

COUPLING OF A LAGRANGIAN PARTICLE MODEL  
(SPRAY) AND NEURAL NETWORK TO IMPROVE THE  
ACCURACY ON IMPACT ASSESSMENT OF AN  
INDUSTRIAL FACILITY.

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# Preliminary considerations

- In complex areas (eg. breeze circulations, complex topography) Gaussian models could not be the correct tool to be used due to its stationary and homogeneous nature;
- On such cases, consequence analysis studies could produce wrong design of effects mitigation and control strategies.
- More complex dispersion models have to be used.
- An improvements on model accuracy can be obtained using non conventional approaches where dispersion models are coupled with statistical ones.
- A net improvents on accuracy of the coupled Gaussian dispersion-NN model system were observed in a previous applications

# Main Goal

- The Lagrangian particle models have demonstrated to better deals with non stationary non homogeneous conditions.
- The accuracy is sometimes poor and it needs to be improved.
- In order to get this aim a Lagrangian particle model was coupled with a neural network.
- This model system (Spray-NN) was applied to reconstruct the pollutant by a cement plant located in a complex area

# Case Study

## The Cement Facility

### Main Parameters

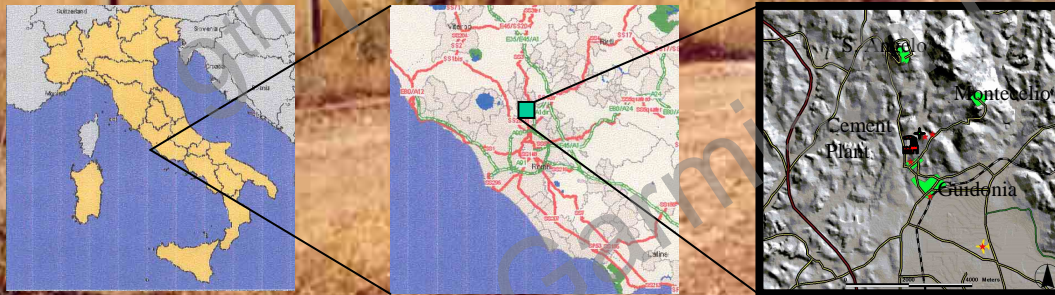
<b>Product capacity</b>	<b>Plant area</b>	<b>stacks</b>	<b>Stack height</b>	<b>Stack diameter</b>
<b>1.7 Mton/y</b>	<b>366,000 m<sup>2</sup></b>	<b>1</b>	<b>54 m</b>	<b>5 m</b>
<b>Emission parameters</b>				
<b>Flow</b>	<b>Temperature</b>	<b>NO<sub>x</sub></b>	<b>SO<sub>2</sub></b>	<b>CO</b>
<b>424,000 Nm<sup>3</sup>/h</b>	<b>100 °C</b>	<b>371 kg/h</b>	<b>3.8 kg/h</b>	<b>76 kg/h</b>



# Case Study

## Description of the modeled area

- Complex orography.
- Complex circulation pattern (breeze, mountain effects).
- Some populated areas.
- The period of November 2nd-5th 2001 was used for test simulations. It can be considered as a typical local atmospheric circulation

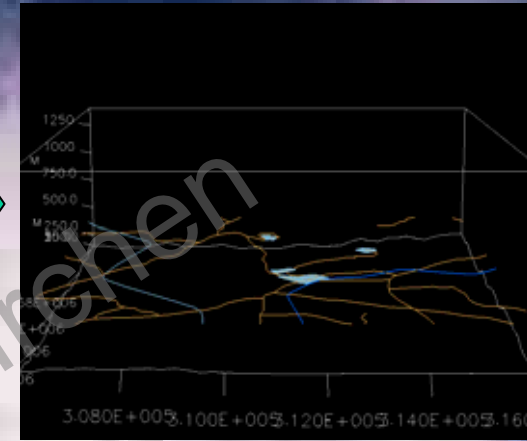
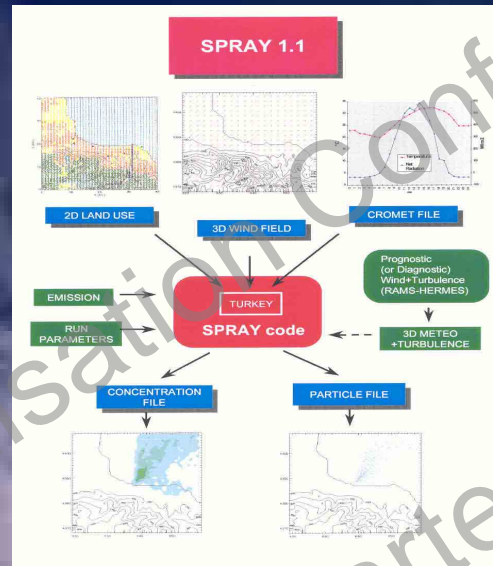
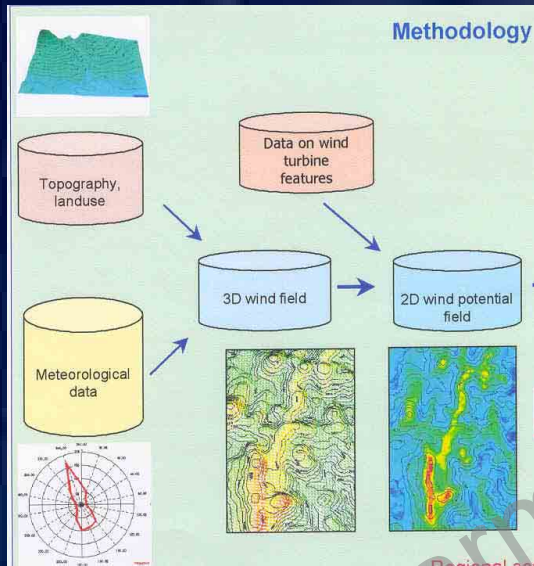


