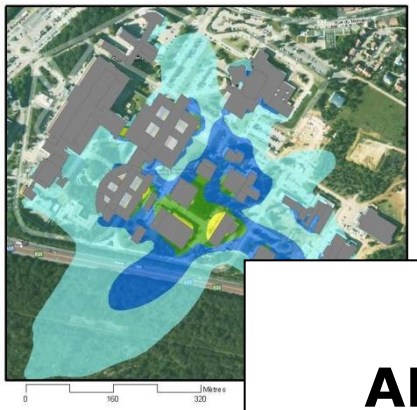

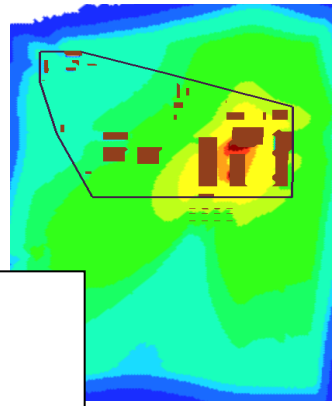

APPLICATIONS OF THE MSS (MICRO-SWIFT-SPRAY) MODEL TO PHOTOCATALYTIC COATING SIMULATIONS

Christophe Olry, Jacques Moussafir, Pierre Castanier
ARIA Technologies, Boulogne-Billancourt, France

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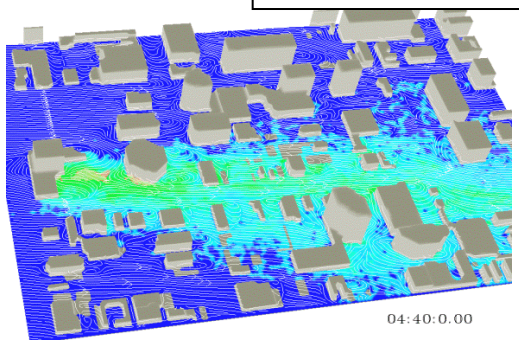
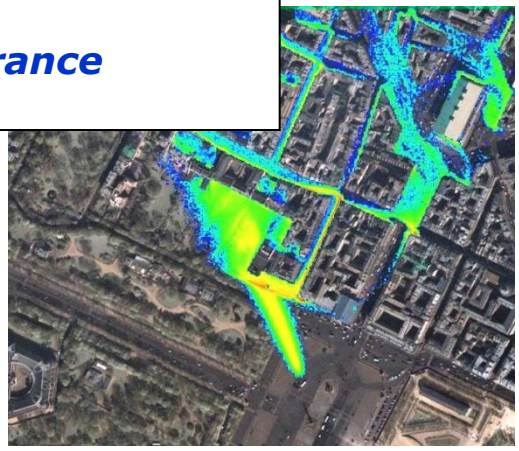
ITALCEMENTI/Ciments Calcia, Guerville, France





jmoussafir@aria.fr

HARMO 13, Paris

June 1st – 4th, 2010

Presentation Map

- **The MSS Model**
  - **Principle**
  - **Development group**

- **Applications to TiO2 photo-catalytic coatings**

- **Presentation of the EXP'AIR package**

The MSS Model

- **MSS is the combination of :**
  - **a simplified CFD model (Micro SWIFT) coupled to**
  - **a LPDM (Lagrangian Particle Dispersion Model) (Micro SPRAY)**

- **MSS was designed to model urban or industrial micro-scale dispersion phenomena with CPU times significantly shorter than the full CFD solutions.**

- **Typical initial MSS emergency response applications:**
  - **Domain size: 1 to 5 km dimension / Cell size: 1 to 10 meters**
  - **Single PC processor CPU time about 1/10th of real simulated time**
  - **Response time: few minutes**

- **MSS is operational into the US-DOD HPAC 5 suite of models**
  - **Coupled to SWIFT meteorological assimilation model**
  - **Coupled to SCIPUFF (Particle to Puff conversion and handoff)**

MSS Development Group

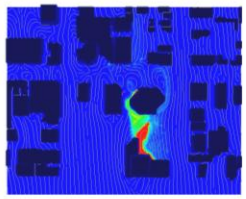
- **MSS is developed by several organizations :**
  - **ARIA Technologies (F)**
  - **ARIANET (I)**
  - **ISAC / CNR (I)**
  - **SAIC (USA)**
  - **CEA (F)**
  - **MOKILI (F)**
  - **CAIRN Développement (F)**

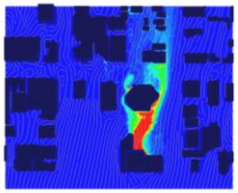
Pr. Domenico ANFOSSI

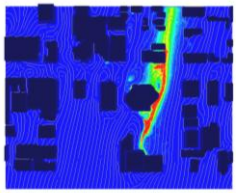
for DTRA

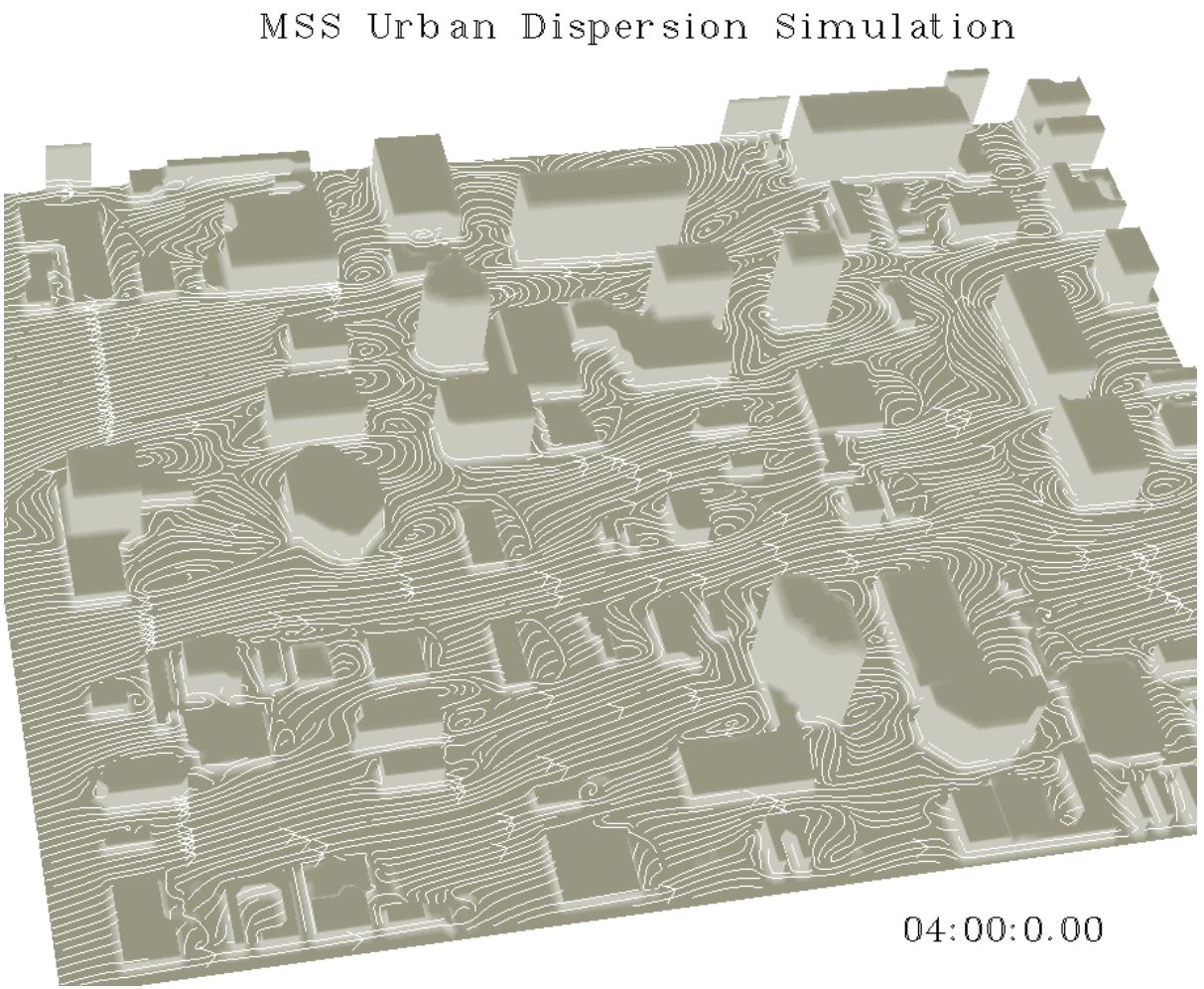
MSS is an urban/industrial site scale tool

Example on Salt Lake City









Resolution in HPAC : 3 to 5 m

Deposition processes in MSS

A fully lagrangian formulation

Boughton B.A, Delaurentis J.M. (1987)
"A stochastic model of particle dispersion in the atmosphere"
BLM 40 pp 147-163

