SENSITIVITY ANALYSIS OF PARAMETERS INFLUENCING ESTIMATED BY A CHEMICAL-TRANSPORT MODEL

RefH11-095

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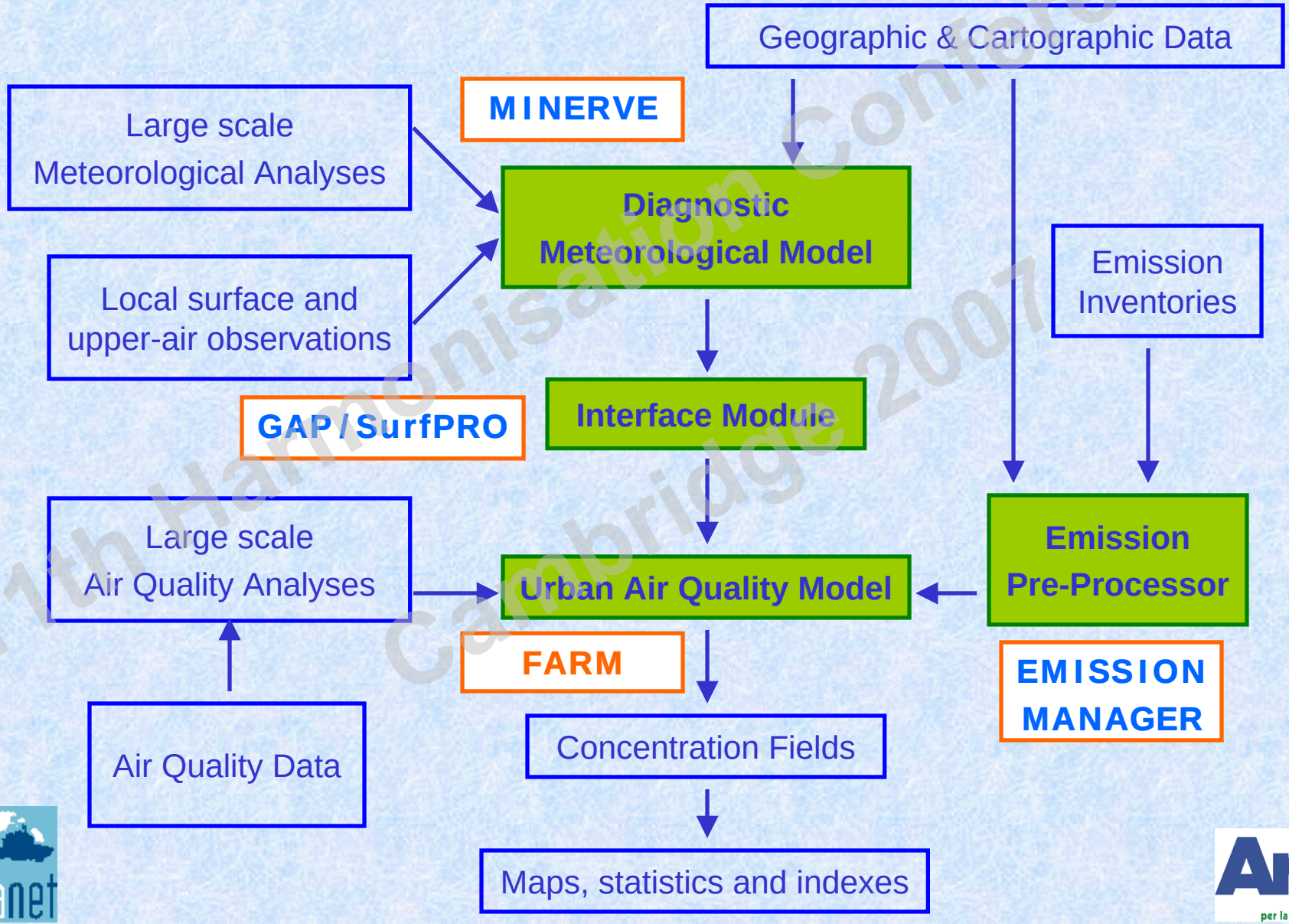
- Modelling system description
- Sensitivity analysis
- Results
- Conclusion

INTRODUCTION

- Italian Legislation appoints the Regional Administrations to assess the air quality
- Since 2004 Arpa performs yearly modelling simulations to support Piemonte Region in AQA
- Accuracy for modelling is defined by EU Directives

MODELLING SYSTEM ARCHITECTURE



GEOGRAPHIC LOCATION AND COMPUTATIONAL DOMAIN

220 x 284 km^2

Δxy: 4 km

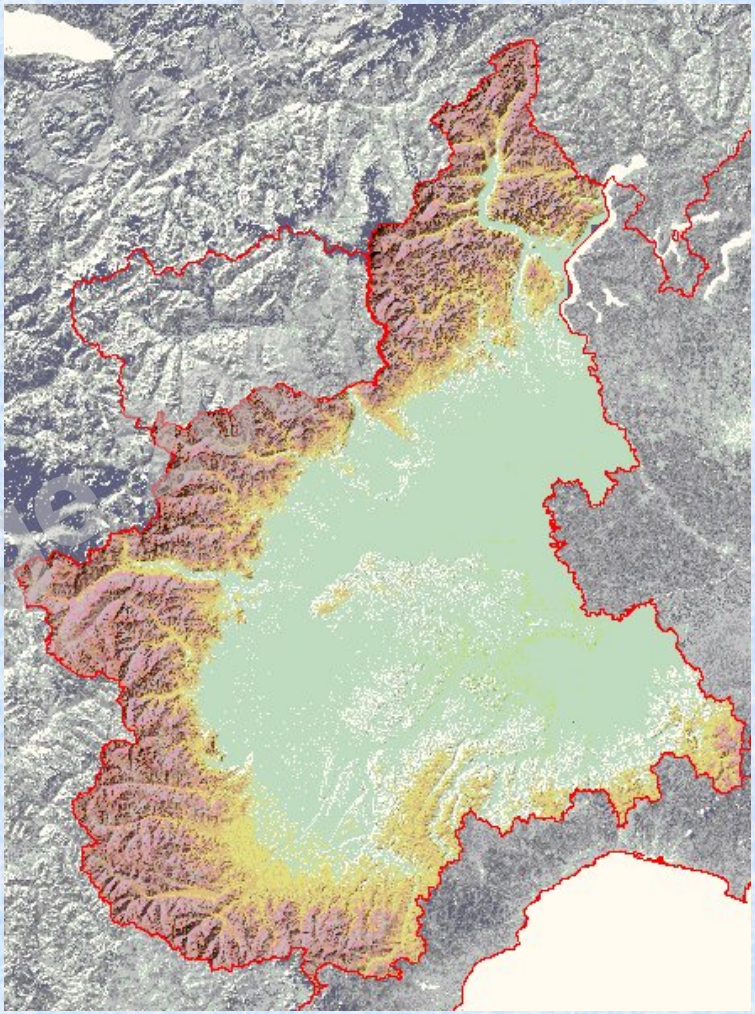
Nx = 56

Ny= 72

Vertical levels: 12 (up to 3500 m agl)

Simulation length: 1 year

Time resolution: 1 hour



SENSITIVITY ANALYSIS

To improve modelling estimation accuracy:

- Tests covering two episodes occurred during year 2004, focused on most critical pollutants in the area (NO_2, PM_{10} and O_3):
  - $10^{th} \div 20^{th}$ February $\Rightarrow PM_{10}$
  - $20^{th} \div 30^{th}$ June $\Rightarrow$ ozone
- Results compared to 2004 simulation considered as “base case”

ATTENTION FOCUSED ON...

