



# PROGRESS IN URBAN AIR QUALITY ASSESSMENT: CFD MODELLING OF A WHOLE TOWN IN SPAIN

E. Rivas<sup>1</sup>, J.L. Santiago<sup>1</sup>, F. Martin<sup>1</sup>, A. Ariño<sup>2</sup>, J.M. Santamaría<sup>3</sup>, J.J. Pons<sup>4</sup>

<sup>1</sup>Atmospheric Pollution Division, Environmental Department, CIEMAT, Spain

<sup>2</sup>Environmental Biology Department, University of Navarra, Spain

<sup>3</sup>Chemistry Department, University of Navarra, Spain

<sup>4</sup>Department of History, History of Art and Geography, University of Navarra, Spain

*esther.rivas@ciemat.es*



Introduction

Area of Study and Experimental Data

Modelling Approach

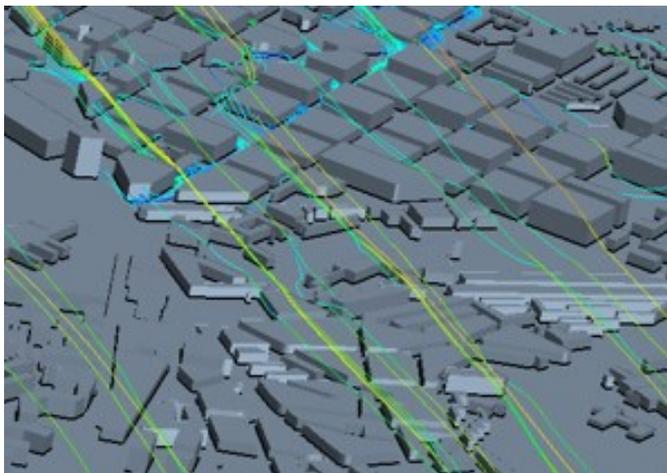
- ❖ *CFD model description and simulation setup*
- ❖ *Numerical methodology*

Results

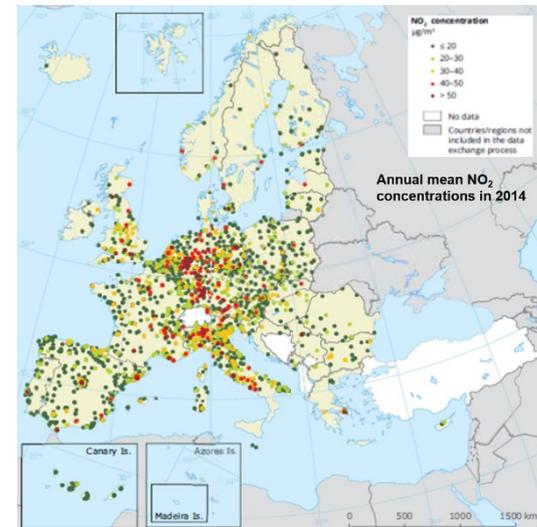
- ❖ *Model evaluation with air quality monitoring stations*
- ❖ *Model evaluation against experimental data from cyclists with microsensors*

Conclusions

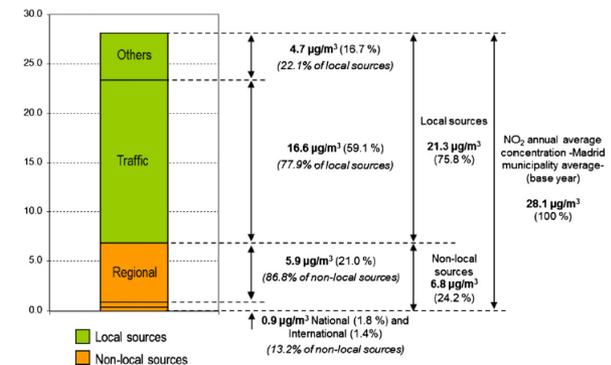
- ❑ *Urban air quality as big environmental problem*
- ❑ *Air pollution vs. human health*
- ❑ *Main source: The road traffic.*



Perspective view of the wind lines in Pamplona when the wind blows North direction.



Red and dark red dots correspond to values above the EU annual limit value and the WHO AQG ( $40 \mu\text{g}/\text{m}^3$ ). Only stations with  $> 75\%$  % of valid data have been included in the map (EEA, 2016a).



Result of the source apportionment analysis (annual  $\text{NO}_2$  mean for the whole Madrid municipality) (Borge et al. 2014).

- ❑ LIFE-RESPIRA project goal: To improve urban air quality and reduce exposure to air pollution by promoting healthy and sustainable mobility.
- ❑ Our LIFE+RESPIRA project task: To develop of an specific tool able to reproduce accurate pollutant maps of the Pamplona's city (Spain).
- ❑ **Objective of this work**: To compute the 2016 hourly  $\text{NO}_2$ ,  $\text{NO}$  and  $\text{NO}_x$  maps for annual and seasonal average days by means of a CFD-RANS methodology.