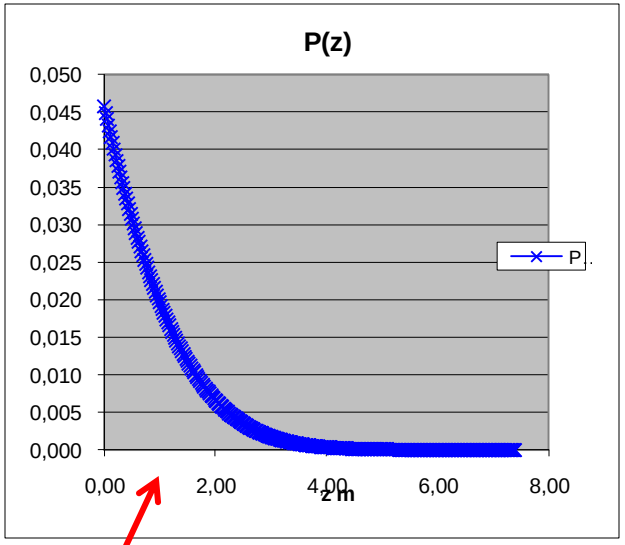
$$P(z_i, \Delta t) = 1 - \int_0^{\infty} p(z, t, z_i, t_i)\, dz$$

$$= \phi[-(z_i - w_s \Delta t)/\sqrt{2K\Delta t}] +$$

$$w_d/(w_d - w_s) \exp(w_s z_i/K)\phi[-(z_i + w_s \Delta t)/\sqrt{2K\Delta t}] -$$

$$(2w_d - w_s)/(w_d - w_s) \exp[w_d z_i/K + w_d(w_d - w_s)\Delta t/K] \times$$

$$\phi\{-[z_i + (2w_d - w_s)\Delta t]/\sqrt{2K\Delta t}\},$$



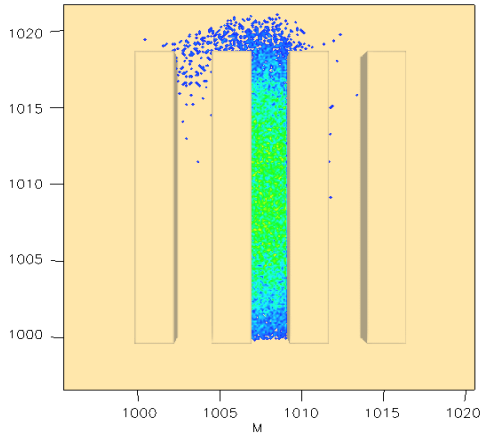
P = Transition Probability during time step
Δt = Model time step (s)
z_i = Particle height (m)
w_d = Deposition velocity (m/s)
w_s = Settling velocity (m/s)
K = Diffusivity near the surface (m2/s)
ϕ= Gaussian cumulated Distribution function

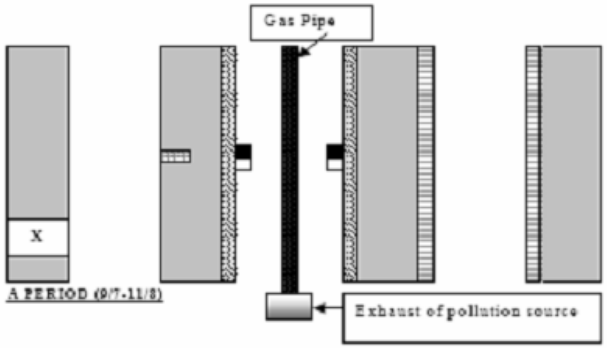
$h_d = \sqrt{2K\Delta t}$ = Deposition length scale

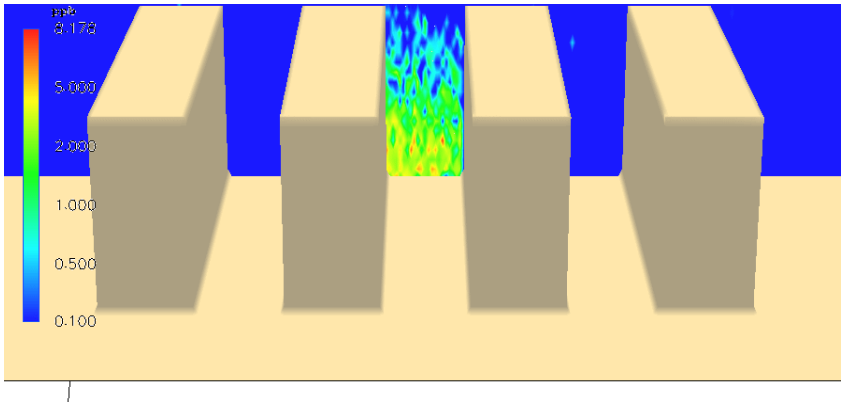
PICADA experiment test case

Test of deposition on facades

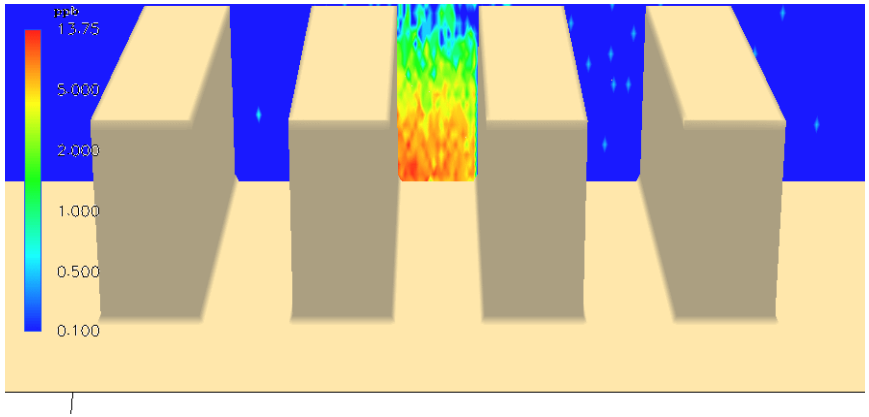
Photocatalytic degradation of NOx using TiO2-mortar panels







WITH TiO2 coating



WITHOUT TiO2 coating

PICADA experiment : courtesy ITALCEMENTI / CALCIA

ARIA TECHNOLOGIES

Deposition in MSS

Current status

- A fully lagrangian deposition scheme is now implemented and tested in MSS at ground, on building roofs, and on building façades

- This scheme has been tested and compares well with more conventional ground deposition Eulerian schemes under stationary conditions, such as :

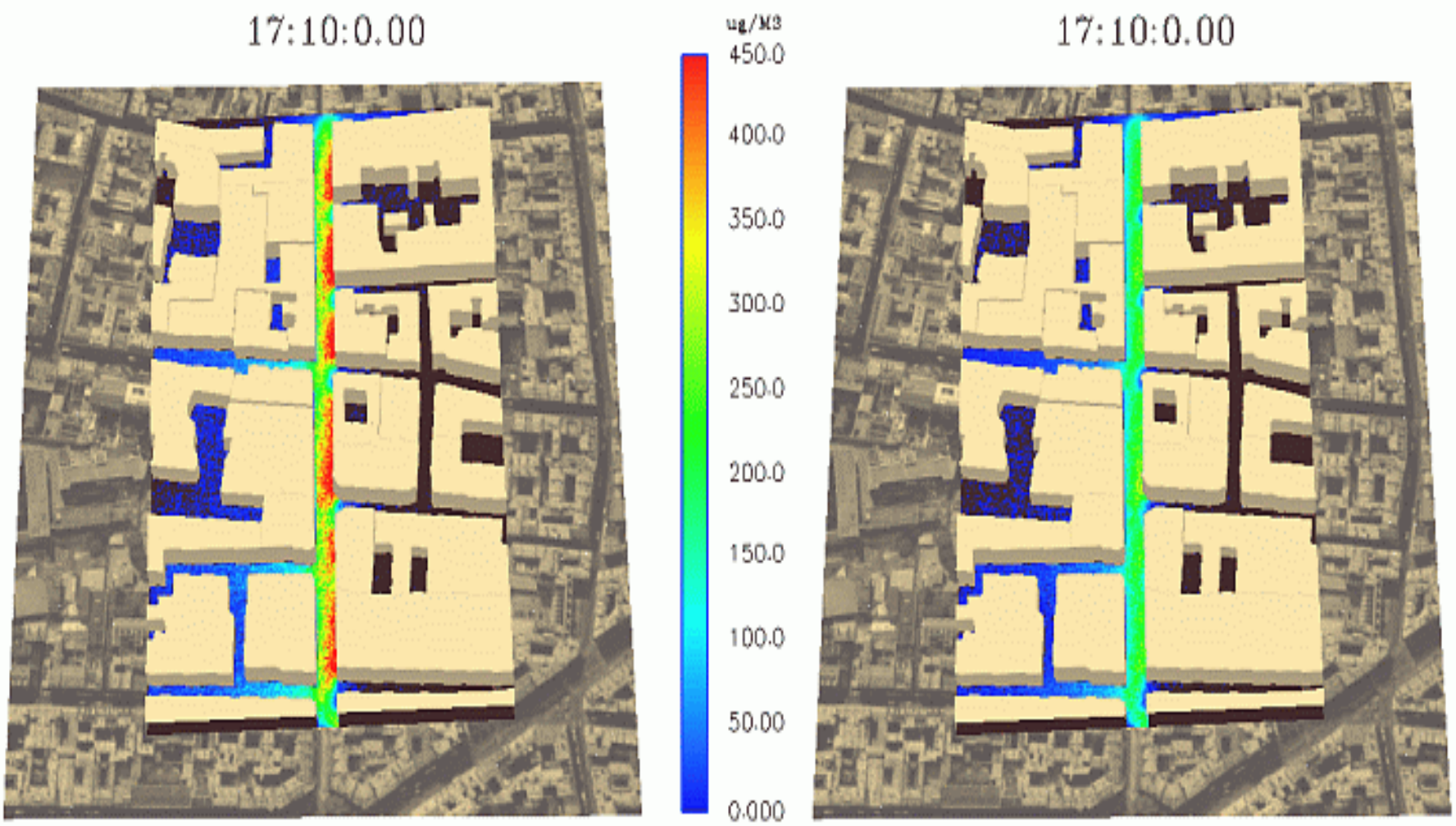
  Deposition flux = $-w_d$. C

- There is a Wild uncertainty on the roughness and deposition parameters to be applied for buildings