1. minimum value for eddy diffusivity;
2. aeolian contribution of mineral dust to particulate emissions;
3. benzene explicit treatment.

SurfPRO

- Meteorological pre-processor for air pollution models based on Monin-Obukhov similarity theory
- Takes into account water bodies, terrain slopes and related shading effects

Input:
topography, land use, meteorological fields (wind, T, RH, cloud, precipitation)

Output:
turbulence scaling parameters, mixing height, horizontal and vertical diffusivities, deposition velocities

FARM

- Chemical Transport Model: Eulerian 3D
- Diffuse and point sources treatment
- Two gas-phase mechanisms (SAPRC90 and SAPRC99)
- Aerosol modules: *aero3* (Models-3/CMAQ) and *aero0* simplified bulk module (based on the Emep Eulerian Unified model approach)
- Yearly simulation performed with ***SAPRC90*** mechanism and ***aero0*** aerosol module

TEST 1

Minimum value for eddy diffusivity (K_z^{min})

K_z^{min}

Introduction of K_z^{min} user-defined values according to the fractional area of urban land use:

$$K_z^{min} = K_z^{min,rural} \cdot (1 - f_{urban}) + K_z^{min,urban} \cdot f_{urban}$$

f_{urban} = urban land use fraction (1-0: urban-rural)

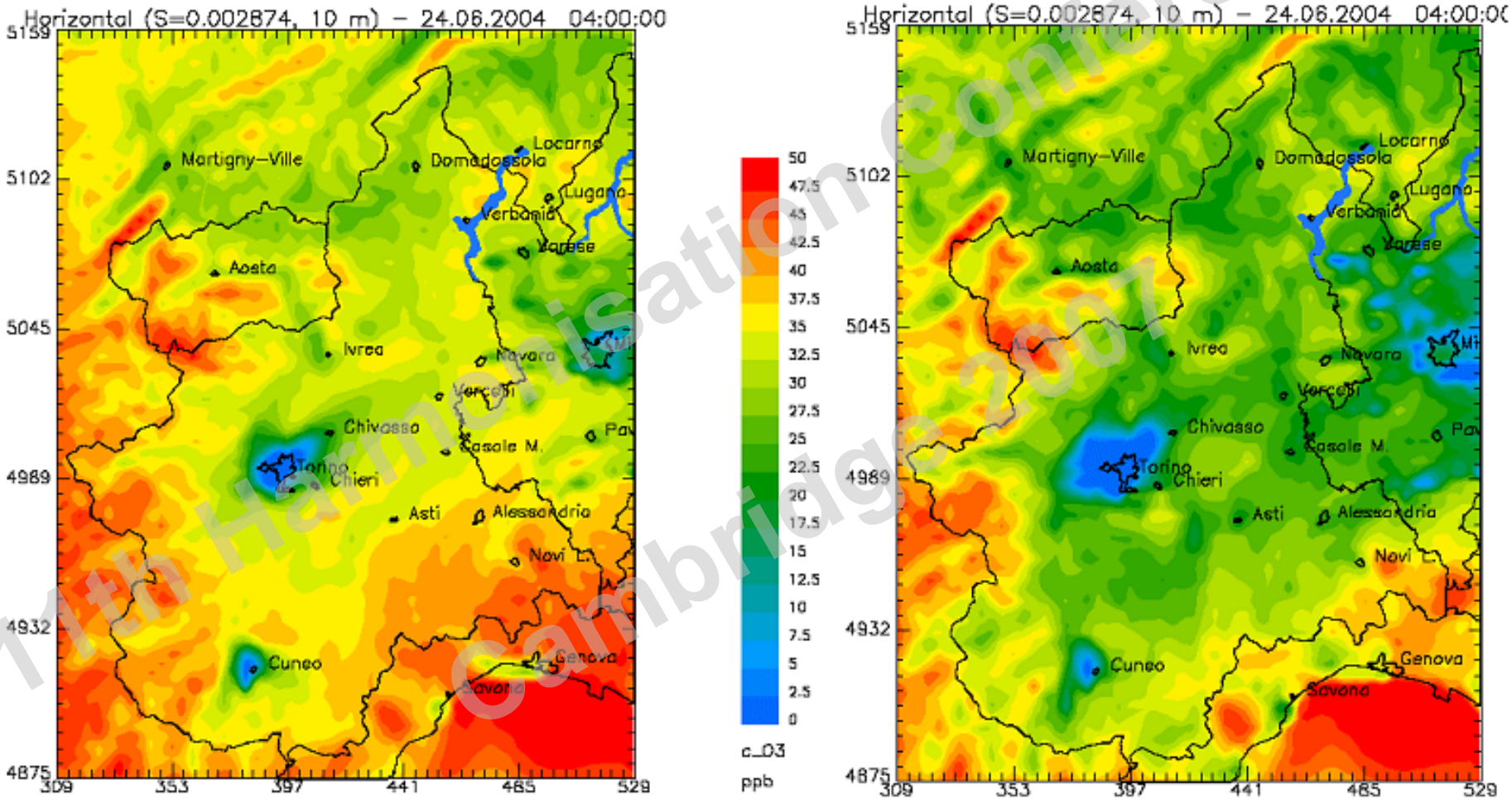
Tested values

Land use	Winter	Summer
Urban	0.2	1
Rural	0.05	0.1

K_z^{min} values ($m^2\ s^{-1}$)

The higher value of K_z^{min} in urban areas is meant to reflect lower nocturnal stability resulting from urban heat island effects.