# The Lagrangian Particles Model System

Meteorological model  
MINERVE

Lagrangian dispersion model  
SPRAY

3D Visualization



- Mass-consistent diagnostic
- Accurate 3D wind fields over complex terrain
- Terrain following coordinates
- From 10x10 to 100x100 Km<sup>2</sup> space scale
- Results: 3D Wind and Temperature fields

- Three basic dispersion components are considered:
  - transport due to the mean velocity;
  - wind turbulent fluctuation;
  - molecular diffusion.
- Results:
  - 3D concentration fields
  - Particles dispersion
  - Turbulence parameters

# Main simulations parameters

## MINERVE

Meteorological model

- 10 x 10 Km<sup>2</sup> domain
- 24 vertical levels
- 1.5 Km top domain
- 250 m resolution
- Interpolation + adjusting
- 10 minutes results
- 1 day simulation

## SPRAY

Dispersion model

- 10 x 10 Km<sup>2</sup> domain
- 15 vertical levels
- 1.5 Km top domain
- 250 m resolution
- Half hourly emission
- Half hour results
- 1 day simulation



# Neural Network Methodology

- Identification of the problem (forecast, classification, 3D reconstruction, etc.)
- Selection of NN architecture (MLP, Kohonen)
- Choice of NN parameters (NNP)
- Choice of Main variables (T, dT/dZ, \*Nox(CLPDM),etc)
- Selection of representative patterns (meteorological surface data of the November 2nd-5th 2001)

## Running of MLP

- Training phases

- Modelling Input/output variables

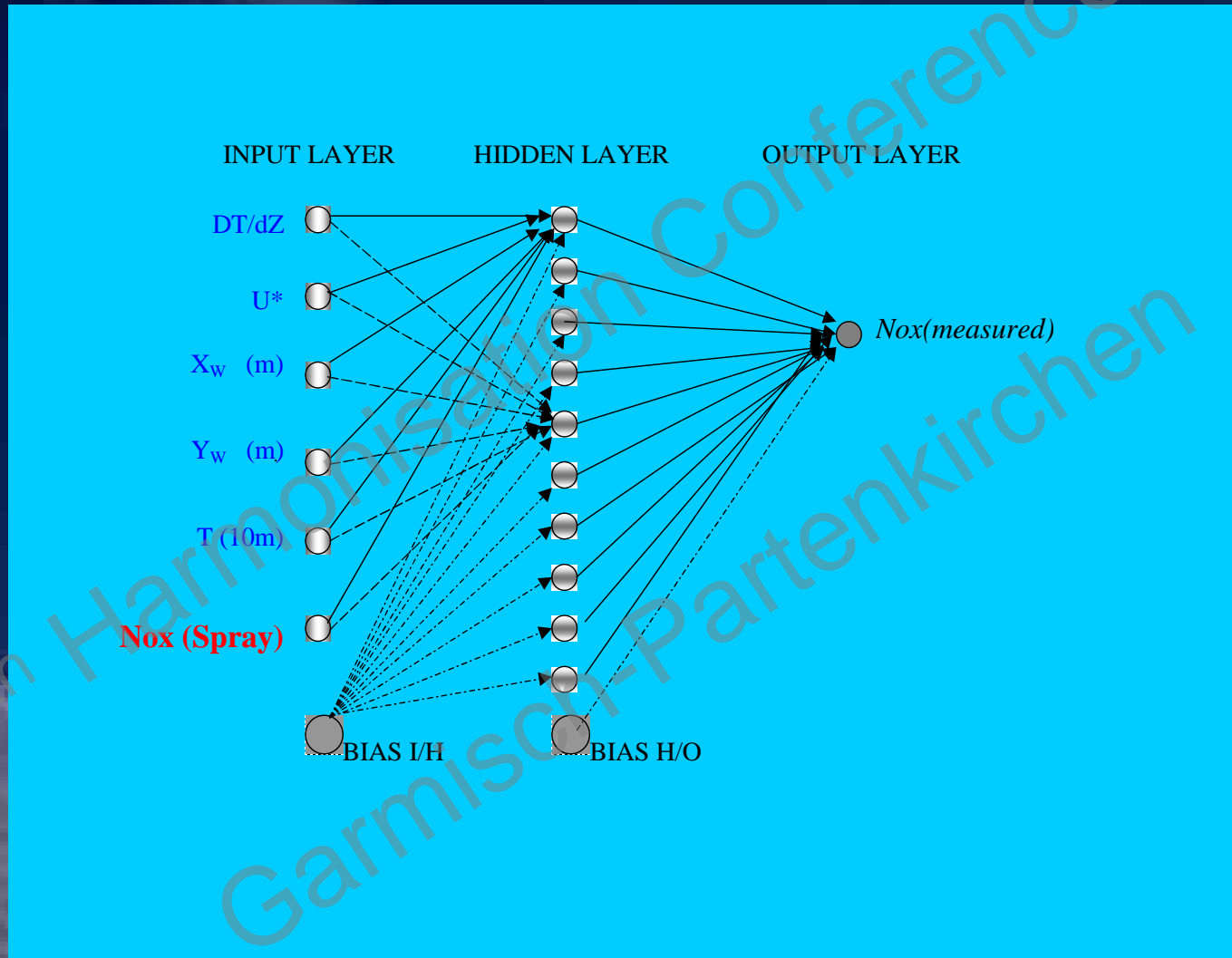
- Amount of input data to be provided
- Tuning of the NN parameters for best performance
- Final NN architecture and parameters