- Current specification of properties is by areas in a given urban landscape (allows to designate one single wall or building, or all buildings in a given area) but provisions for the description of pertinent parameters for each building are made

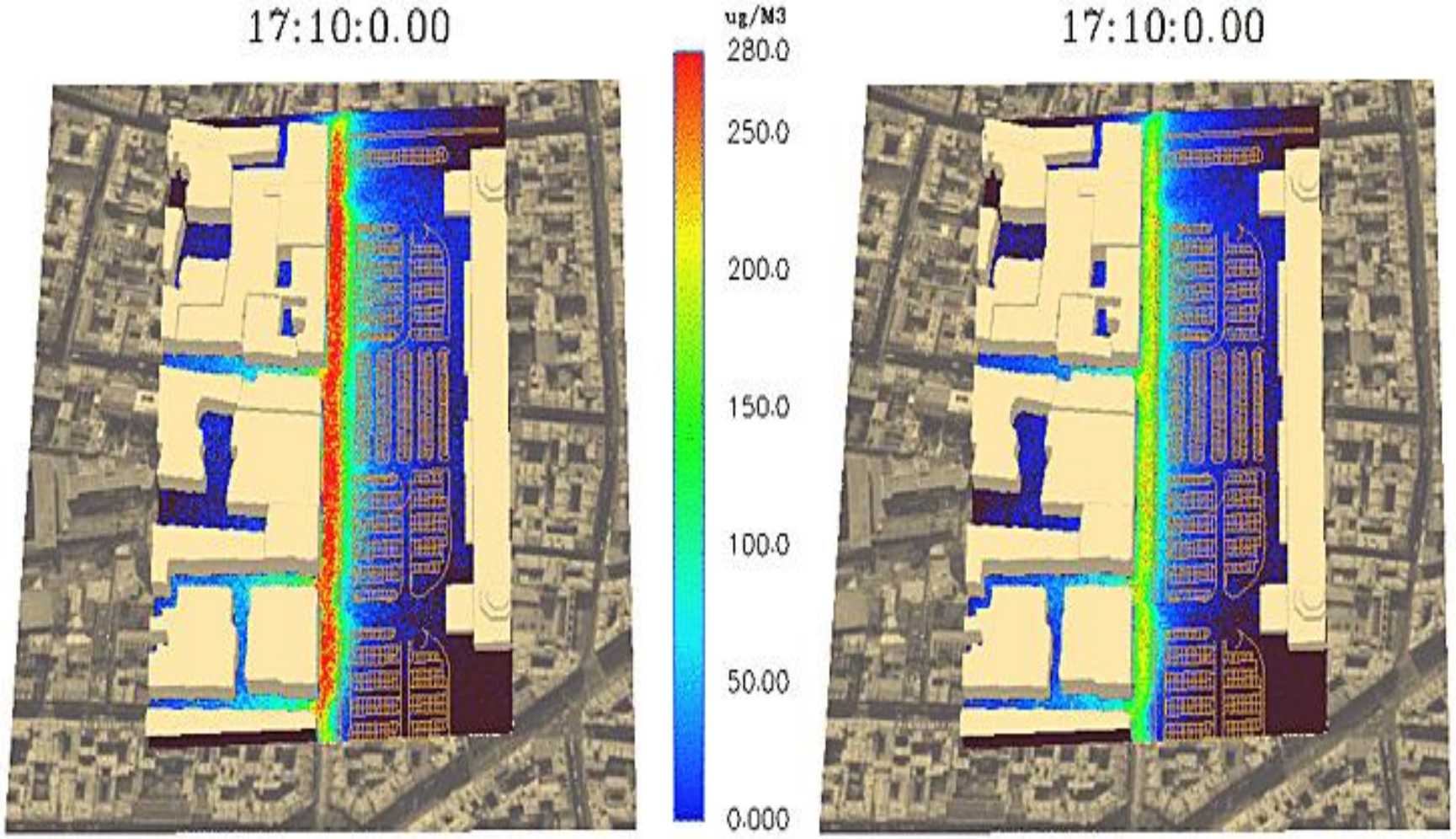
- Desire to make choices compatible with GEDIS/GIS development and u-WRF (Urbanized WRF) solutions

EXP'AIR Base case : street canyon



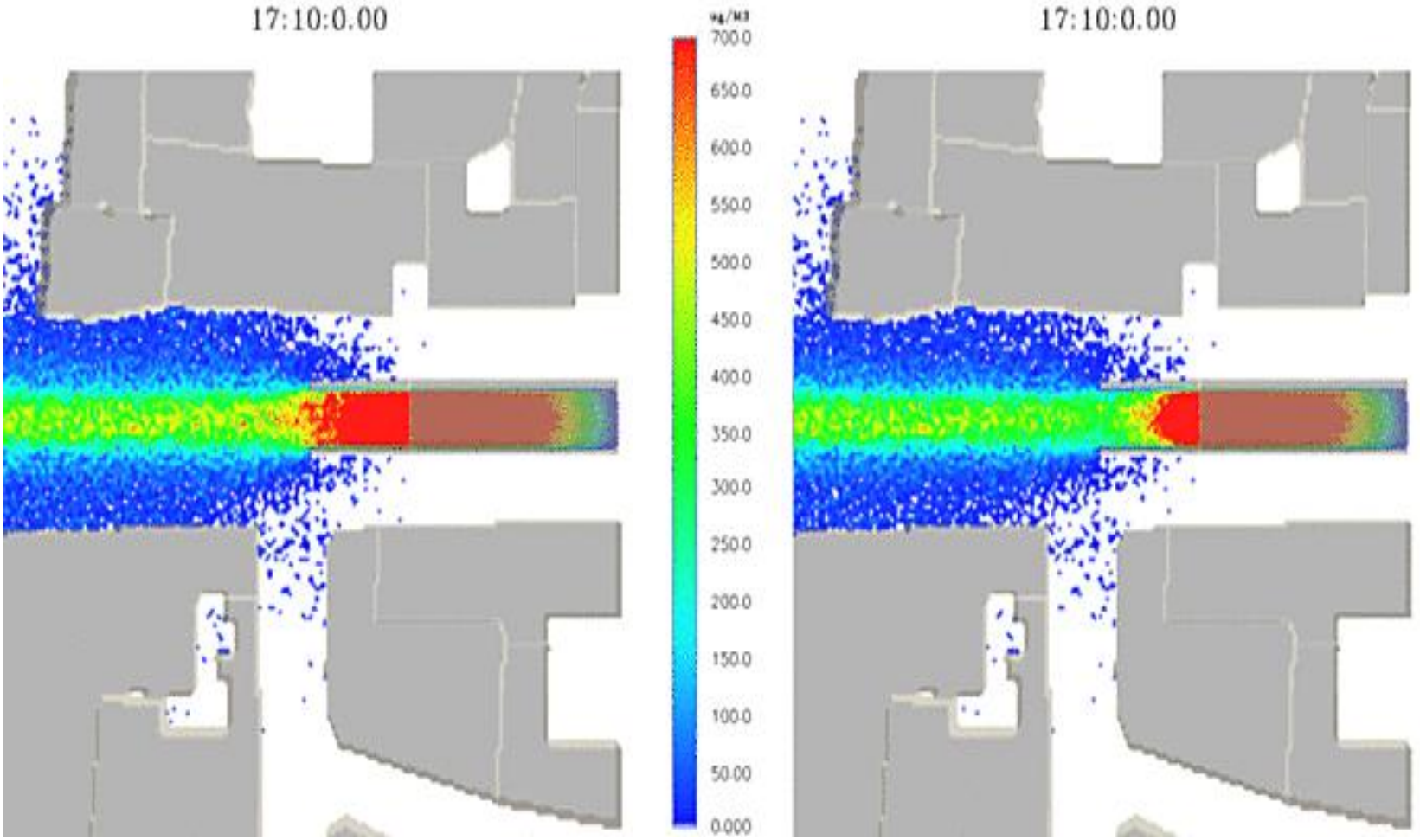
- **Comparison without/with on a street canyon**