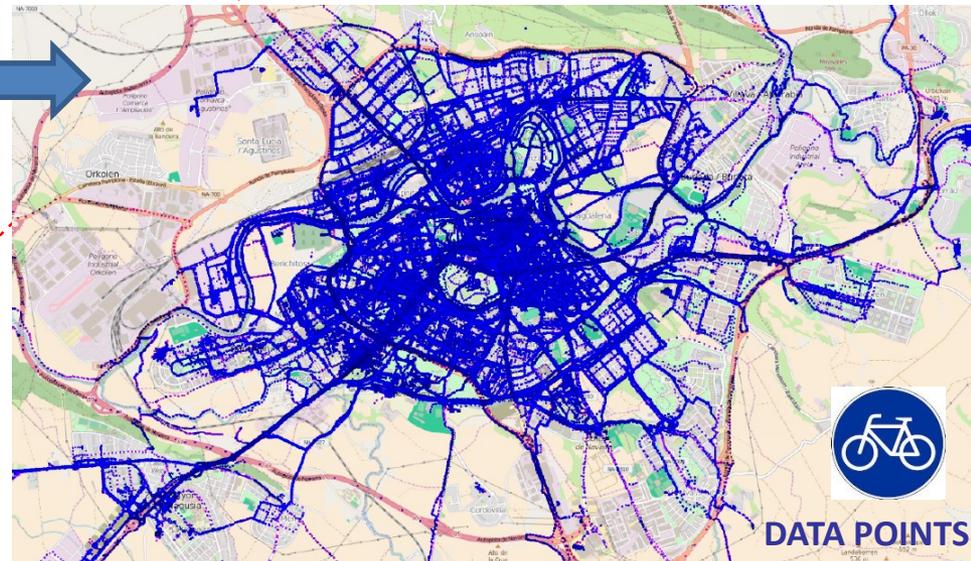


# Area of Study and Experimental Data

## Urban Morphology and Large-scale monitoring



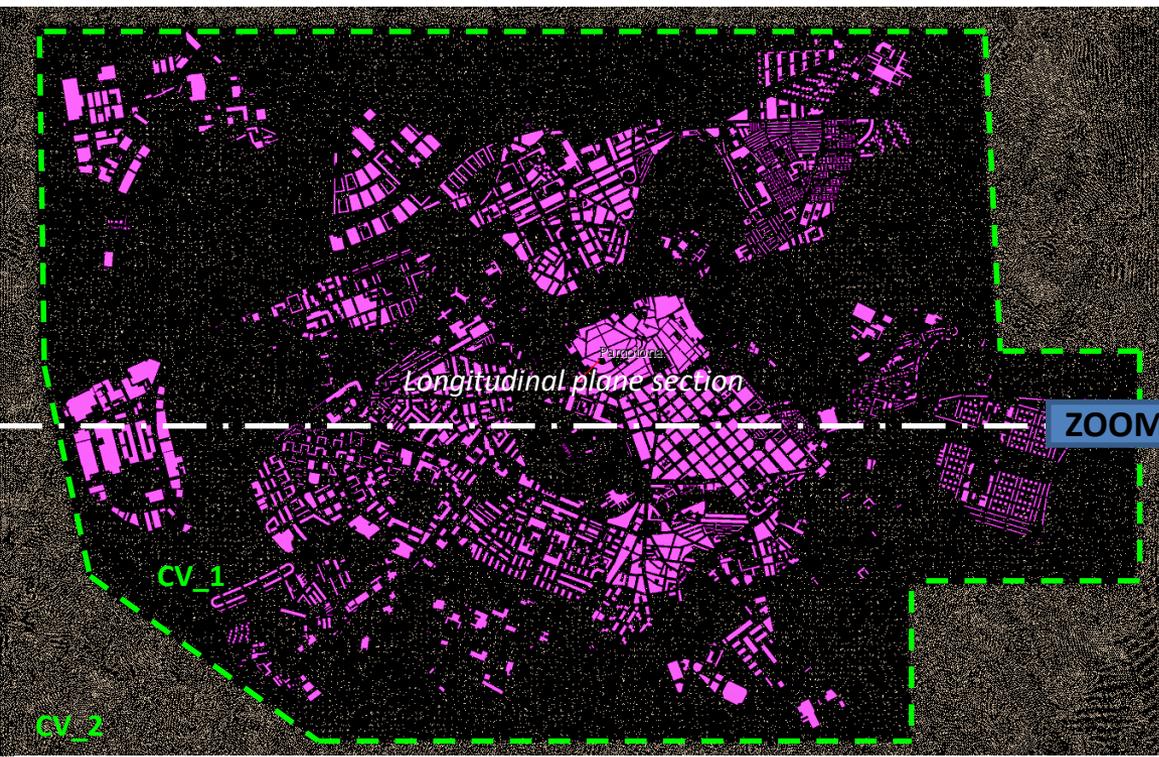
Pamplona  
(Source: Google Earth)



Aerial view of Pamplona's City  
(Source: Google Earth)

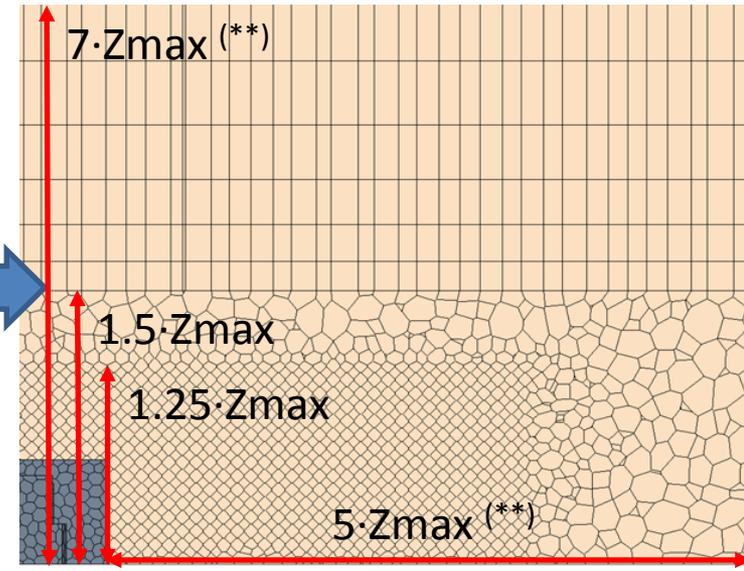
Roads traveled by cyclists during 2016  
(provided by University of Navarra)

## CFD model description and simulation setup: Mesh Model



CFD Mesh model (\*)

Total number of cells:  $44.6 \times 10^6$



$Z_{max} = 70\text{m}$

(\*) CFD tool: STAR-CCM+9.04.011®

(\*\*) Franke et al. 2007

## CFD model description and simulation setup: Physical Models

*Steady State Simulations*

*Segregated Flow Model*

*RANS as turbulent approach:*

- *Realizable K- $\epsilon$  Two-Layer model*
- *All Y+ wall hybrid treatment*

*Neutral atmospheric conditions*

*Constant air density*

*Default values of STAR-CCM + 9.04.011<sup>®</sup> as free parameters of the turbulent model*