SUMMER EPISODE: OZONE



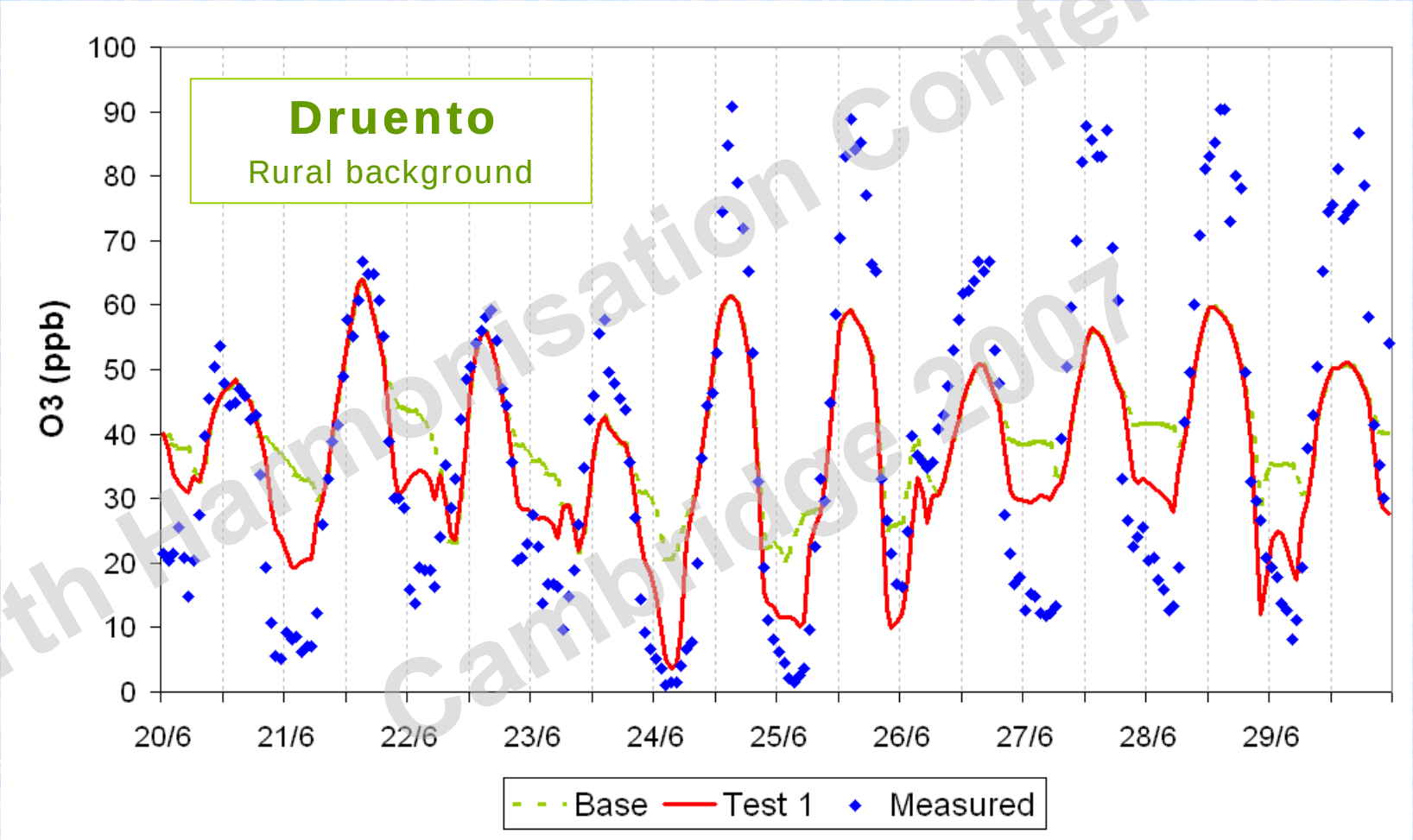
Base case

K_z^{min} = 1.0 m²/s

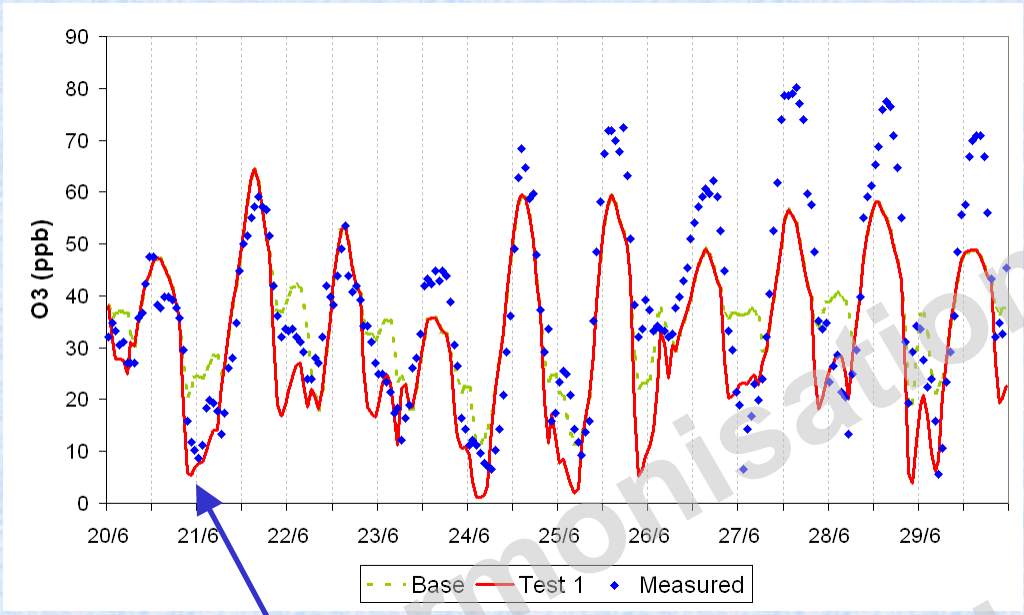
04:00 a.m.