EXP'AIR Base case: facade configuration



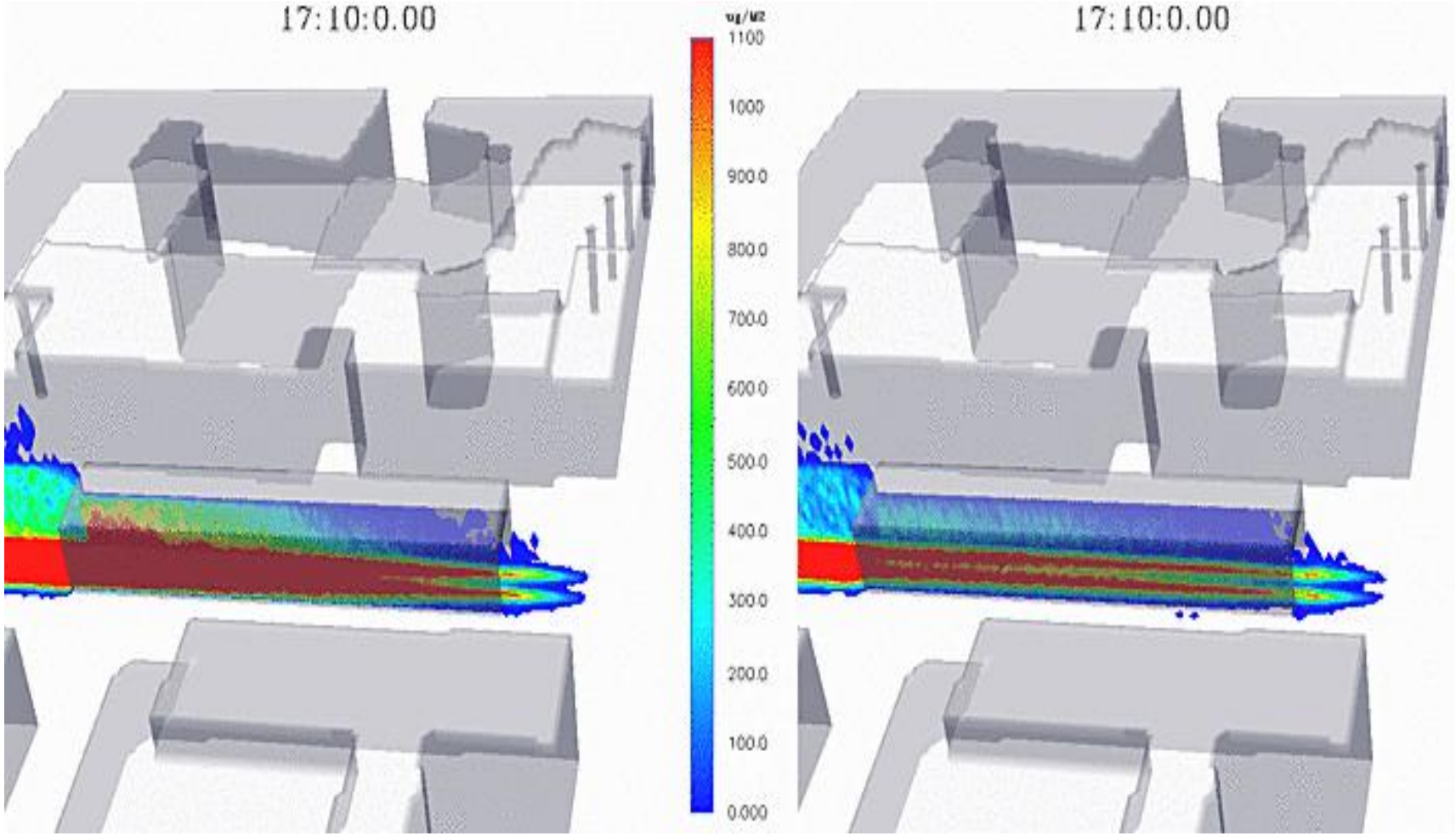
- **Comparison without/with for the façade configuration**

EXP'AIR Base case : tunnel access



- **Comparison without/with on a tunnel access**

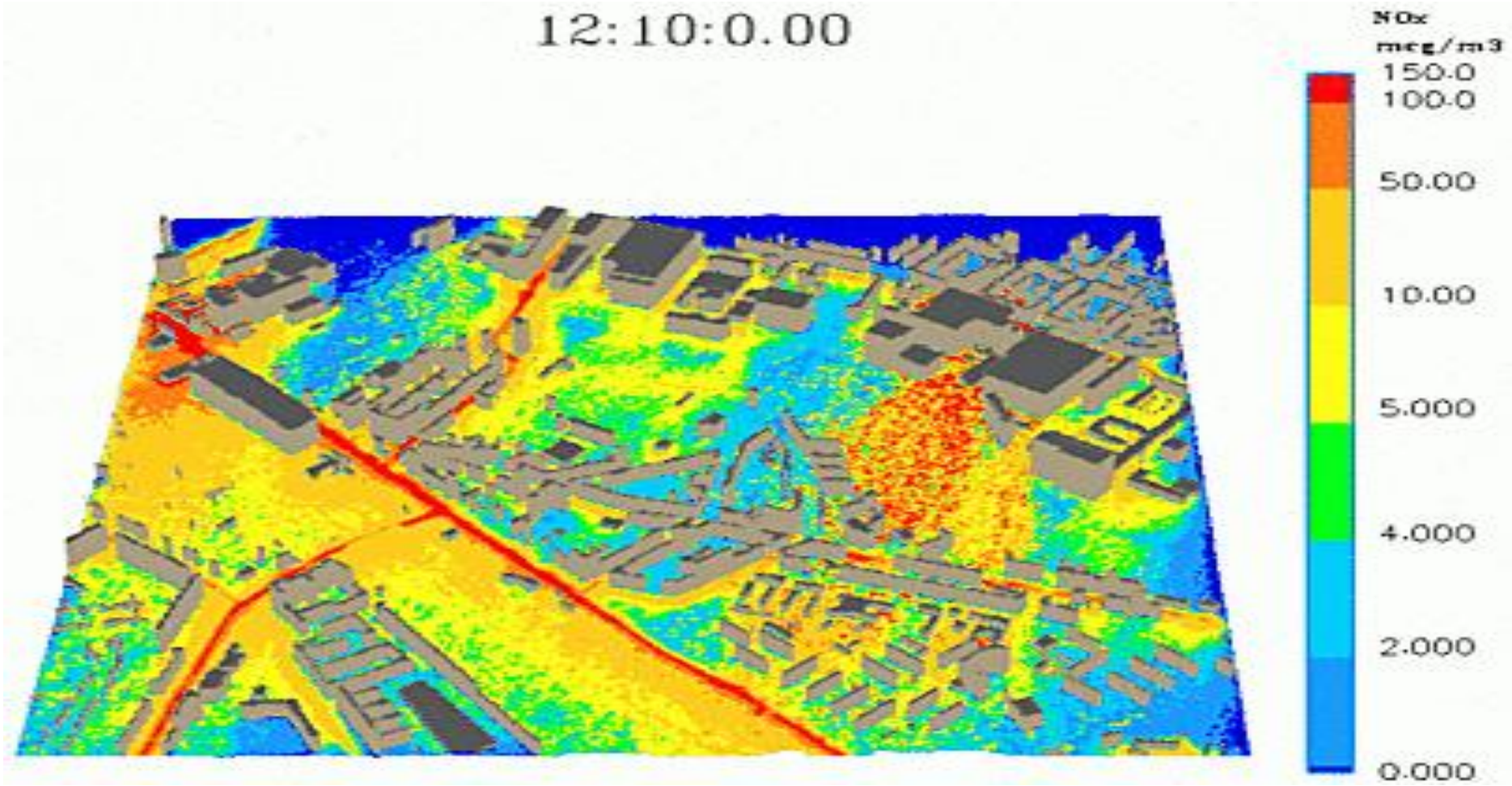
EXP'AIR Base case : tunnel



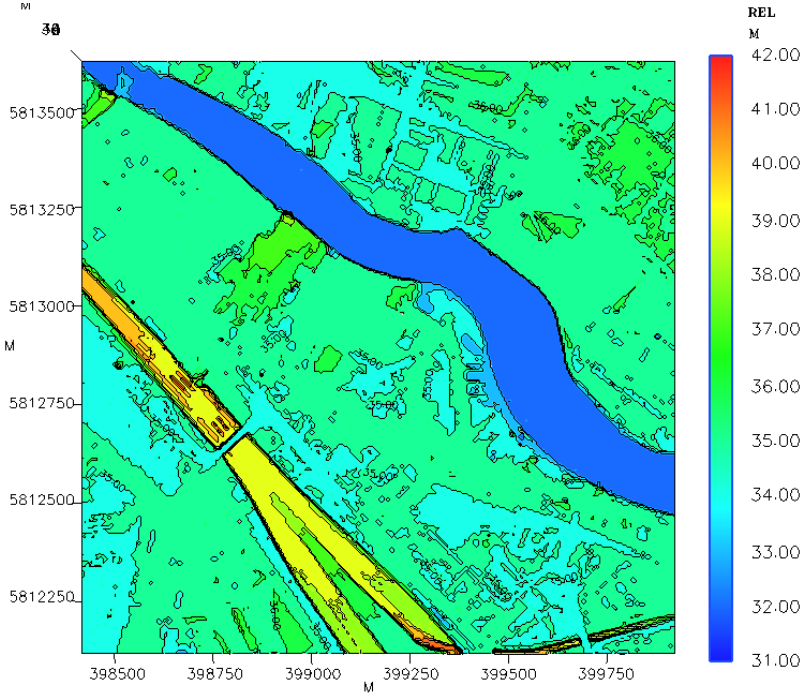
- **Comparison without/with on a tunnel**