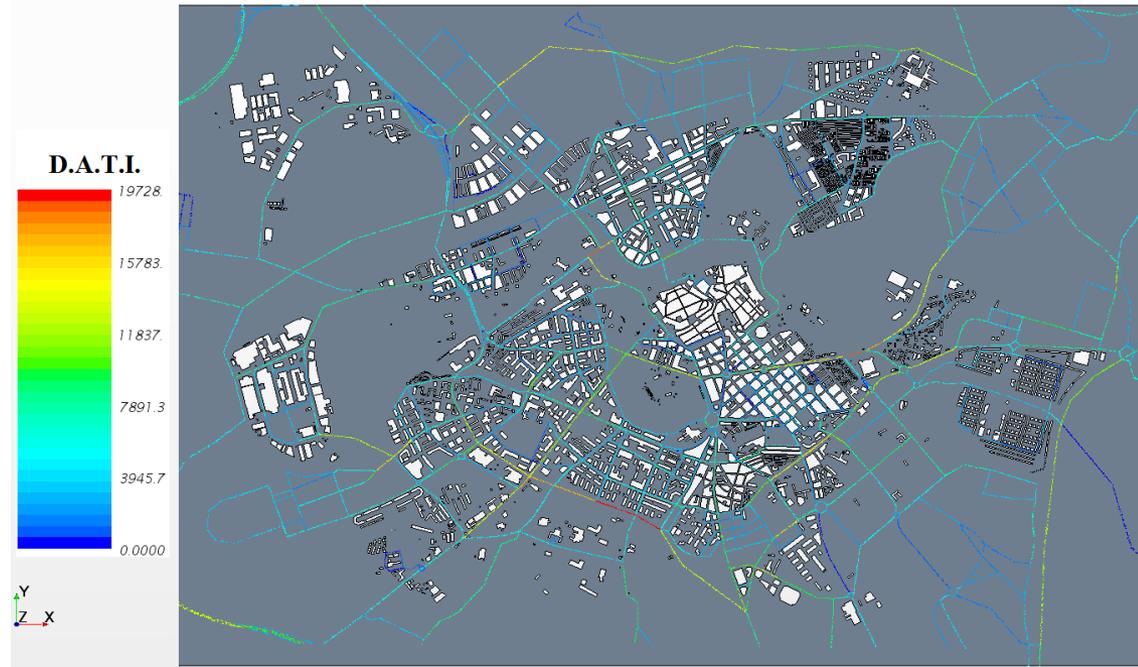
## CFD model description and simulation setup: NOx dispersion

+ *an additional passive scalar transport equation*

$$\left\{ \partial_j \left( \rho u_j C_{CFD}(\vec{r}) - \frac{\mu_{eff}}{Sc_t} \partial_j C_{CFD}(\vec{r}) \right) = S_C \right\}_{j=x,y,z}$$

+ *Pollutant emissions at roads proportional to traffic intensity*

+ *Without atmospheric chemistry*



Daily Average Traffic Intensity map in Pamplona's city

## CFD model description and simulation setup: Boundary Conditions

□ Building: Solid boundary with surface specification: smooth

□ Ground: Solid boundary with surface specification: roughness

□ Inlet<sup>(\*)</sup>:  $u(z) = \frac{u_*}{\kappa} \ln\left(\frac{z + z_0}{z_0}\right); k = \frac{u_*^2}{\sqrt{C_\mu}}; \varepsilon = \frac{u_*^3}{\kappa \cdot (z + z_0)}$

□ Outlet:  $\Delta P_{in-out} = 0$

□ Top: Symmetry boundary condition

(\*) Richards & Hoxey 1993

# Modelling approach

## Numerical Methodology (\*)

CFD Simulations  
 $\{u_M\}_{i=1,\dots,16}$  - scenarios

$\{C_{CFD,i}\}_{i=1,\dots,16}$

Meteorological Data: Pamplona GN Met. St. (\*\*)  
 $i$ -scenario  $\rightarrow \{f_i(t), \overline{u_{ref,i}(t)}\}_{t=1,\dots,24}$  - hour

Pollutants Conc. Data: Pamplona Pza. Cruz A.Q. St.  $\vec{r}_0$   
 $\{(\overline{C_O(\vec{r}_0,t)})_{NO_x}, (\overline{C_O(\vec{r}_0,t)})_{NO_2}, (\overline{C_O(\vec{r}_0,t)})_{NO}\}_{t=1,\dots,24}$

**NO<sub>x</sub> maps**

$$(C_M(t))_{NO_x} = \left[ \sum_{i=1}^{16} f_i(t) \cdot C_{CFD,i} \cdot \frac{u_M}{u_{ref,i}(t)} \right] \cdot E(t)$$