- Generalisation phases

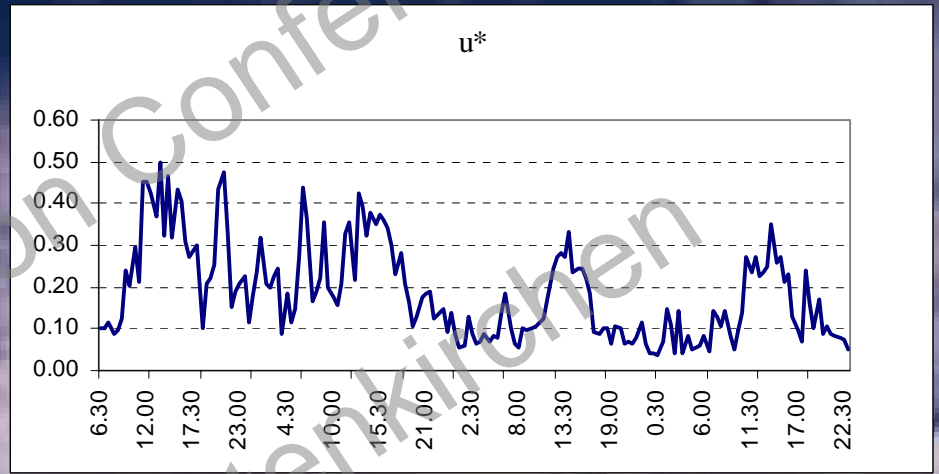
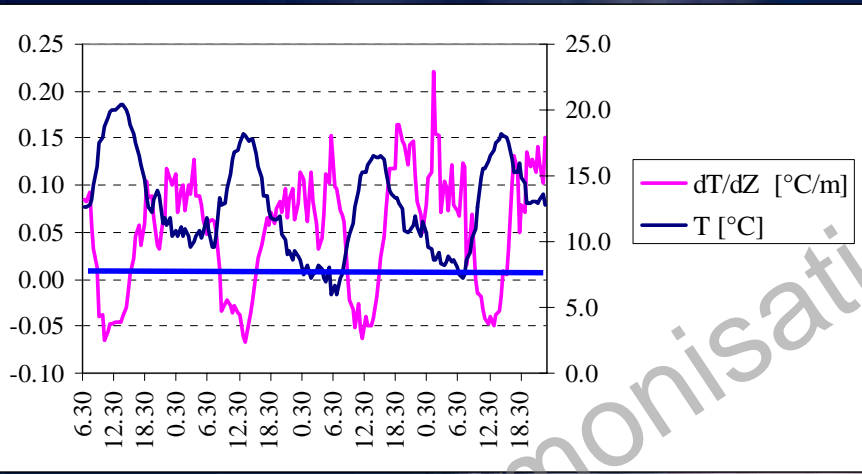
- Testing and comparison of NN results respect to the target observed values