Test 1

SUMMER EPISODE: OZONE

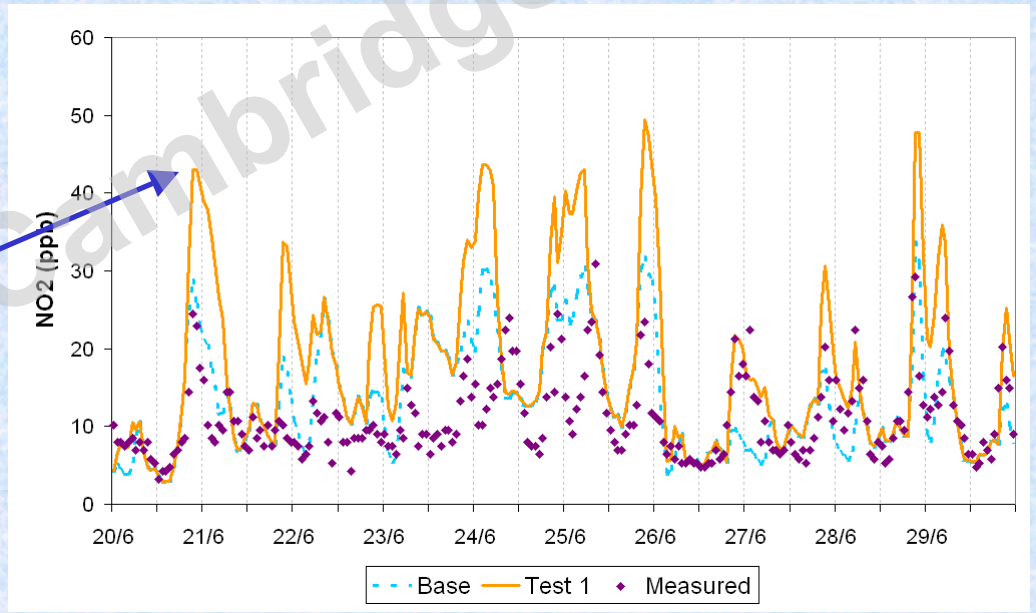


SUMMER EPISODE: O_3 AND NO_2



Borgaro

Suburban background



TEST 2

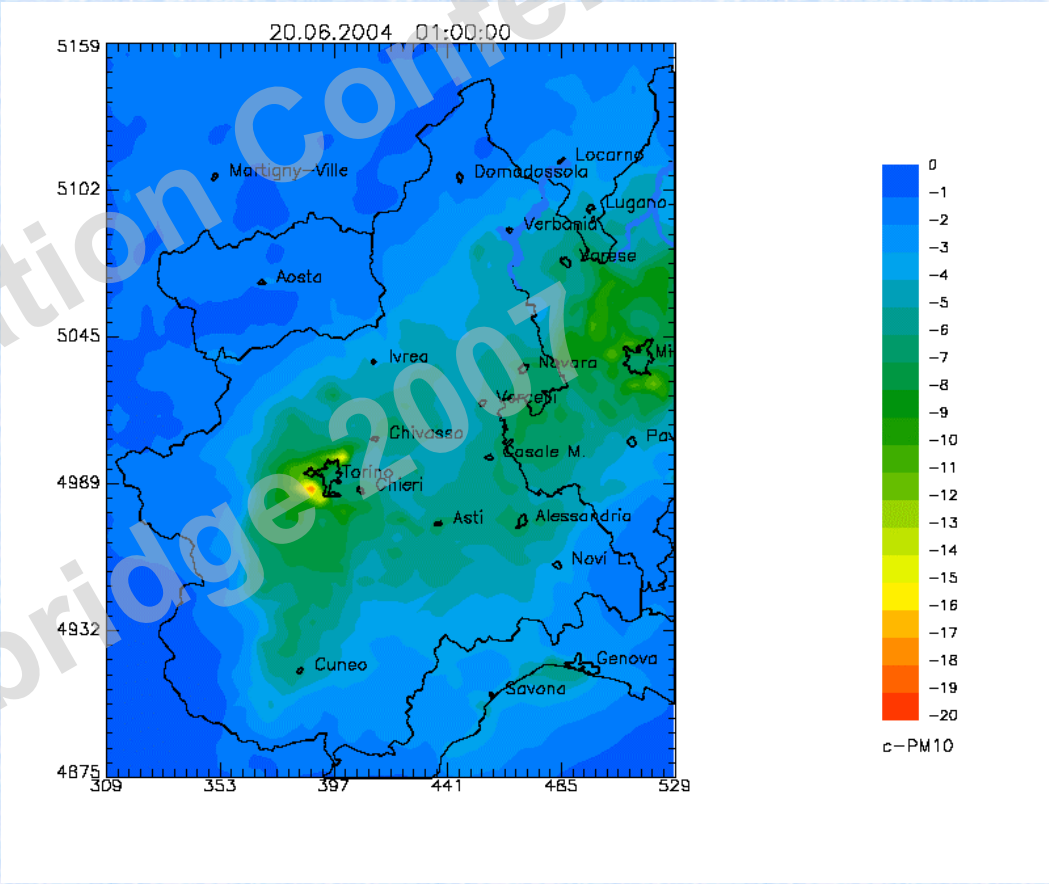
Erosion/resuspension processes

DUST EMISSION FROM LOCAL EROSION/RESUSPENSION

- Evaluation of dust emission contribution from local erosion/resuspension to improve estimation of PM_{10} concentrations
- Introduction of a simplified bulk scheme in Surf*PRO* (Vautard, 2005)
- Significant differences appear during the summer episode in correspondence of stronger winds
- Rather small influence during winter episode

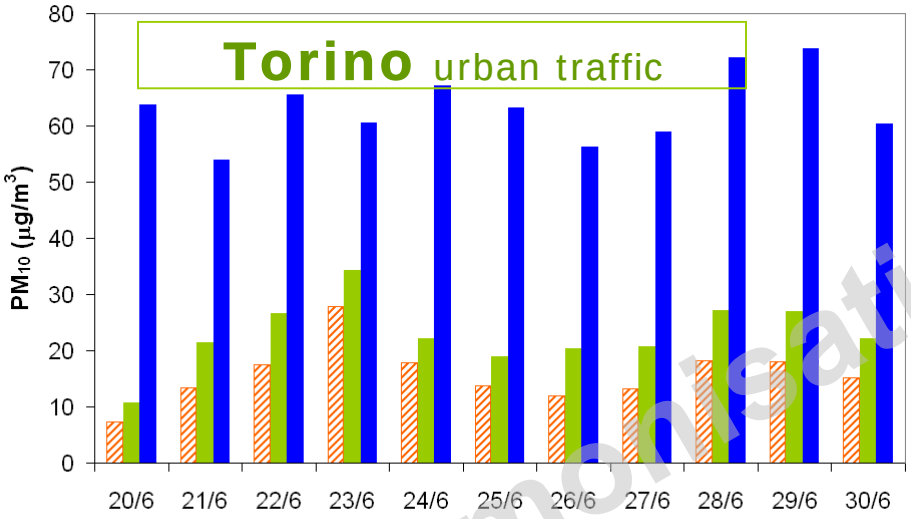
SUMMER EPISODE: PM_{10}

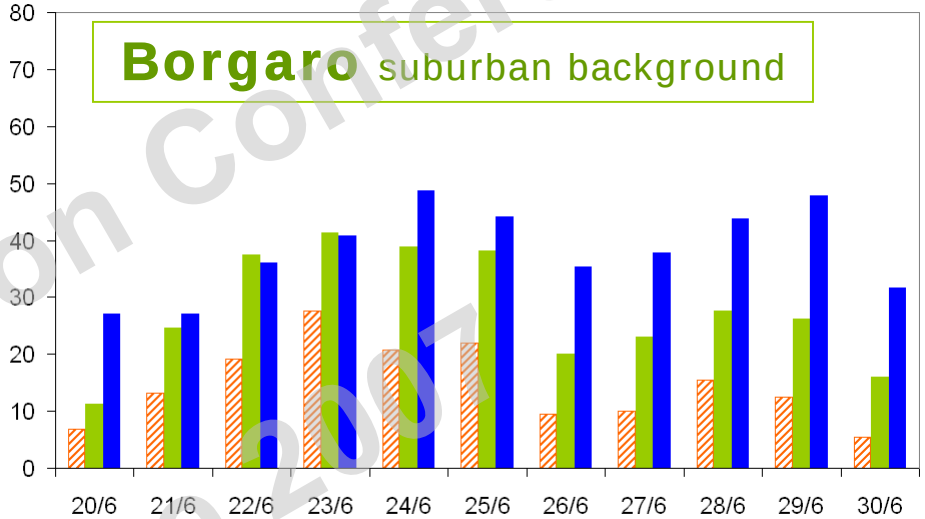
Difference between concentrations averaged over the period show a maximum increase of 20 $\mu g/m^3$ with the contribution of the erosion/resuspension processes.