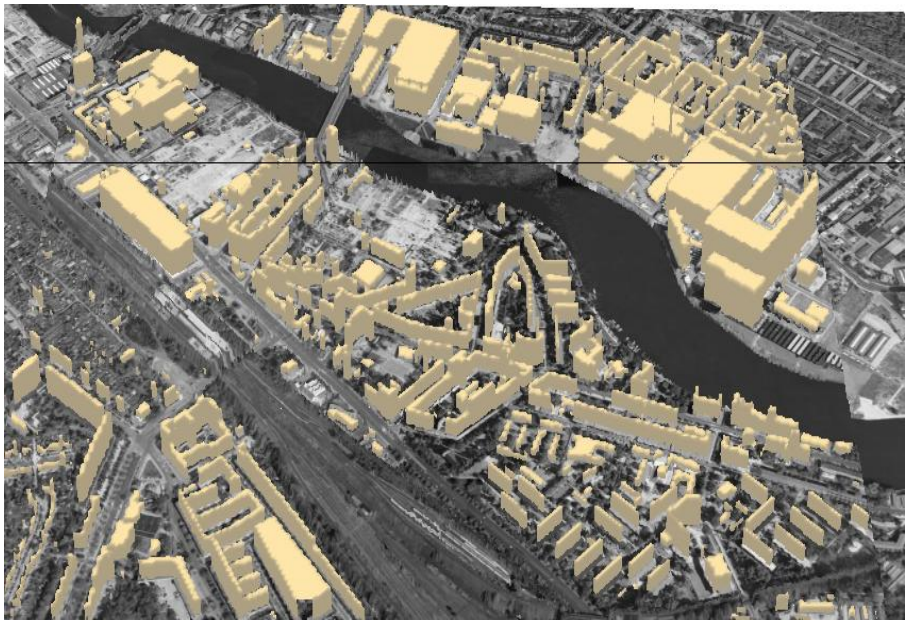
District case

Realistic situation on Berlin area



District study details

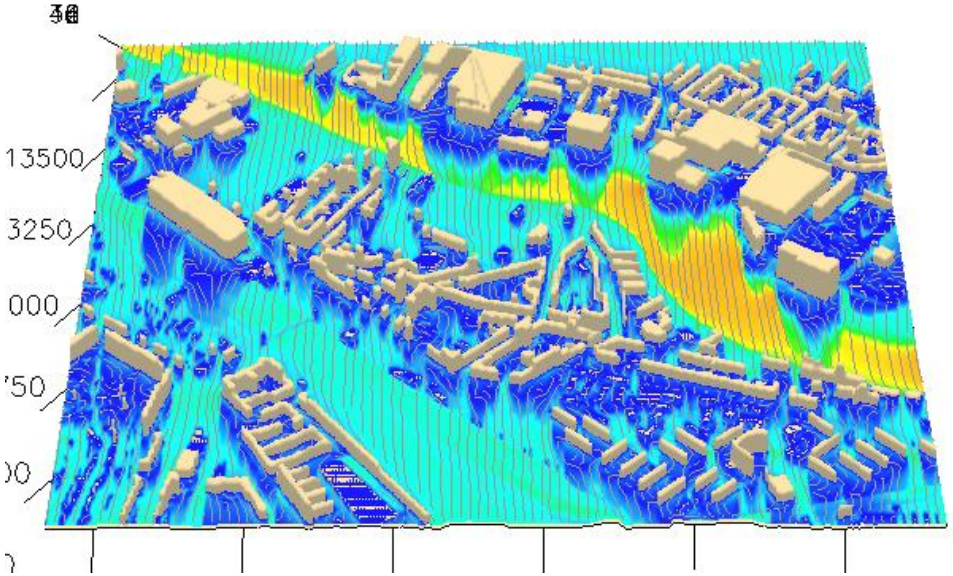


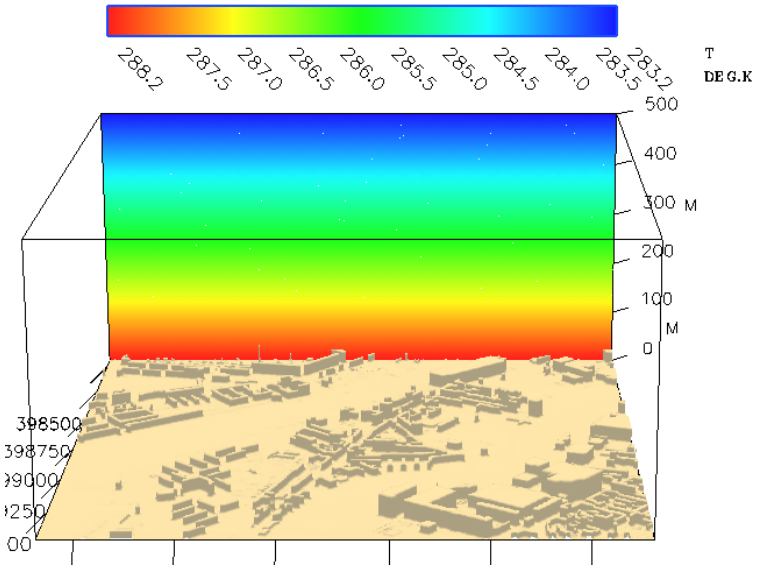


- **Berlin neighbourhood: 1,5 km x 1,5 km**
- **Grid cell size : 5 m**
- **Grid size: 301 x 302 x 27**
- **Domain top : 500 m**
- **High resolution vertical grid within obstacles, coarser and expanding above**

District study: met conditions

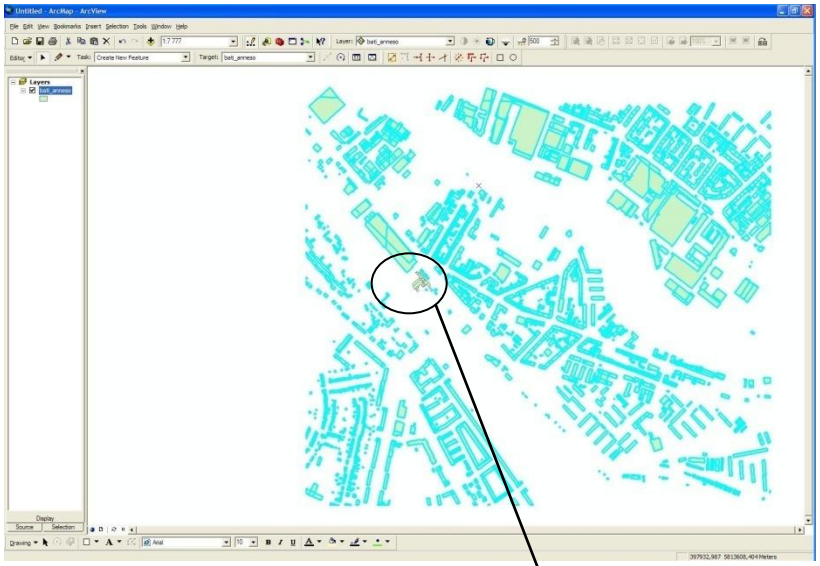
- **Academic inflow wind profile (power law) identical to other EXP'AIR cases**
- **Time-dependent wind rotation over one hour: 0° (North) to 90° (East)**
- **Wind speed at 5 m above ground set to 2 m/s**
- **Flow influenced by roughness and buildings**
- **Neutral conditions (most likely in urban conditions)**