# MLP Architecture



# Characteristics of the input variables of NN

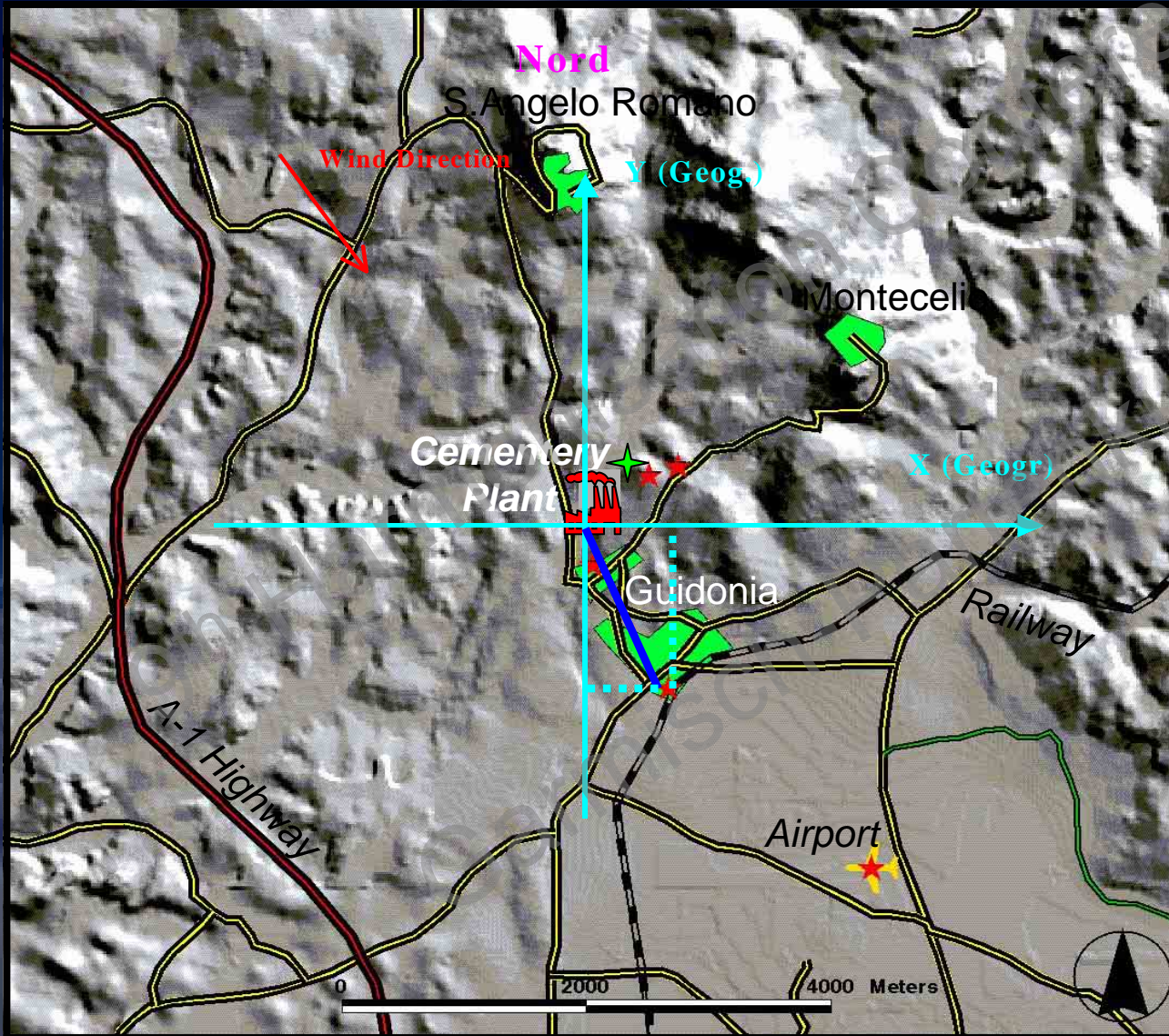


	TEMP (°C)	dT/dZ (°C/m)	u* (m/s)	NOx Spray (mg/m <sup>3</sup> )	NOx meas. (mg/m <sup>3</sup> )
<b>SD</b>	3.6	0.06	0.12	29.1	22.8
<b>Mean</b>	13.1	0.05	0.20	13.5	23.0

# New system of coordinates

- The aim is provide NN the information related with downwind-upwind conditions and impact distances.
- The geometrical coordinates of the monitoring stations  $X_{geo}$  and  $Y_{geo}$  are linked to the Fixed System Coordinates (FCS) and are time independent.
- In this FCS we measured a variation of wind direction and a fixed distance between chimney and monitoring station.
- The new system of coordinates are linked with the wind direction and the stack-monitoring stations distance