$E(t) : (C_M(\vec{r}_0,t))_{NO_x} = (\overline{C_O(\vec{r}_0,t)})_{NO_x}$

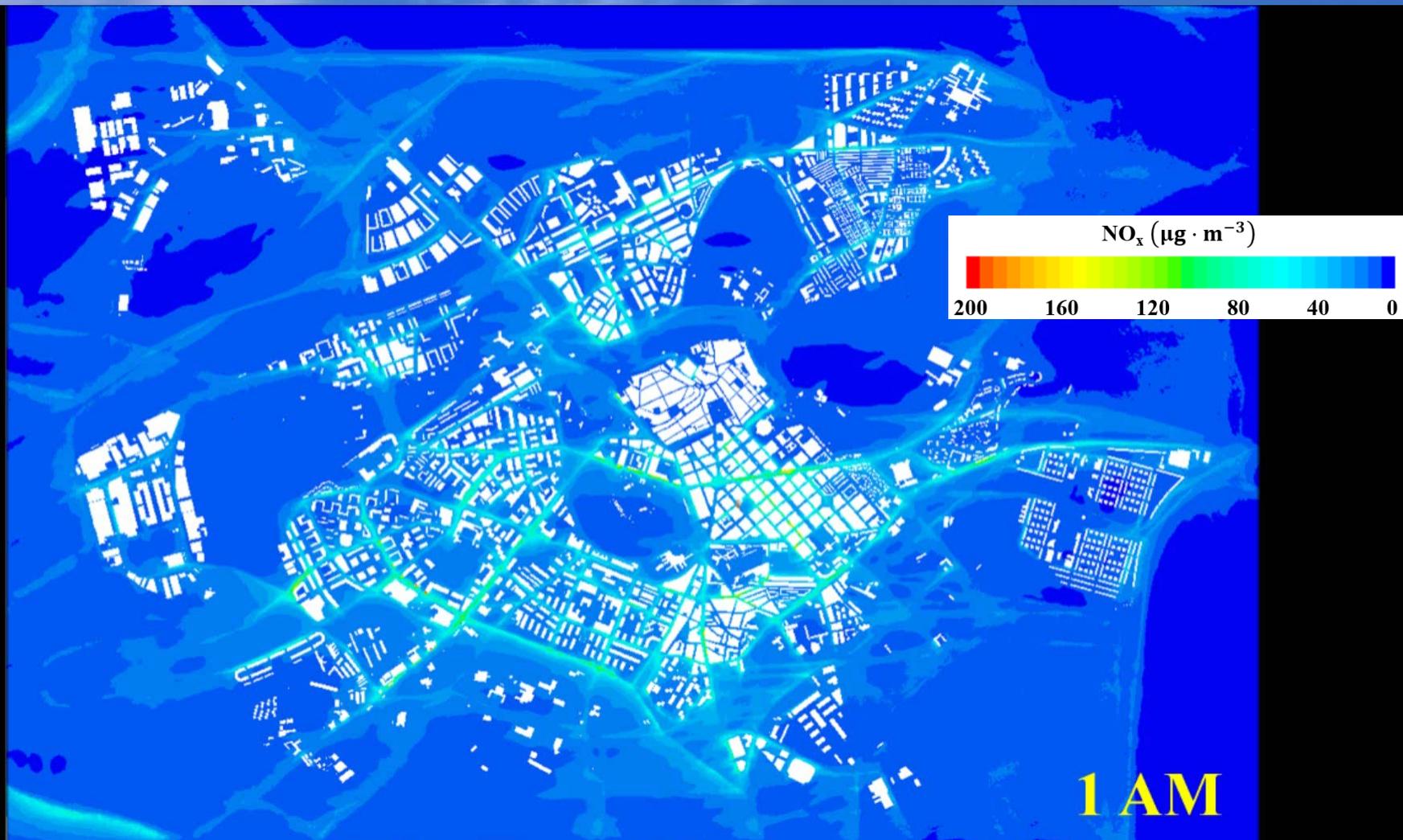


**NO and NO<sub>2</sub> maps**

$$(C_M(t))_{NO_2 \text{ or } NO} = (C_M(t))_{NO_x} \cdot \frac{(\overline{C_O(\vec{r}_0,t)})_{NO_2 \text{ or } NO}}{(\overline{C_O(\vec{r}_0,t)})_{NO_x}}$$

(\*) Parra et al. 2010  
 Santiago et al. 2013  
 Santiago et al. 2017  
 (\*\*) Source: GN

# Results

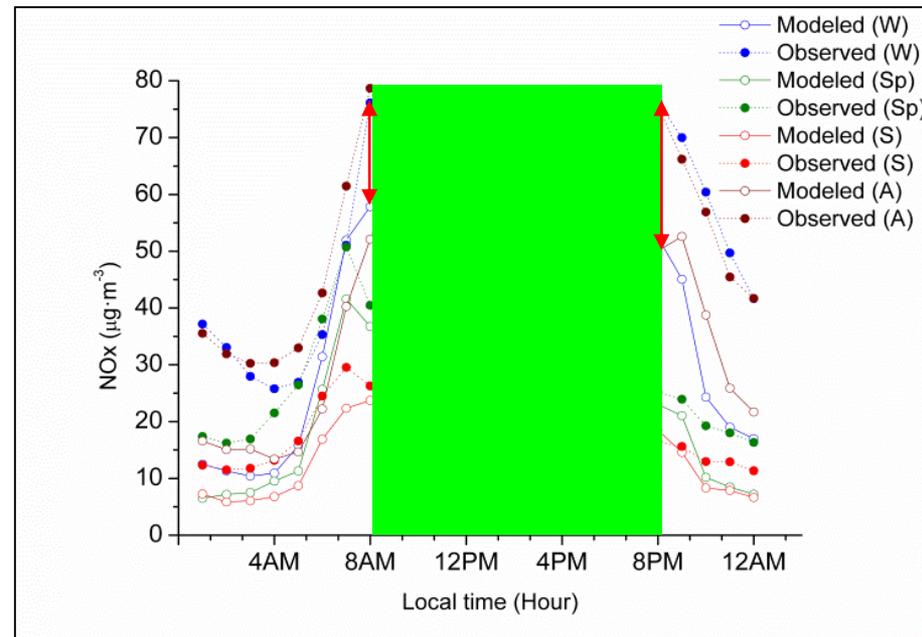
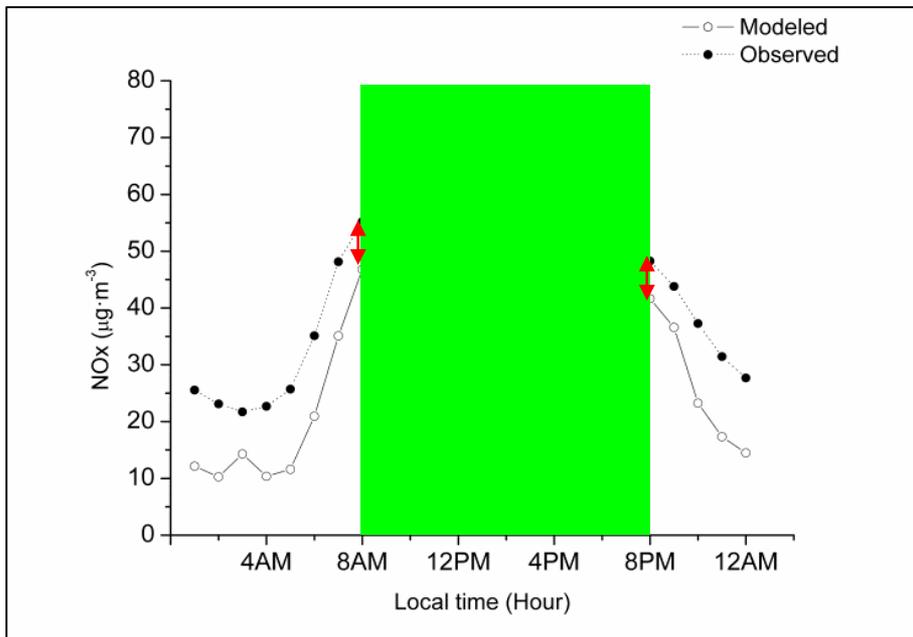


High resolution hourly maps of NO<sub>x</sub> annual averaged concentration during 2016 at pedestrian level