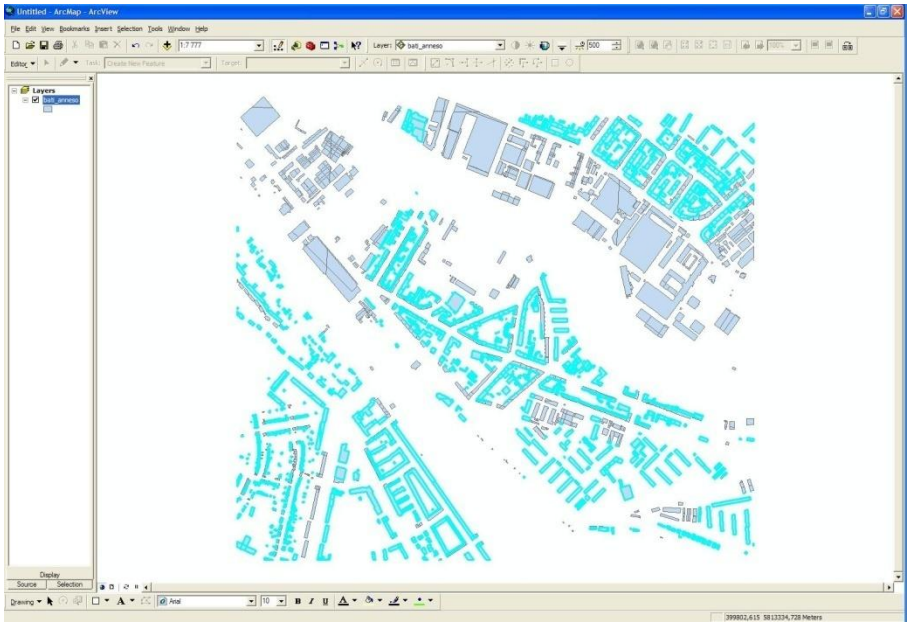
District study: roof process

At roof level, except for the train station, all roofs processed



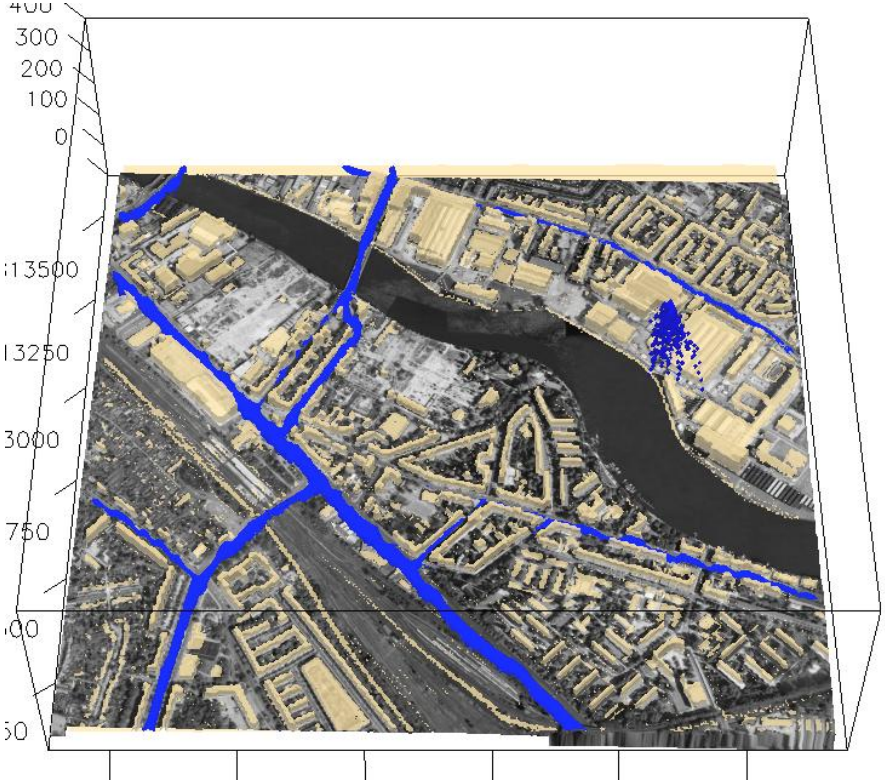
District study: facades process

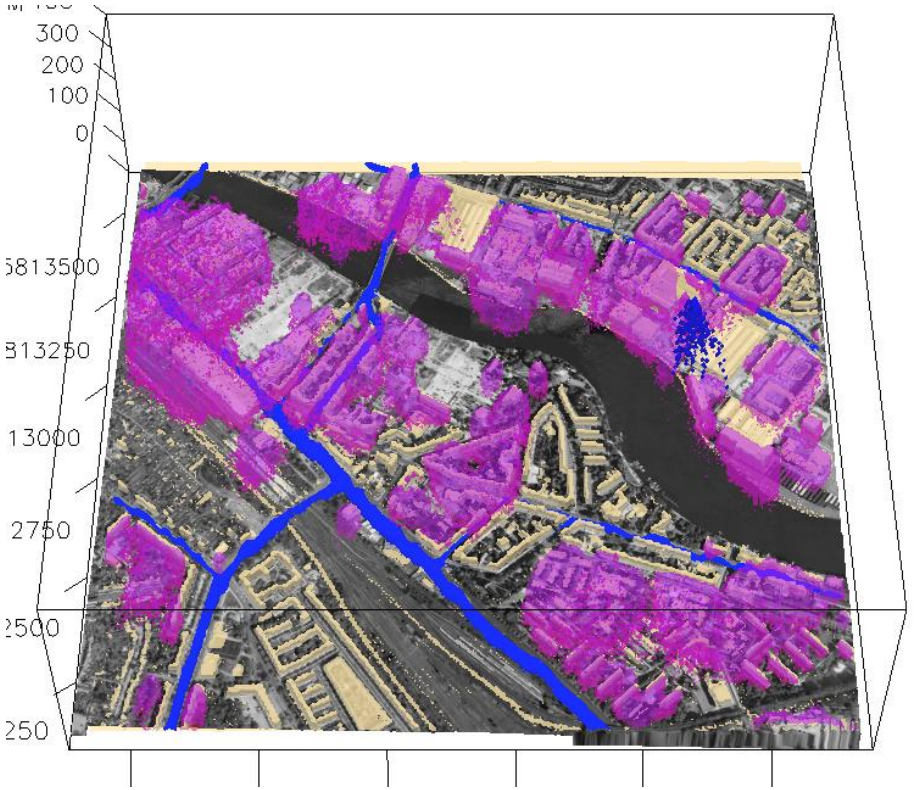
- **Facades: GIS selection of processed facades**



District study: emissions

- **Area sources:** 667 area sources for NOx considered at roof level
- **Line sources:** 49 traffic links
- **Point source:** 1 stack only





District study: control volumes

The control volumes where concentrations are computed to estimate percentage reductions are the following, in the district case :

- **« canopy » volume : between ground (0m) and 42 m AGL**
- **« residential » volume : between ground (0 m) and 20 m AGL,**
- **« traffic » volume : between ground (0 m) and 3 m AGL**
- **« roof » volume: between 20 m and 42 m AGL**

In all cases, we ignore full cells (buildings) and cells above the river;

District study: sample results

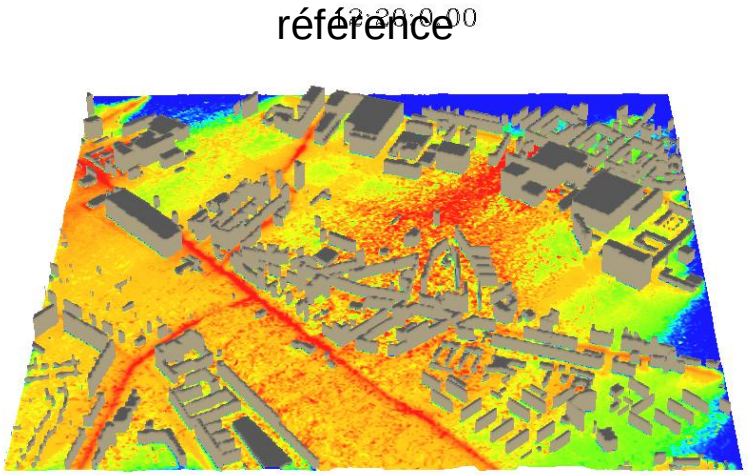
Traffic + area sources

- Roof processed : 6,5 % to 8,5 % reduction on average Nox concentration;
- Steet and facade process : 33% (volume roof) to 40,9 % (volume residential) : 37% in canopy

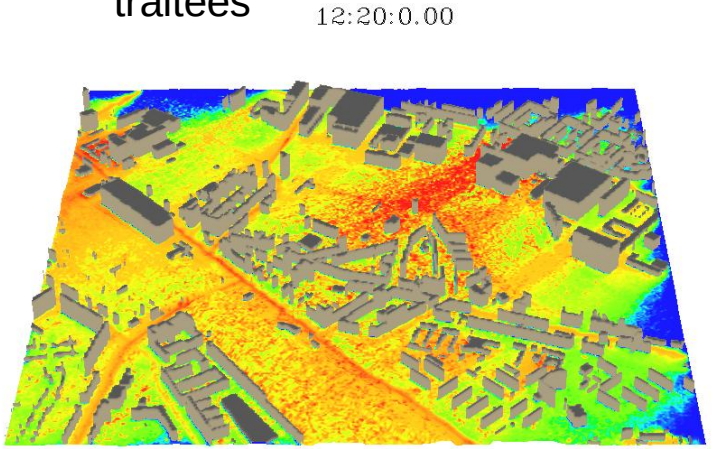
	Cas référence	Chaussée+mur+toit		Chaussée+mur		Toit	
	Concentration (µg/m3)	Concentration (µg/m3)	Ecart relatif (%)	Concentration (µg/m3)	Ecart relatif (%)	Concentration (µg/m3)	Ecart relatif (%)
Volume canopée	14,67	8,30	43,41	9,23	37,13	13,58	7,48
Volume habitation	15,58	8,36	46,37	9,21	40,90	14,57	6,48
Volume trafic	15,61	8,68	44,36	9,66	38,12	14,88	4,64
Volume toit	13,83	8,24	40,42	9,25	33,17	12,65	8,54