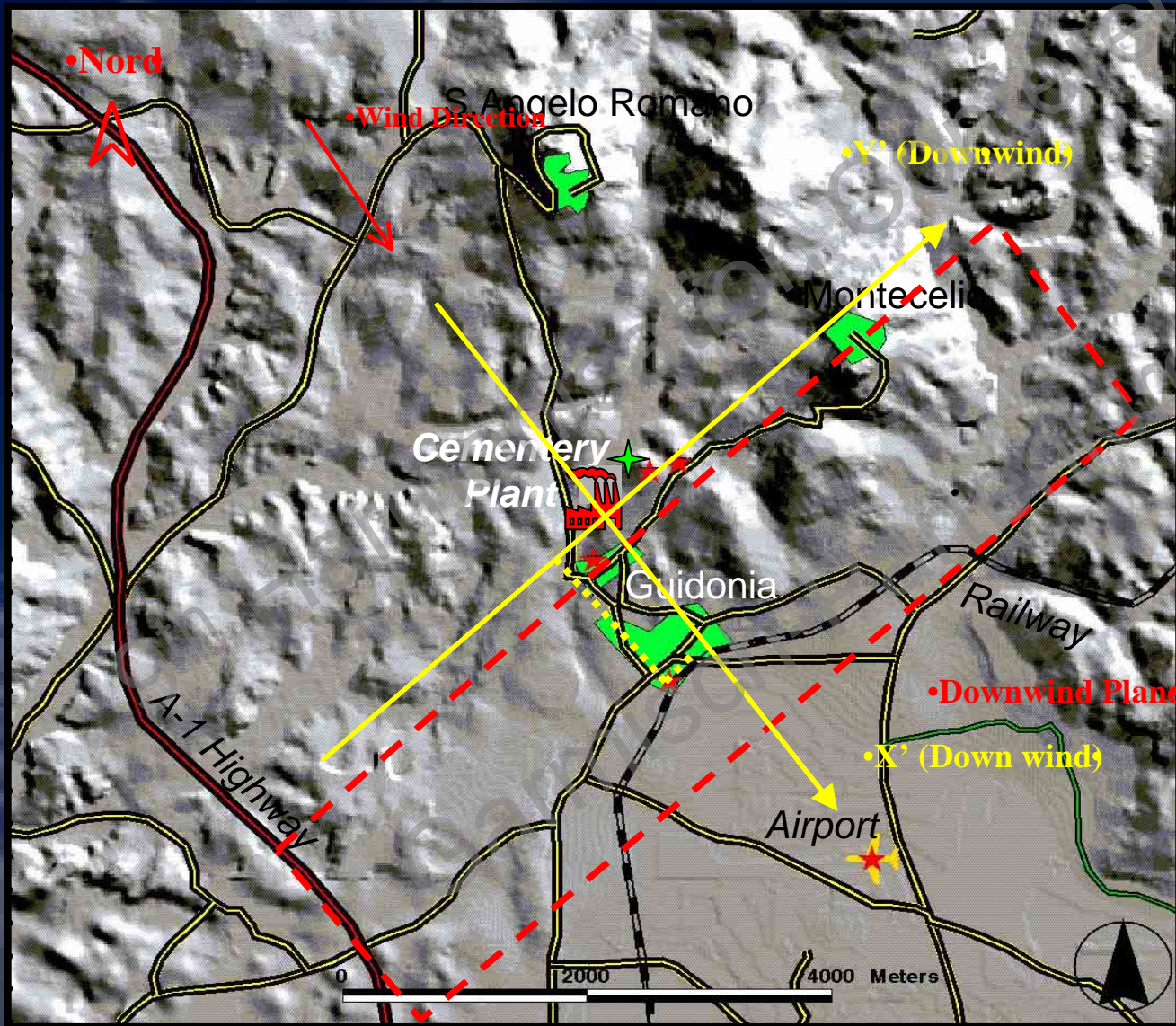
# Fixed System Coordinates of Monitoring Stations



- ★ Ground stations
- ★ meteo/chemical
- ★ Upper air stations



# New system of mobile coordinates linked with wind direction



- ★ Ground stations meteo/chemical
- ★ Upper air stations

# Rules of transformation of the coordinates

The rotation matrix  $R$  is defined by:

$$R = \begin{pmatrix} \cos(\mathcal{G}_c) & \text{sen}(\mathcal{G}_c) \\ -\text{sen}(\mathcal{G}_c) & \cos(\mathcal{G}_c) \end{pmatrix}$$

The axis inversion (to maintain the chirality of the coordinates system) is defined by:

$$R_{180} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

the product of the two matrixes gives the passage to the coordinates in the leeward system  $X_W Y_W$  to starting from  $X_{geo} Y_{geo}$ :