## Model evaluation with air quality monitoring stations



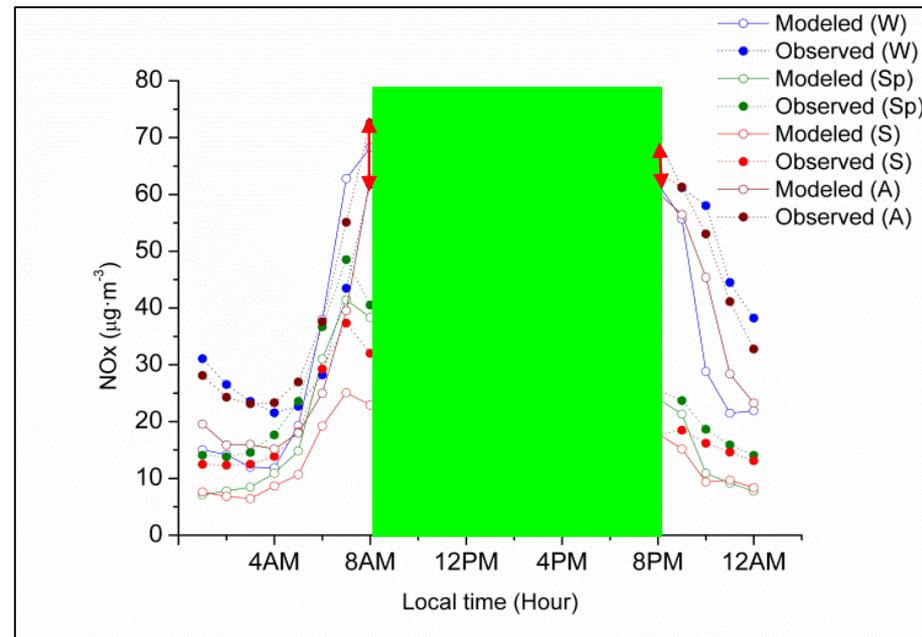
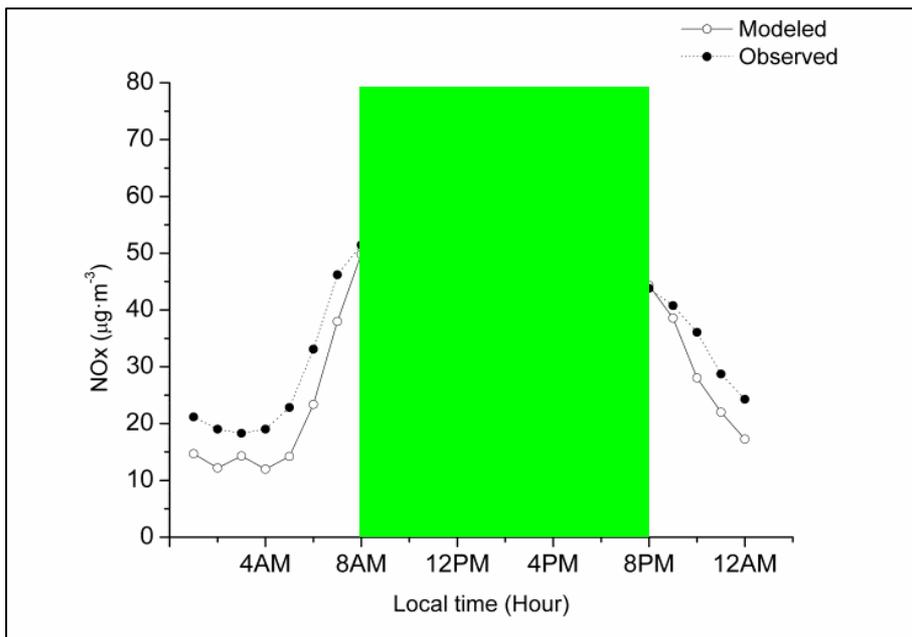
## Model evaluation with air quality monitoring stations: NO<sub>x</sub>



	Pamplona-Rotxapea					
	RE Max	Hour	R	NMSE	FB	FAC2
2016-average annual day	55.5	2AM	0.843	0.080	-0.282	83.3
2016-average spring day	62.7	1AM	0.807	0.108	-0.298	70.8
2016-average summer day	50.1	11AM	0.666	0.108	-0.103	100.0
2016-average autumn day	55.9	4AM	0.826	0.099	-0.325	83.3
2016-average winter day	66.4	1AM	0.814	0.161	-0.439	70.8

NMSE < 1.5  
 - 0.3 < FB < 0.3  
 (\*) Chang & Hanna 2005  
 Goricsán et al. 2011

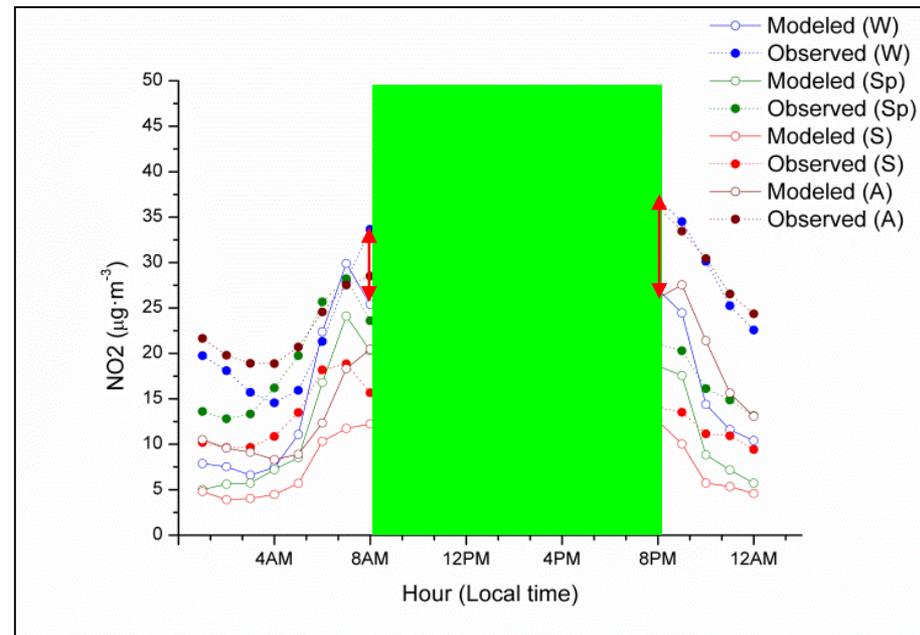
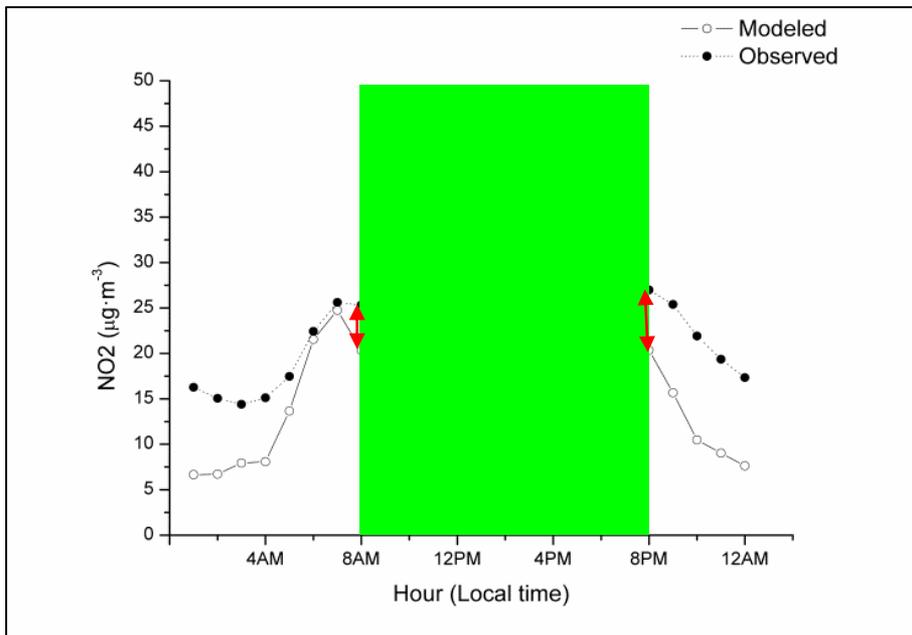
## Model evaluation with air quality monitoring stations: NO<sub>x</sub>