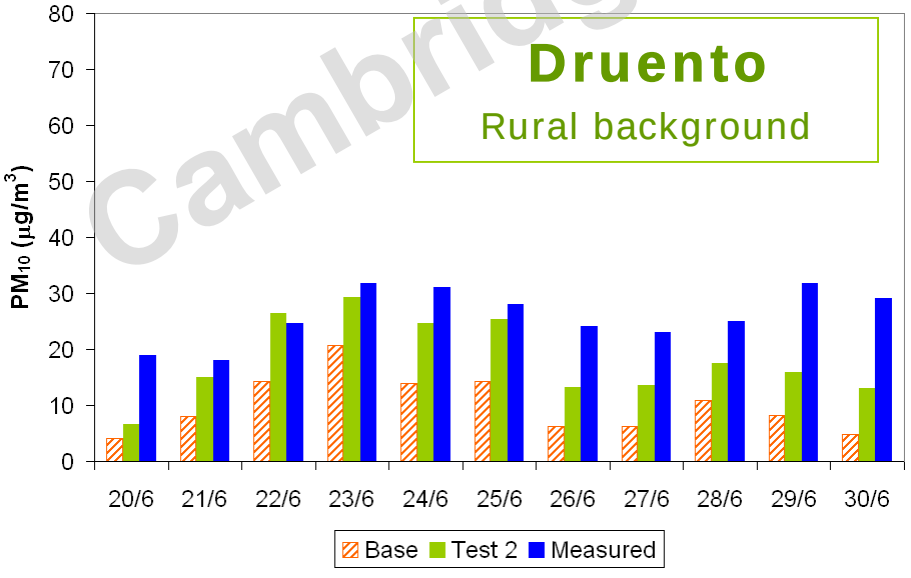


Base case – Test 2

SUMMER EPISODE: PM_{10}







TEST 3

Benzene explicit treatment

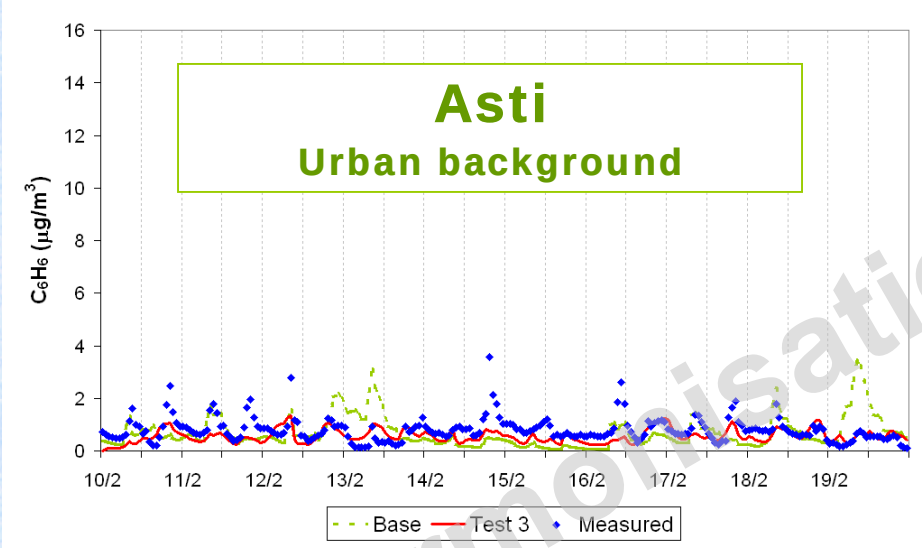
EXPLICIT TREATMENT OF BENZENE

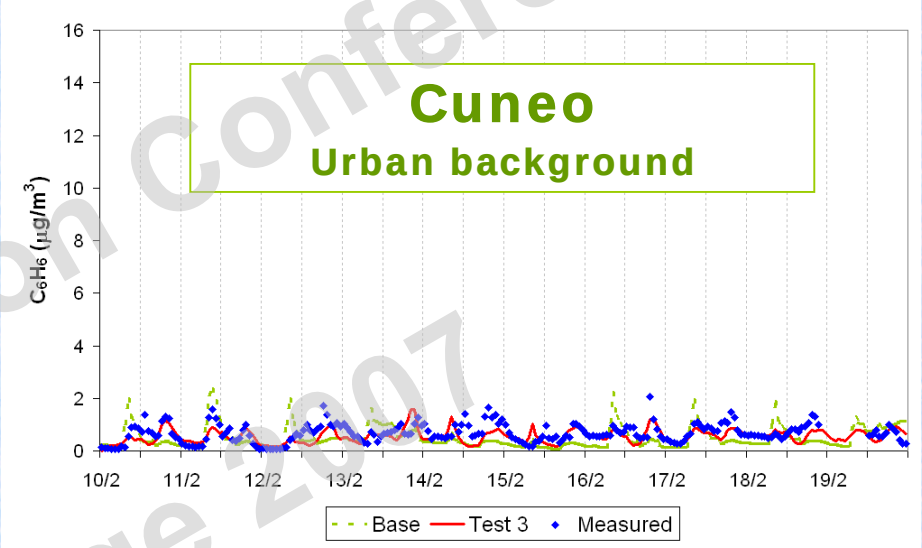
- SAPRC90 chemical mechanism considers benzene as included in the ARO1 lumped species (in previous studies over Piemonte region, benzene has been considered as 20% of resulting ARO1 concentrations)