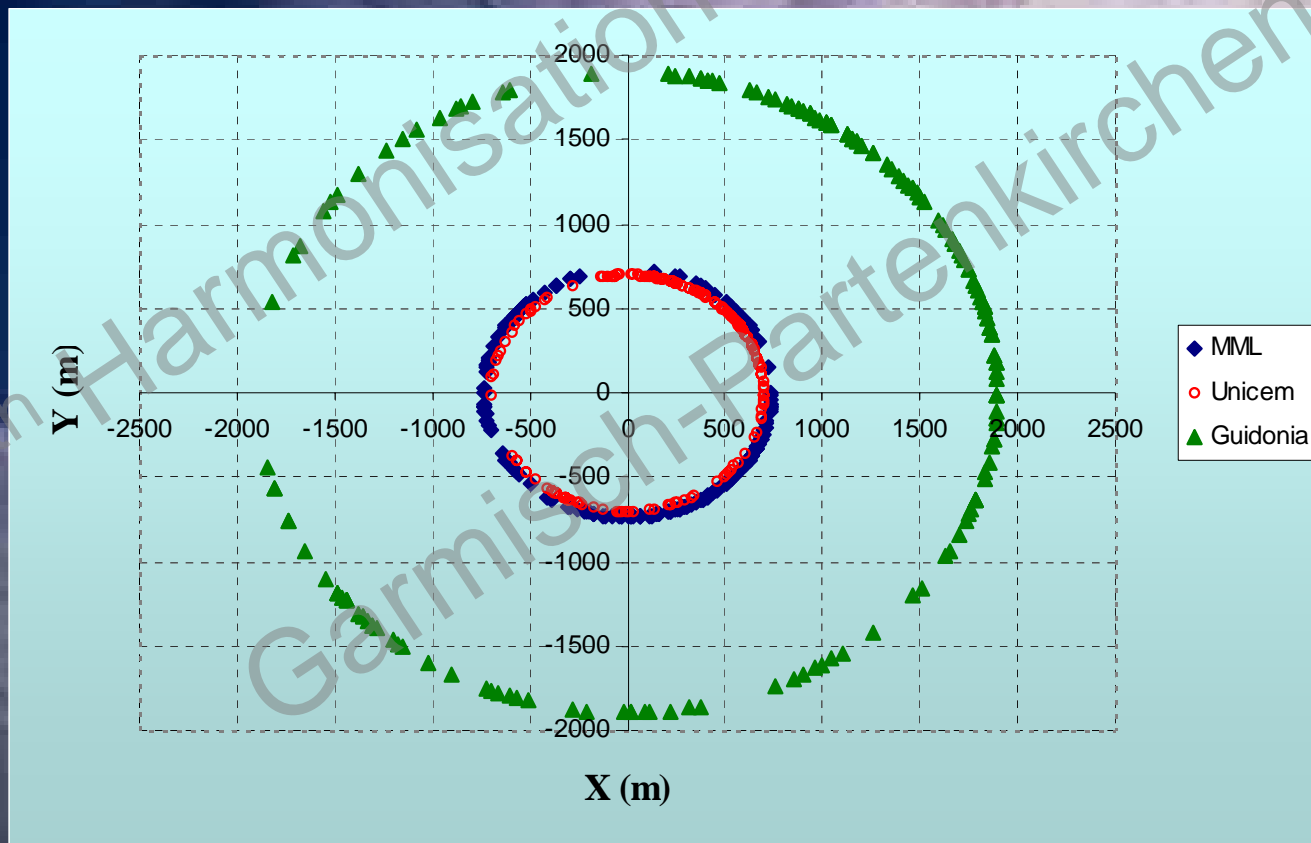
$$R_{tot} = R_{180} \cdot R = \begin{pmatrix} -\cos(\mathcal{G}_c) & -\text{sen}(\mathcal{G}_c) \\ +\text{sen}(\mathcal{G}_c) & -\cos(\mathcal{G}_c) \end{pmatrix}$$

It follows that the new coordinates  $X_W Y_W$  of the monitoring station are:

$$\begin{pmatrix} X_W \\ Y_W \end{pmatrix} = \begin{pmatrix} -\cos(\mathcal{G}_c) & -\text{sen}(\mathcal{G}_c) \\ +\text{sen}(\mathcal{G}_c) & -\cos(\mathcal{G}_c) \end{pmatrix} \begin{pmatrix} X_{geo} \\ Y_{geo} \end{pmatrix}$$

-As a result the point of coordinates  $X_w(t), Y_w(t)$  moves on a circumference of radius equal to the stack-station distance (736.2m, 698.9 m and 1859.3 m for the stations of the ISP, of the UNI and of the GUID respectively) according to the wind direction.