	Pamplona-Iturrama					
	RE Max	Hour	R	NMAE	FB	FAC2
2016-average annual day	37.8	5AM	0.890	0.179	-0.094	100.0
2016-average spring day	49.6	1AM	0.895	0.214	-0.173	100.0
2016-average summer day	48.5	3AM	0.811	0.247	-0.187	100.0
2016-average autumn day	47.4	5PM	0.860	0.212	-0.097	100.0
2016-average winter day	51.8	11PM	0.817	0.245	-0.193	87.5

NMSE < 1.5  
 - 0.3 < FB < 0.3  
 (\*) Chang & Hanna 2005  
 Goricsán et al. 2011

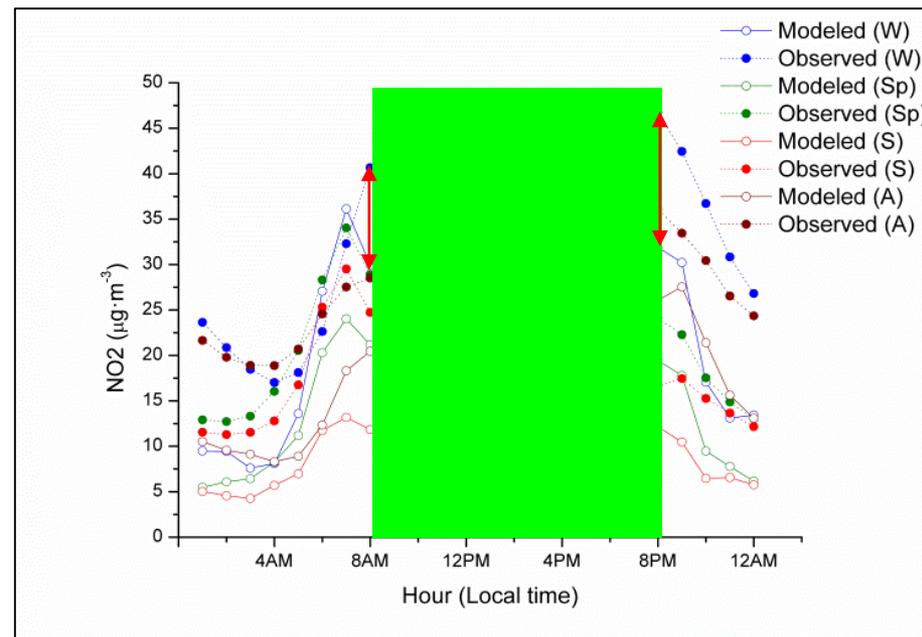
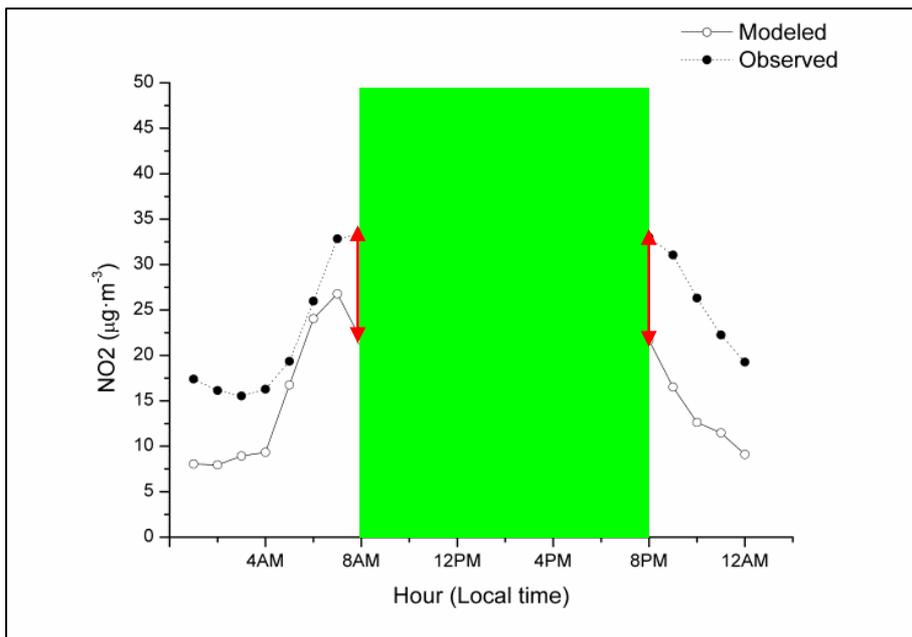
## Model evaluation with air quality monitoring stations: NO<sub>2</sub>



	Pamplona-Rotxapea					
	RE Max	Hour	R	NMAE	FB	FAC2
2016-average annual day	59.1	1AM	0.683	0.250	-0.310	79.2
2016-average spring day	63.1	1AM	0.699	0.268	-0.321	70.8
2016-average summer day	59.4	2AM	0.492	0.308	-0.296	70.8
2016-average autumn day	58.3	5AM	0.893	0.307	-0.396	75.0
2016-average winter day	60.1	1AM	0.780	0.286	-0.364	75.0

NMSE < 1.5  
 - 0.3 < FB < 0.3  
 (\*) Chang & Hanna 2005  
 Goricsán et al. 2011