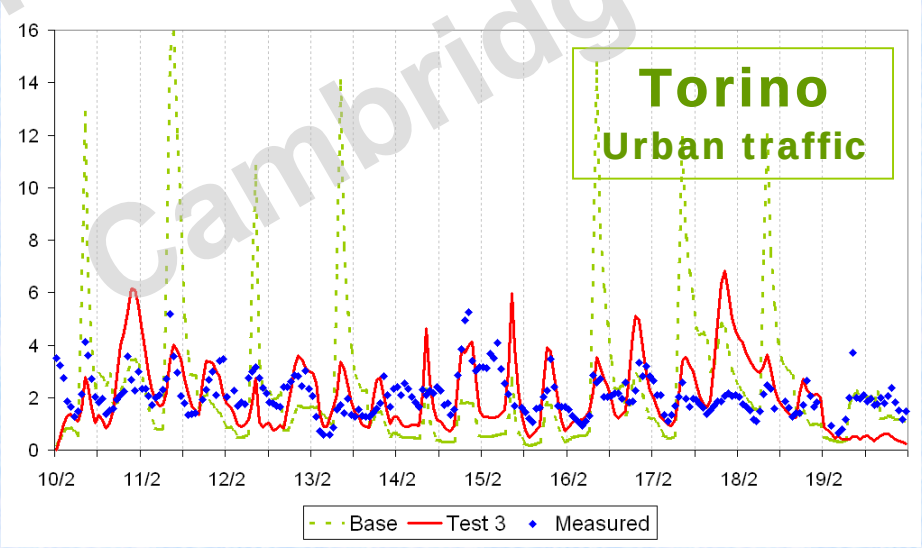
- Explicit treatment of benzene has been introduced in the mechanism:

$$C_6H_6 + HO = 0.236 \cdot CRES + 0.764 \cdot RO_2\_R + \\ + 0.236 \cdot HO_2 + 0.764 \cdot C\_O_2$$

WINTER EPISODE: BENZENE







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CONCLUSIONS (1)

- K_z^{min} differentiated for urban and rural areas lead to a better reproduction of nighttime ozone concentrations during summer (even though some overestimation of primary pollutants occur in areas with mixed land use features);
- Introduction of dust erosion and resuspension processes results in a better estimation of PM_{10} levels (especially during summer period);
- Explicit treatment of benzene in the SAPRC90 mechanism gives better reproduction of simulated levels (particularly during the winter period).

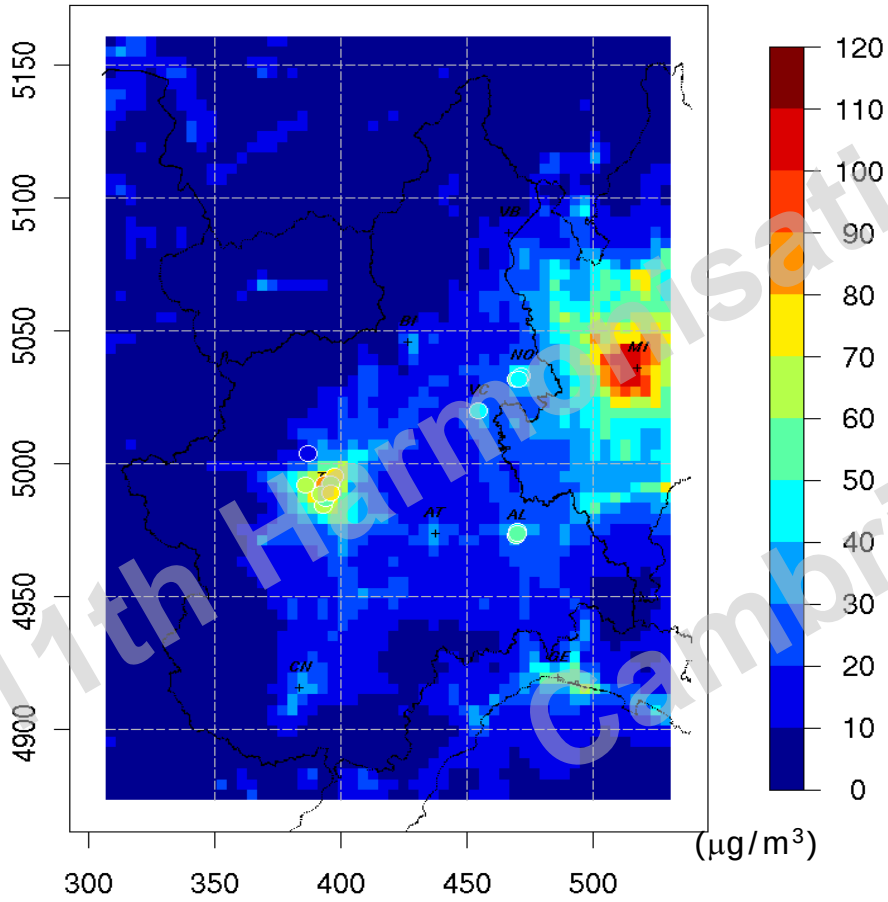
CONCLUSIONS (2)

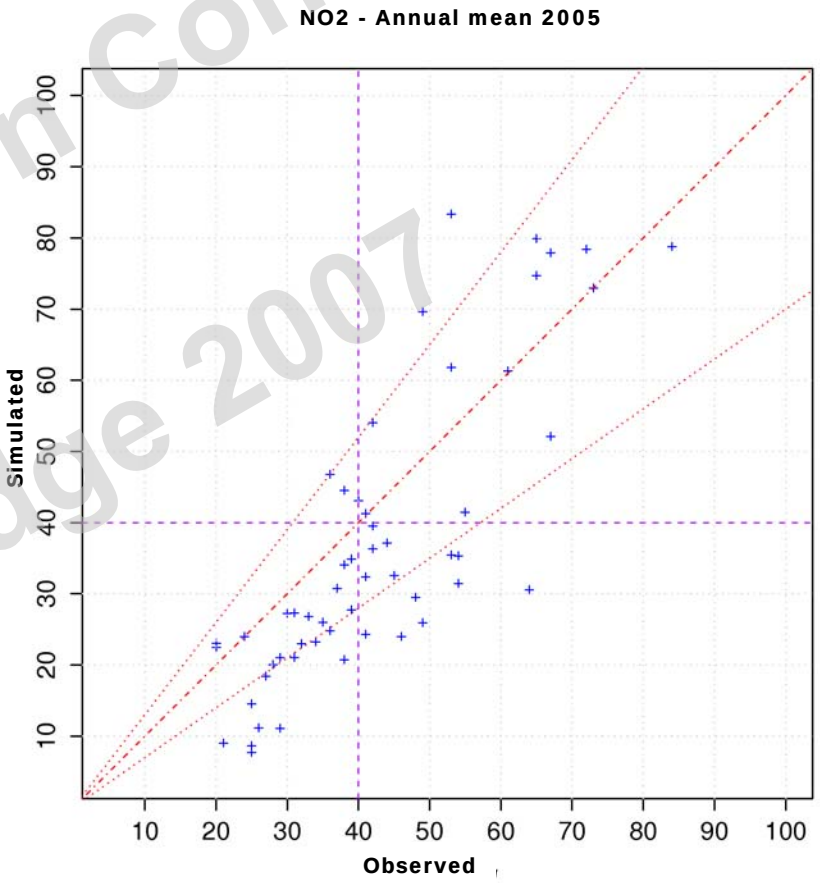
- Sensitivity analysis considering summer and winter episodes (year 2004) were performed to define simulation settings to be used for 2005 yearly simulations
- Annual simulations for years 2005 and 2006 have been realized with the introduction of:
  - vertical diffusivity differentiated for rural/urban areas;
  - dust erosion/resuspension processes;
  - benzene explicit treatment.
- Further investigations being accomplished verify the performance SAPRC99 chemical mechanism (a more efficient integration scheme is needed to lower computational time) and to evaluate the use of aero3 aerosol module to improve secondary particulate estimation.