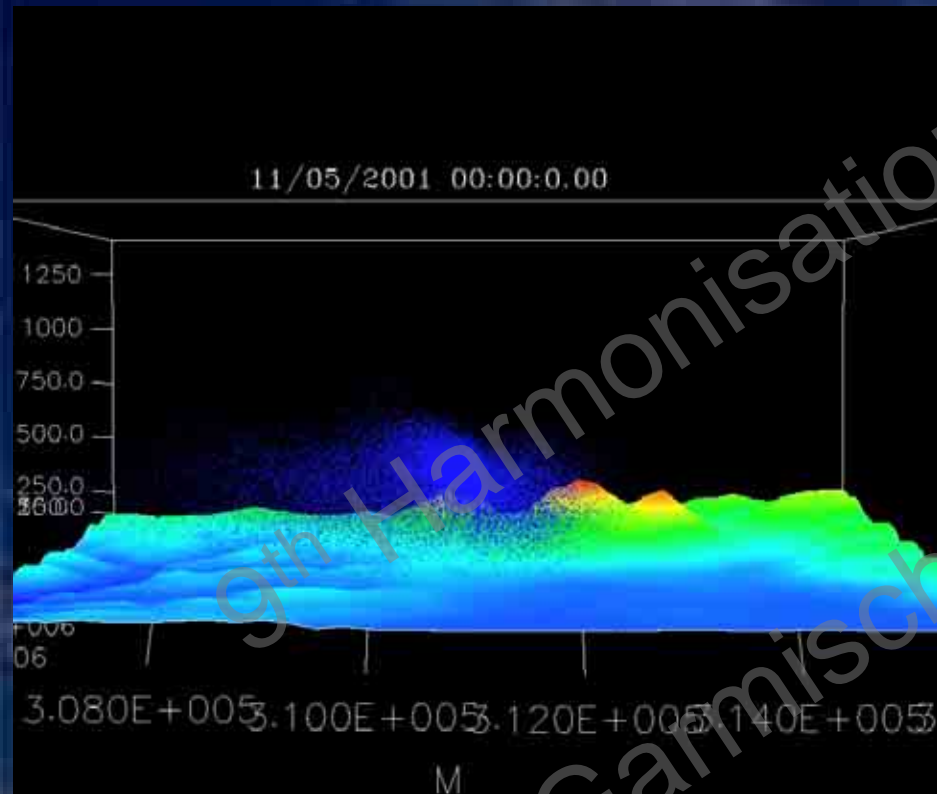
-The different anemological conditions correspond to different upwind distances ( $Y < 0$ ) and downwind ( $Y > 0$ ) for the three stations.