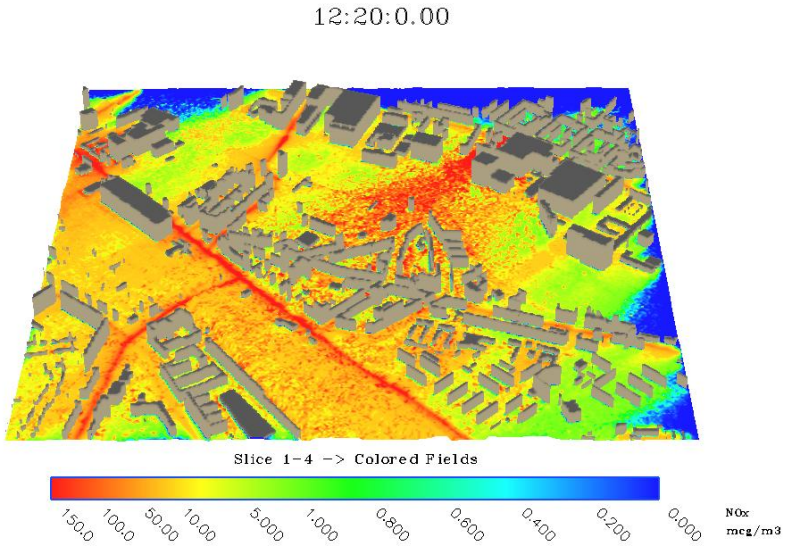
Concentrations at 1,5 m AGL

Cas de référence

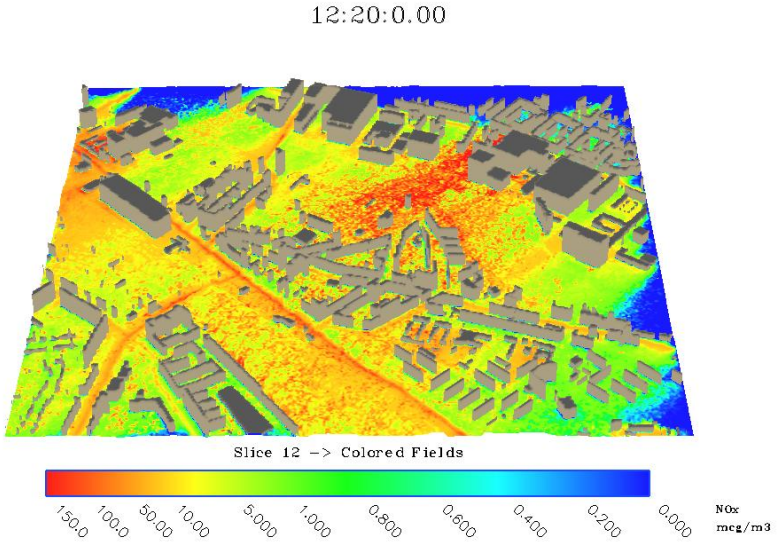


Chaussées et façades traitées





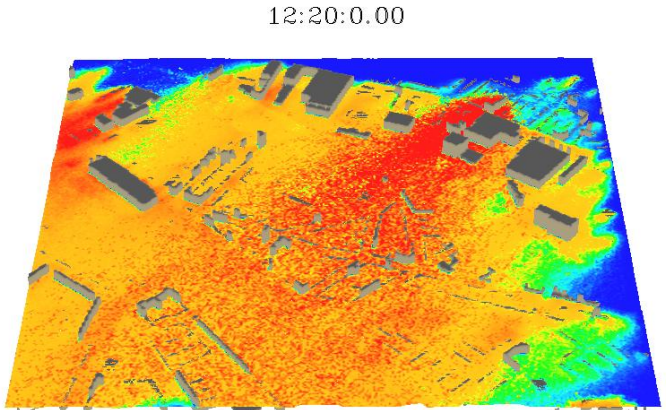
Toits traités



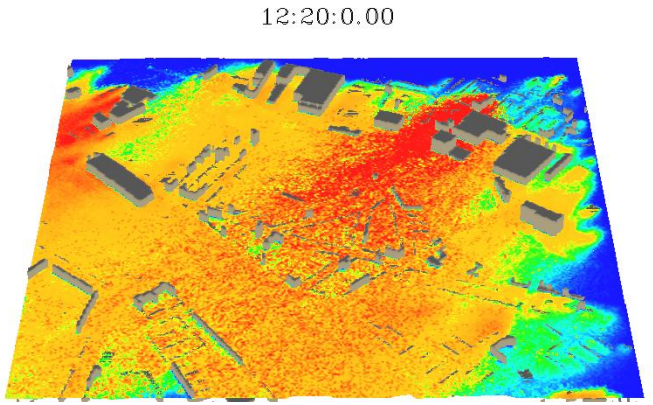
Chaussées, toits et façades traités

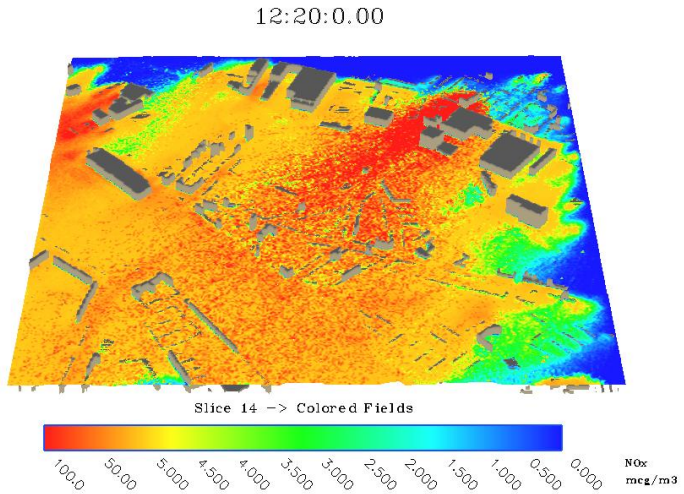
Concentrations at 15 m AGL

Cas de référence

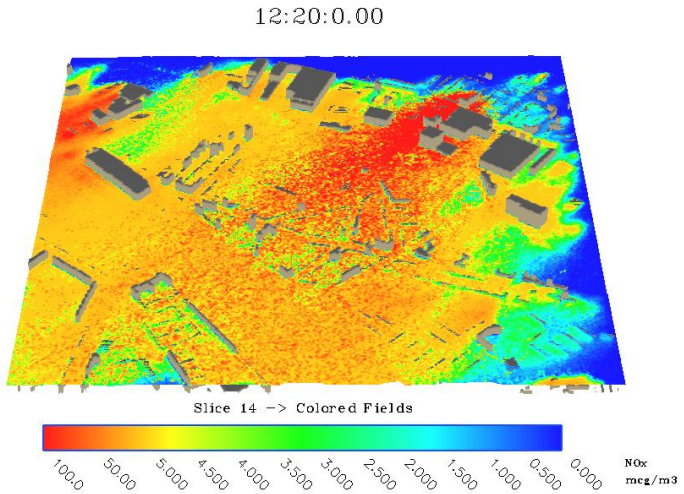


Chaussées et façades traitées





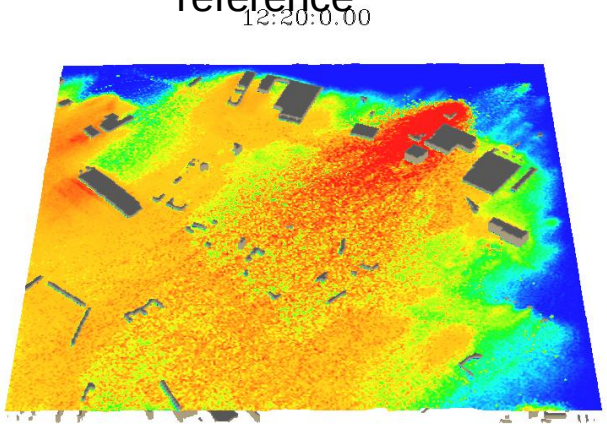
Toits traités



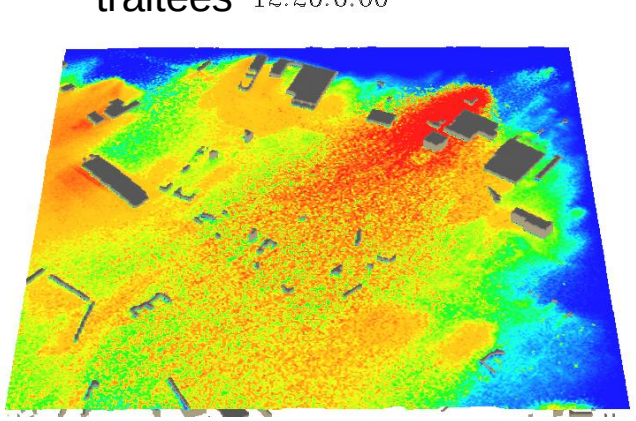
Chaussées, toits et façades traités

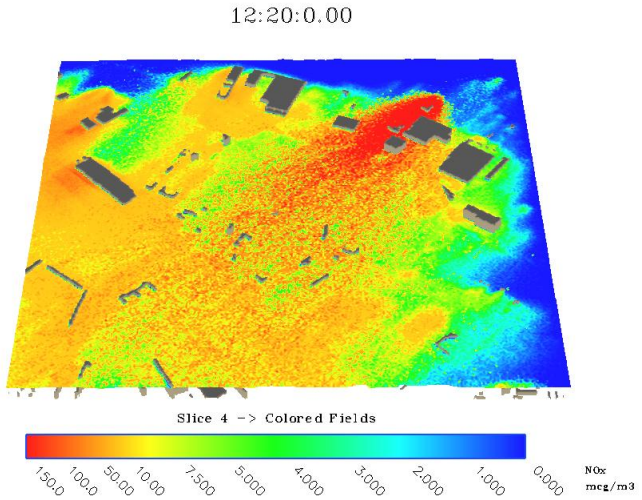
Concentrations at 25 m AGL

Cas de référence