2005 ANNUAL SIMULATION RESULTS

NITROGEN DIOXYDE

Annual mean



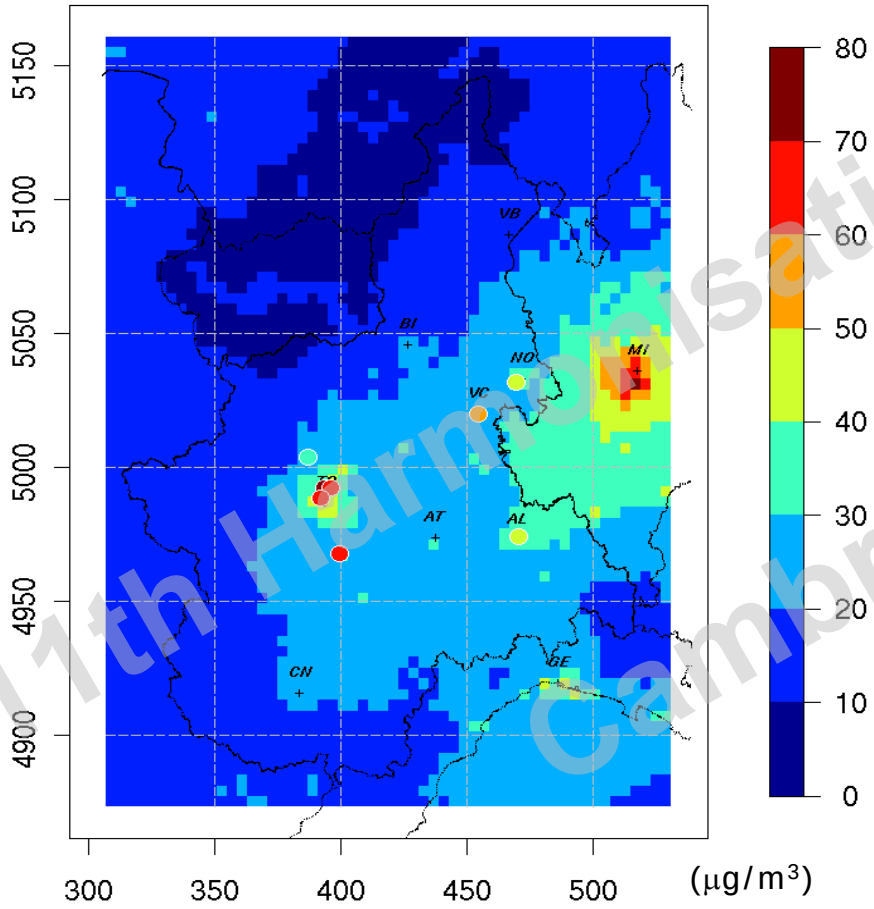


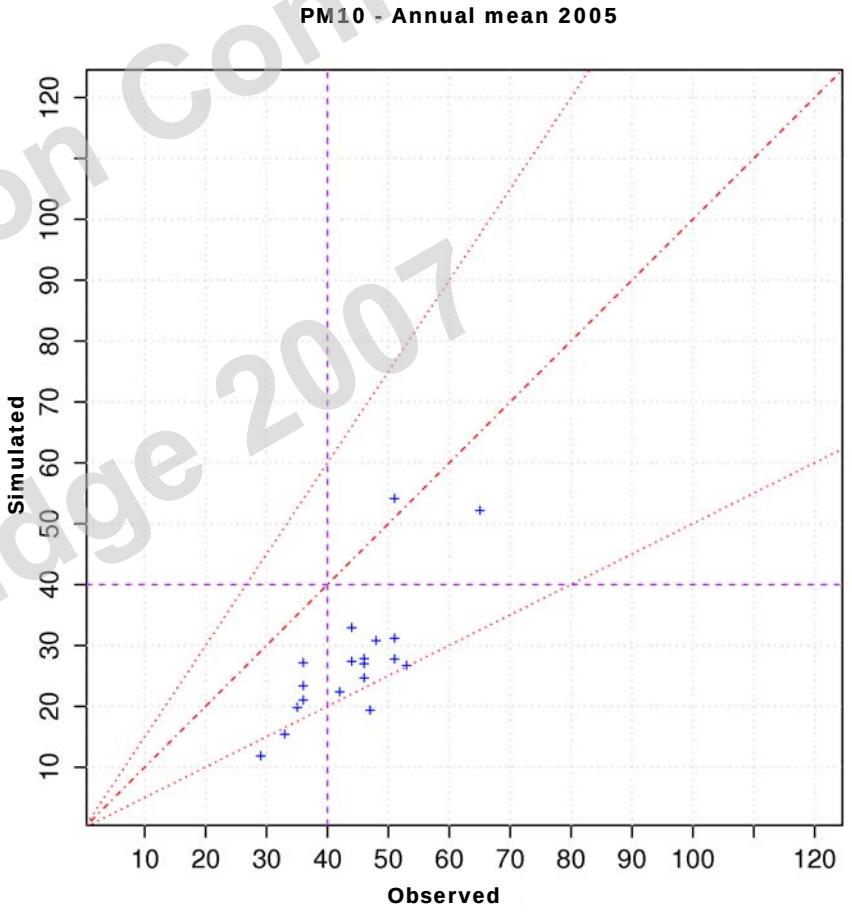
Observed/simulated

Modelling accuracy 30 %

PM10

Annual mean

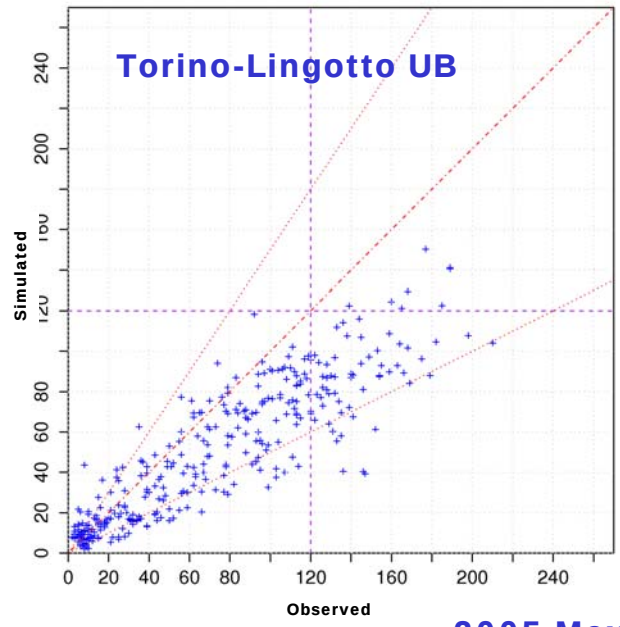


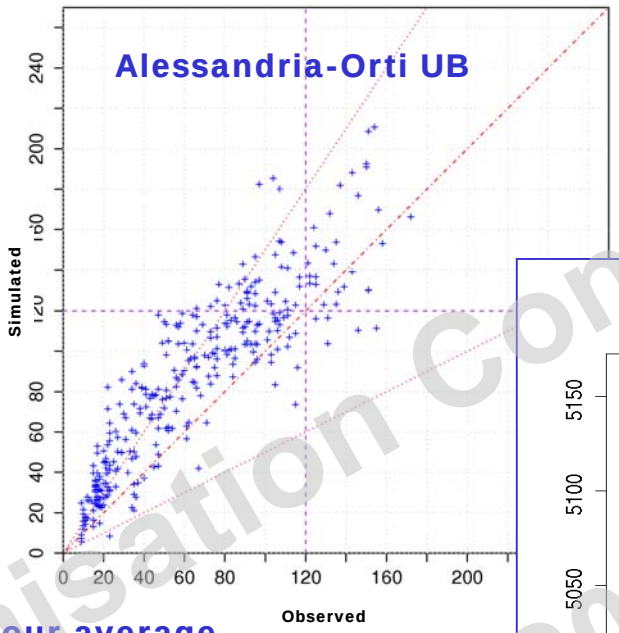


Observed/simulated