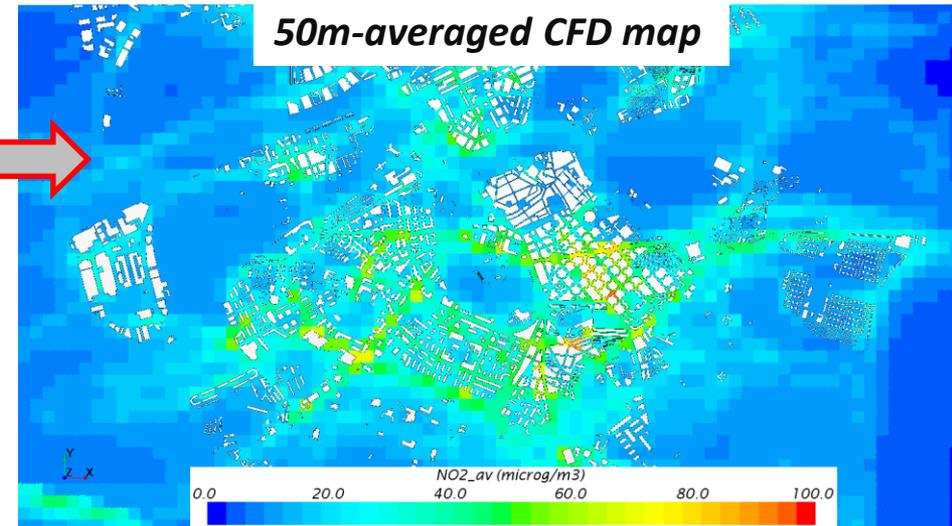
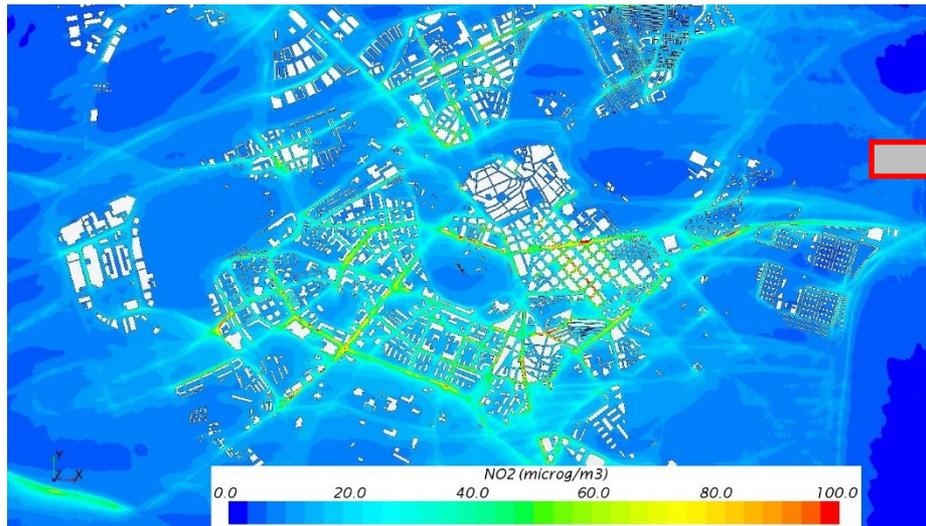
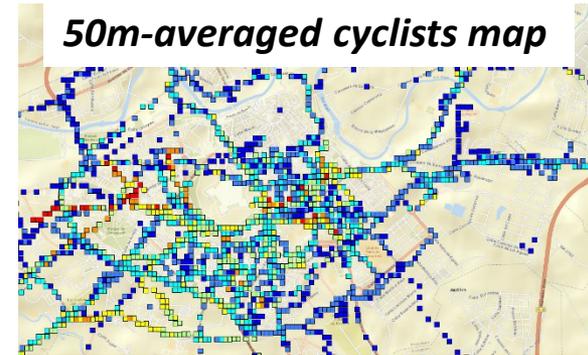
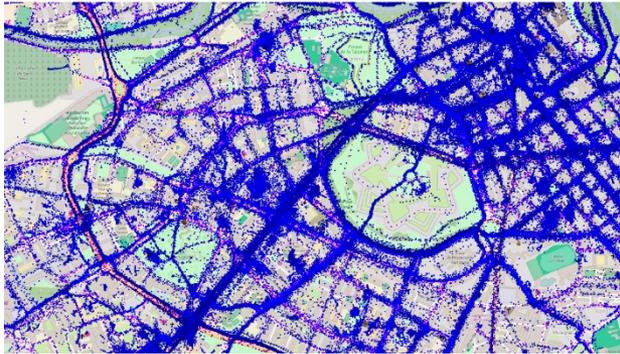
## Model evaluation with air quality monitoring stations: NO<sub>2</sub>



	Pamplona-Iturrama					
	RE Max	Hour	R	NMAE	FB	FAC2
2016-average annual day	53.7	1AM	0.754	0.296	-0.375	83.3
2016-average spring day	57.4	1AM	0.880	0.292	-0.370	83.3
2016-average summer day	62.9	3AM	0.741	0.392	-0.526	54.2
2016-average autumn day	53.5	4AM	0.853	0.346	-0.440	75.0
2016-average winter day	59.9	1AM	0.770	0.350	-0.427	75.0

NMSE < 1.5  
 - 0.3 < FB < 0.3  
 (\*) Chang & Hanna 2005  
 Goricsán et al. 2011

## Model evaluation against experimental data from cyclists with microsensors



High resolution map of NO<sub>2</sub> annual average concentration during 2015 at pedestrian level<sup>(\*)</sup>

Annual average concentration map of NO<sub>2</sub> spatially-averaged in cells of 50 x 50 m<sup>2</sup><sup>(\*)</sup>

<sup>(\*)</sup> Lechón Y. et al. *Externalities assessment of traffic related NO<sub>2</sub> emissions in the city of Pamplona (Spain)*. 14<sup>th</sup> ASAAQ Conference. 29 - 31 May 2017 – Strasbourg, France.