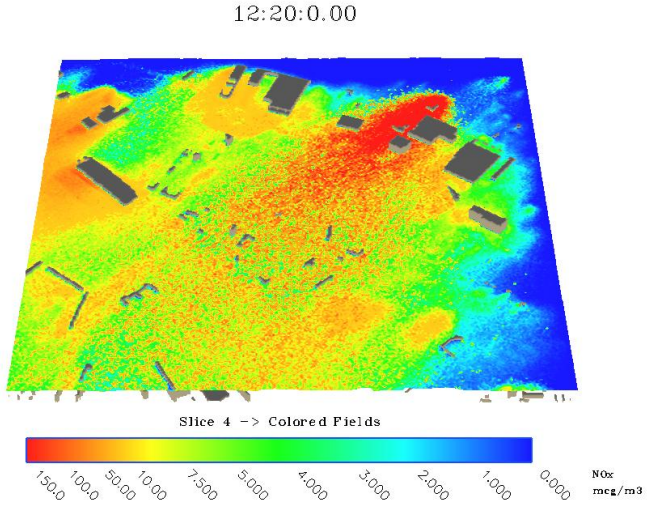


Chaussées et façades traitées



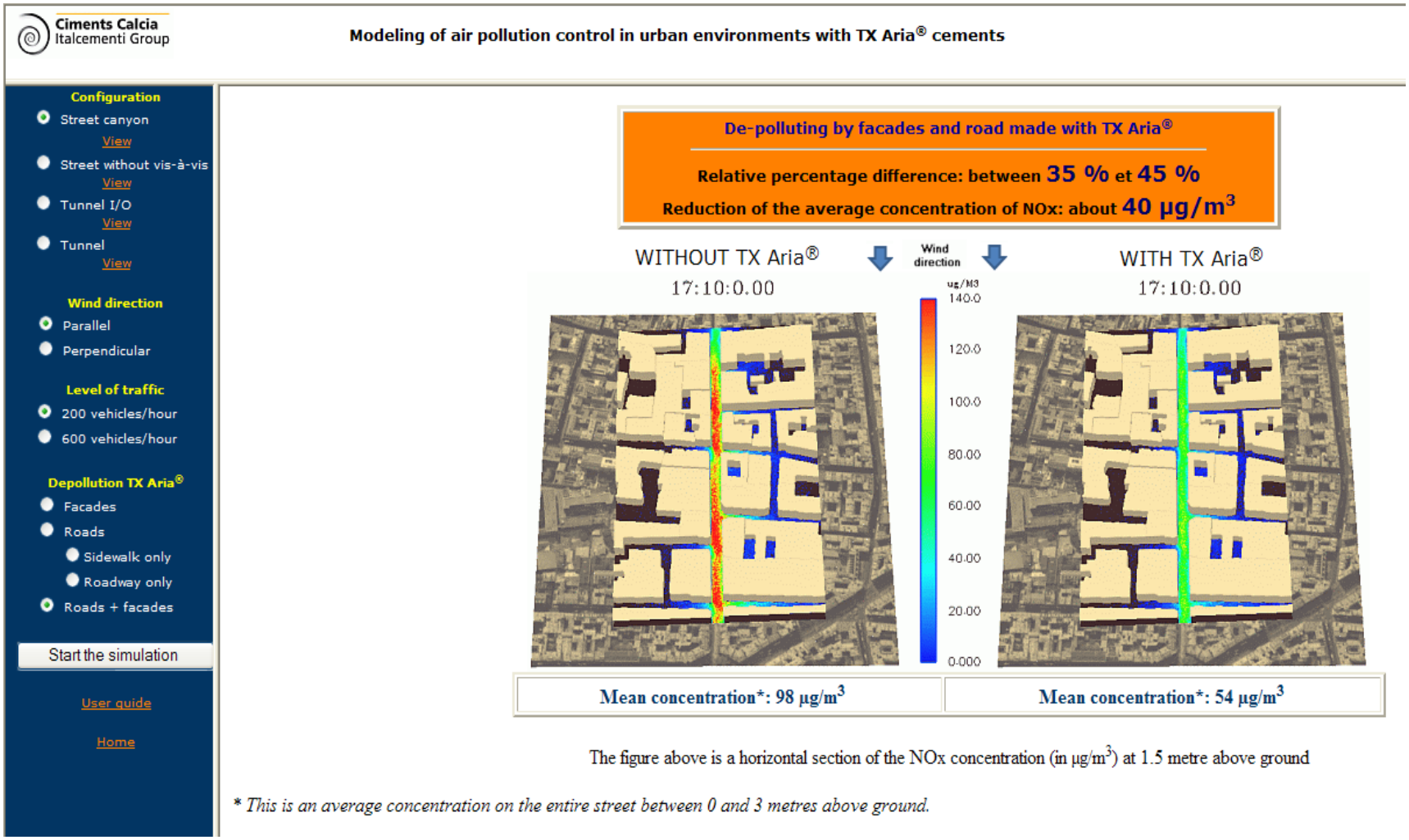


Toits traités



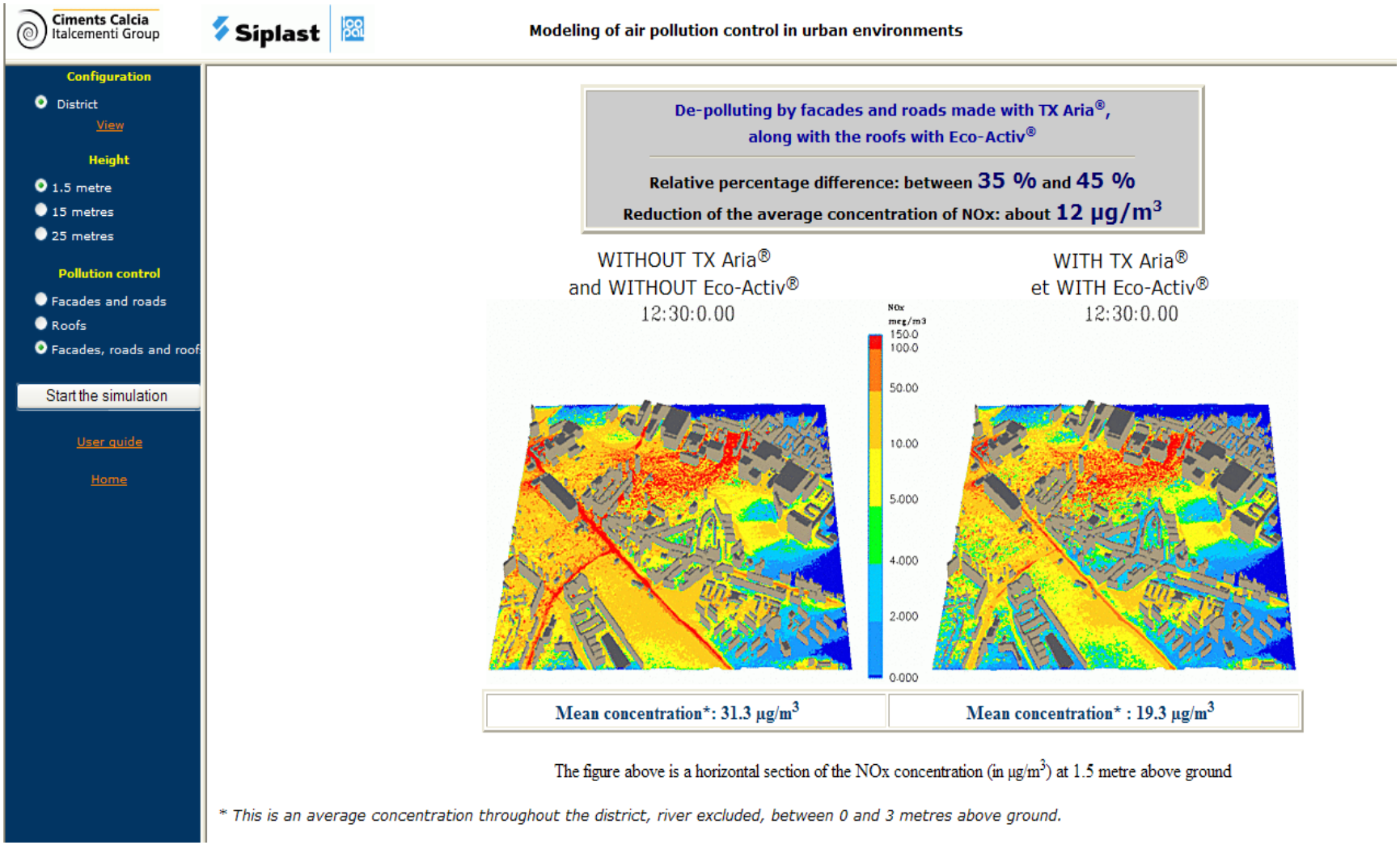
Chaussées, toits et façades traités

EXP'AIR GUI / Base cases



- **Comparison without/with on a canyon street**

EXP'AIR GUI / District case



- **Comparison without/with on a district basis**

Conclusions

- **Tool developed**
- **Open to completion with full CFD results**
- **Link to be made with PHOTOPAQ Project (see Nick MOUSSIOPOULOS for details)**
- **Operational data needed for various types of coatings (deposition velocity).**

ARIA TECHNOLOGIES

Thank you for your attention

Questions ?