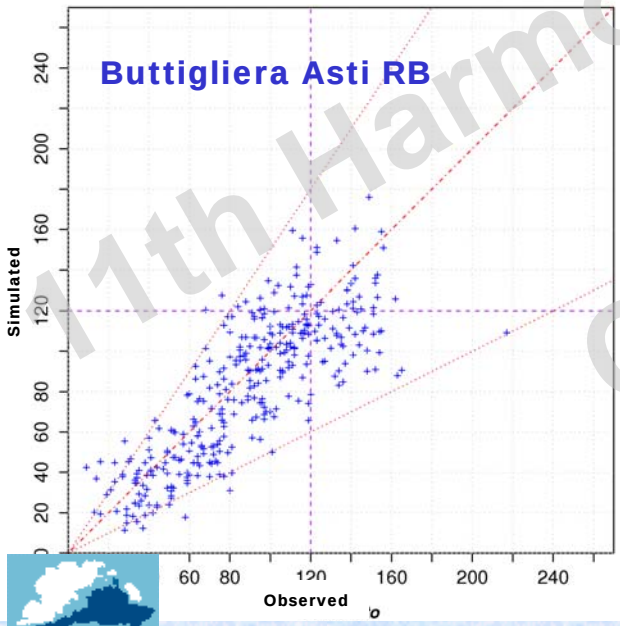
Modelling accuracy 50 %

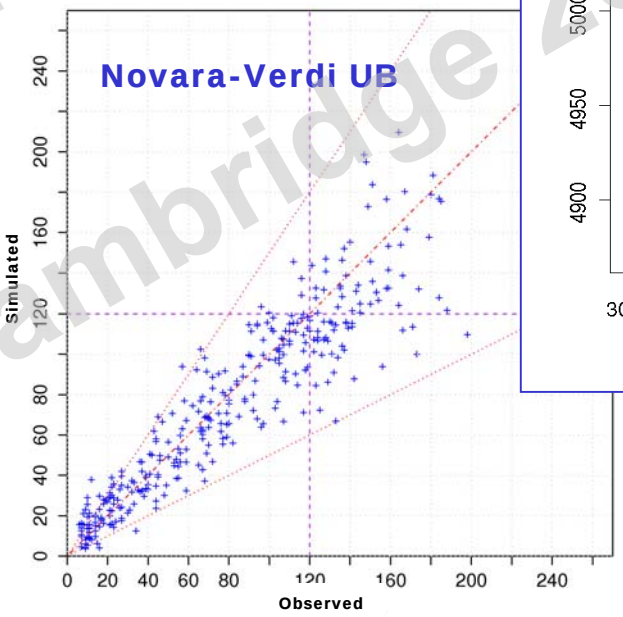
OZONE

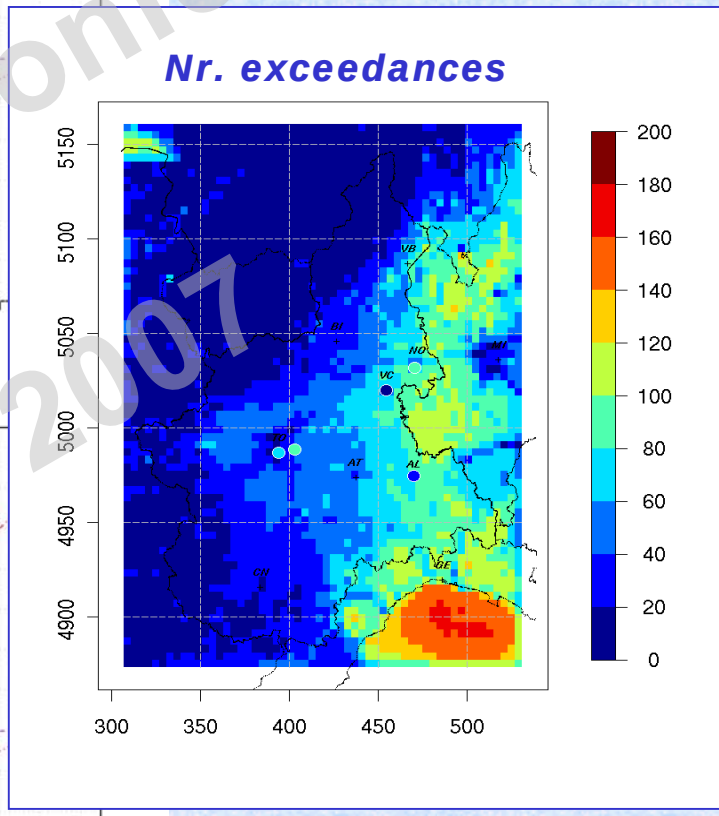




2005 Max 8 hour average







Observed/simulated

Modelling accuracy 50 %

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THANK YOU
FOR YOUR ATTENTION!