## Model evaluation against experimental data from cyclists with microsensors

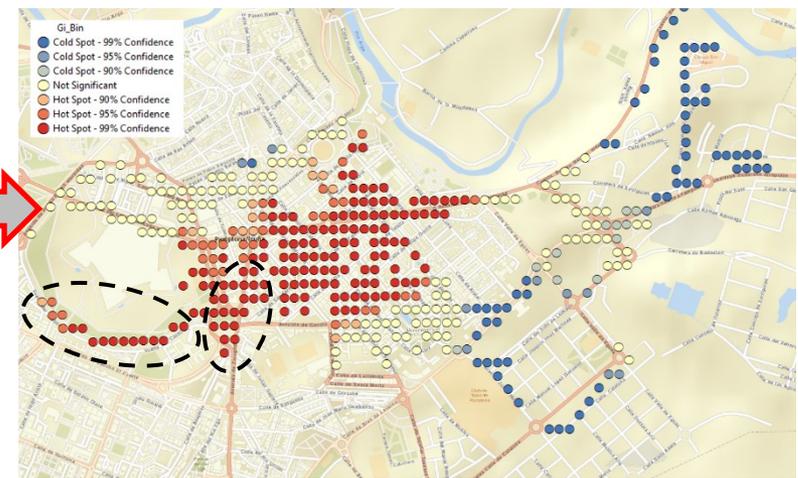
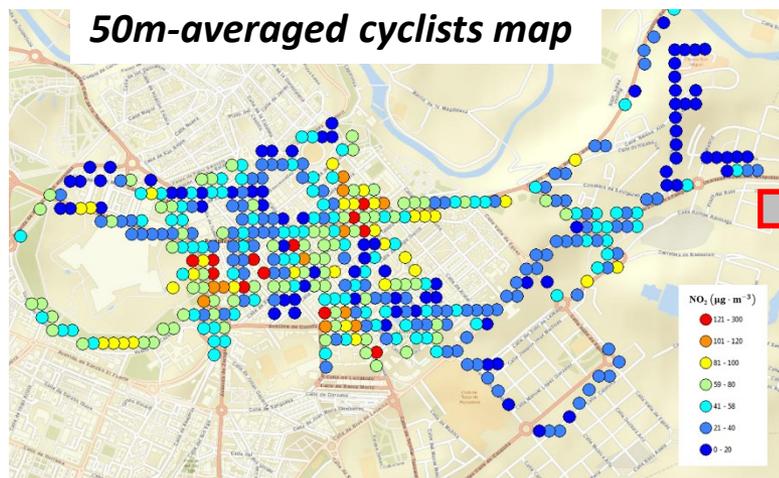
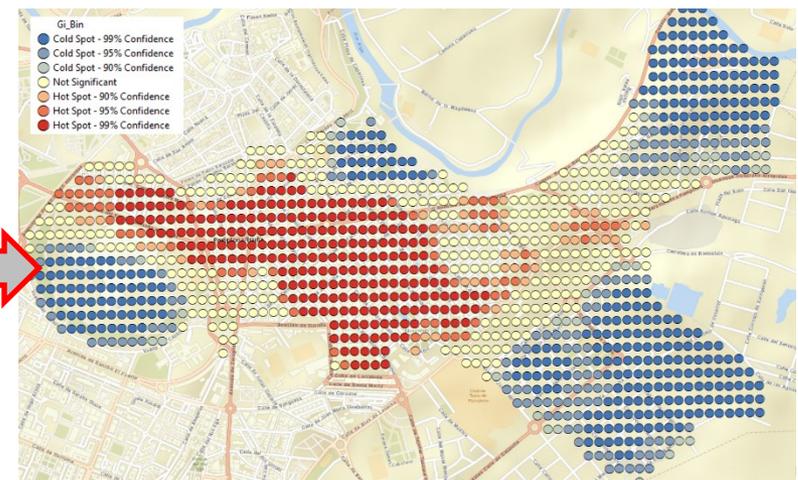
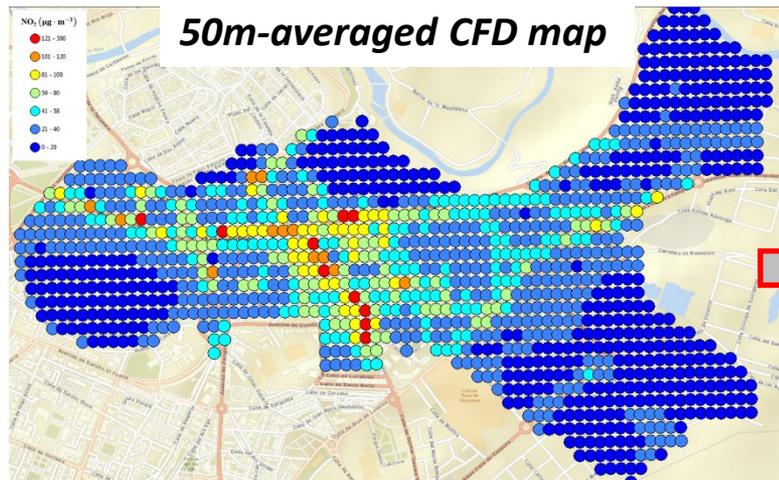
Comparison *50m-averaged CFD maps vs 50m-averaged cyclists maps* presents several difficulties:

1. In **CFD maps**, the concentration represents the average value over all cell, while in **cyclists maps**, concentration represents the average value but only over the portion of the cell where the cyclists travel.
2. Measurements from cyclists are accompanied by a certain spatial uncertainty due to: the microsensors sampling time and the movement of cyclists. These instruments send data every 10 s (time-averaged concentration and GPS position), but during this period there are uncertainties about the actual GPS positions traveled by cyclists.
3. The total number of cyclists in some cells could not be enough to obtain a representative average concentration value.

Therefore, a direct comparison (point-by-point) seems not be suitable ...



## Model evaluation against experimental data from cyclists with microsensors: NO<sub>2</sub>, 8PM



- ❑ *A CFD-RANS methodology has been modified and applied to the entire city of Pamplona to compute high resolution NO<sub>x</sub>, NO<sub>2</sub> and NO maps at pedestrian level.*
- ❑ *This modelling approach is able to reproduce the data from air quality monitoring stations located within the domain, especially during daytime hours (from 8 A.M. up to 8 P.M.).*
- ❑ *Data from cyclists could not be directly compared (point-by-point), therefore a comparison by using a spatial statistical method that identifies clusters of high and low values of pollutant concentrations is applied. A preliminary analysis indicates that, in general, similar locations of maxima and minima of concentration are obtained in both, experimental and numerical maps.*
- ❑ *This methodology seems to be adequate to compute high resolution concentration maps for an entire city.*

Thank you for your attention!

[esther.rivas@ciemat.es](mailto:esther.rivas@ciemat.es)