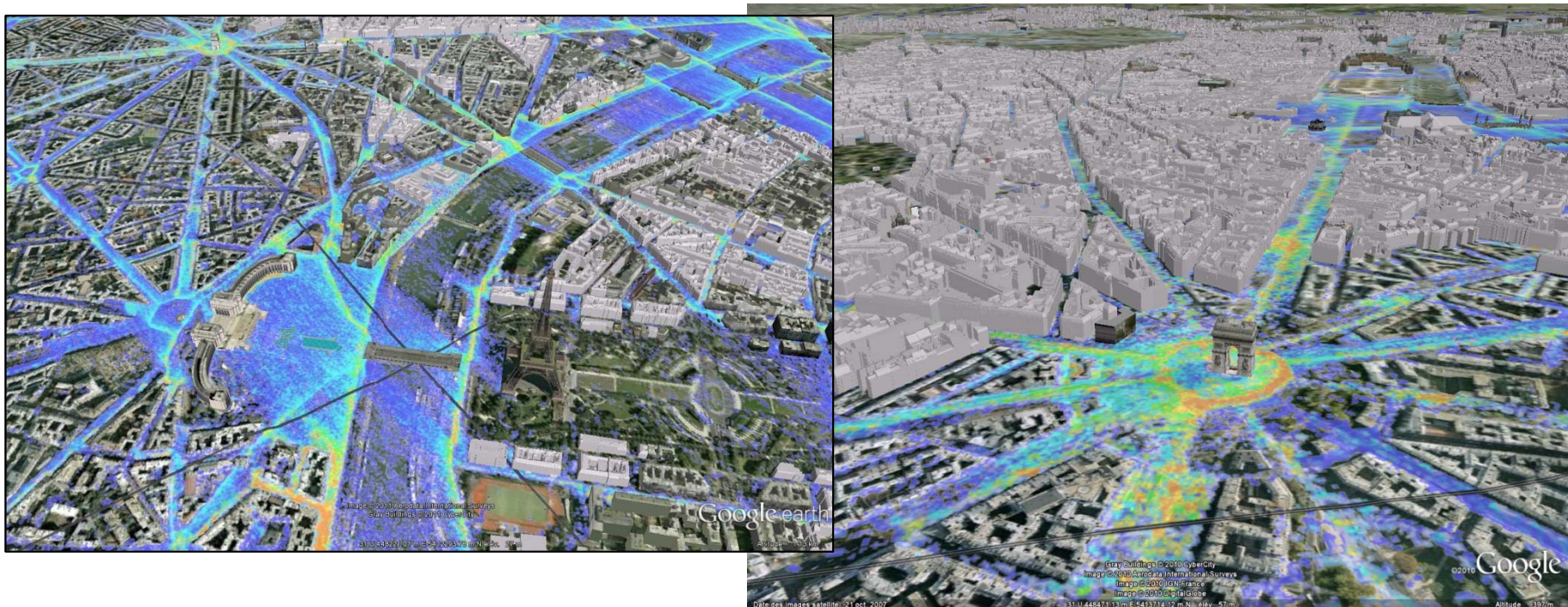
- **The current LPDM model was extended to include chemical reaction and self induced turbulence**
- **The segregation term is not important at street scale but should be included for large plume whose magnitude is much smaller than the turbulence scale.**
- **$\text{NO}/\text{NO}_x=0.75$ for Paris area and is not a free parameter of the model**
- **It is important to well assess NO_2 background when modeling an isolated district**
- **The whole set of GRS equation should be solved only in case that there is a large background concentration of RP**

Next step :



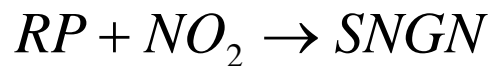
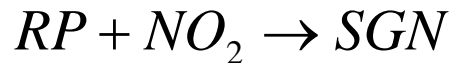
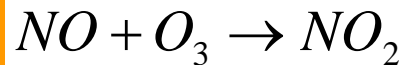
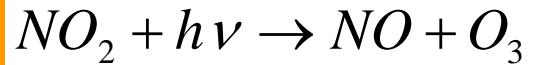
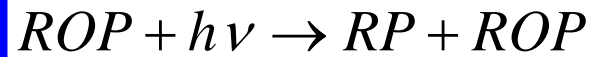
NO₂ for « AirCity » Project

- Compute and forecast meteorological and air quality parameter within a 3m resolution
- Need of HPC : Ex Paris at 3M resolution 360 CPU



█ Thank you for your attention !

The generic reaction set (GRS)



ROP- Reactive organic products

RP- Radical Products

SGN- Stable gaseous nitrogen products

SNGN- Stable nongaseous nitrogen products