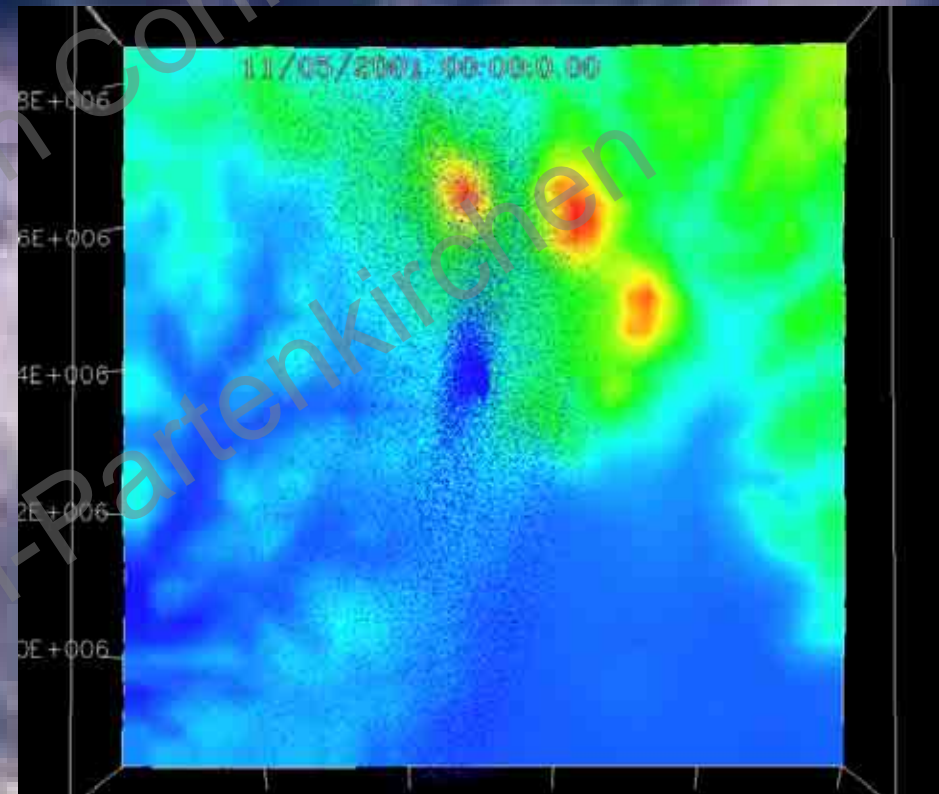


# SPRAY Particles dispersion

Side view

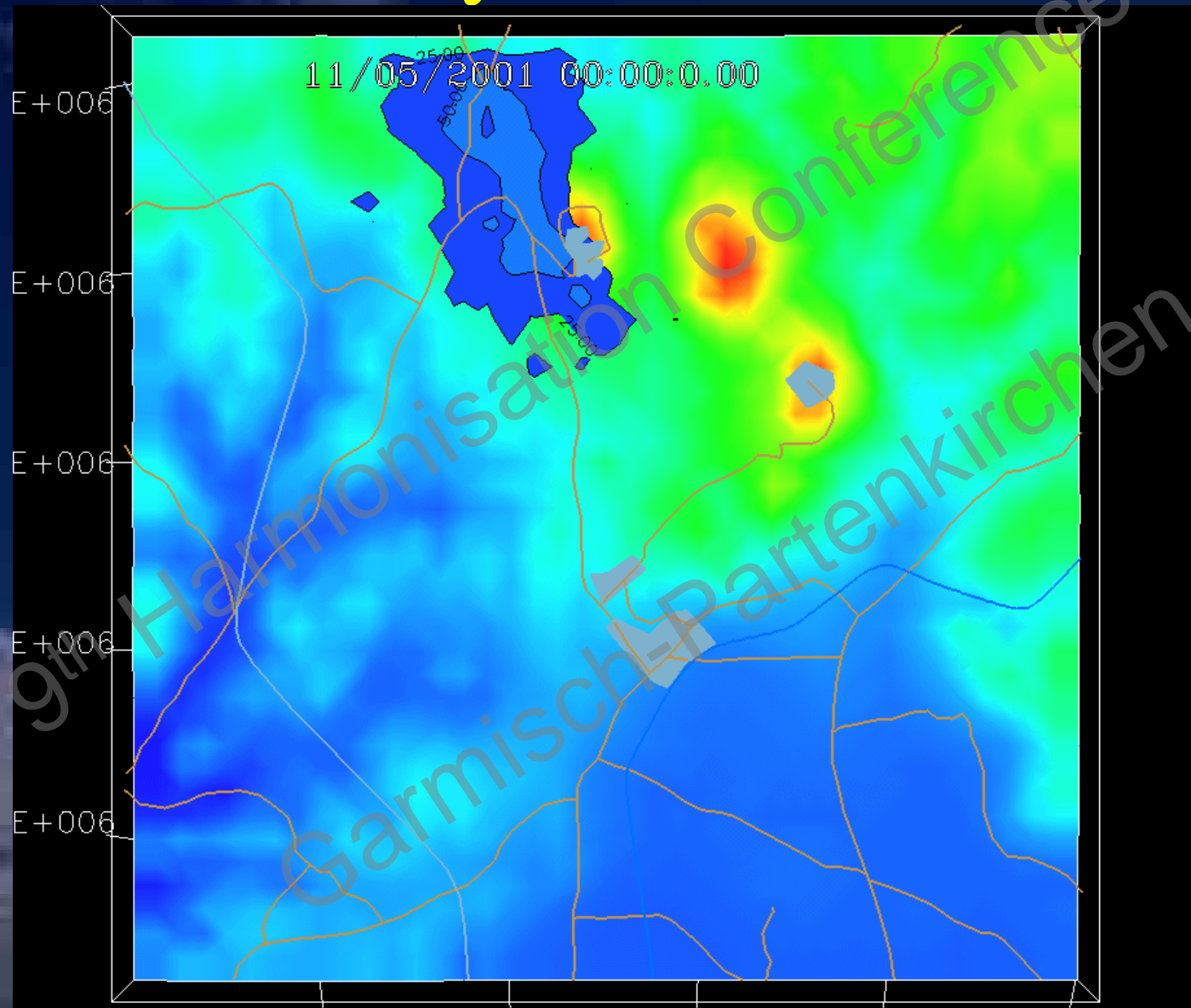


Top view





# Half hourly SPRAY Results



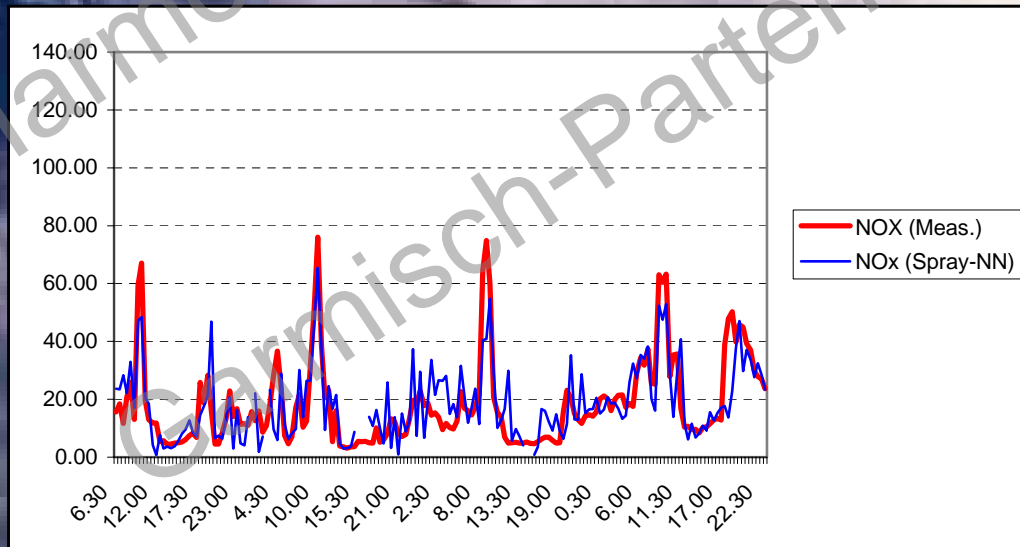
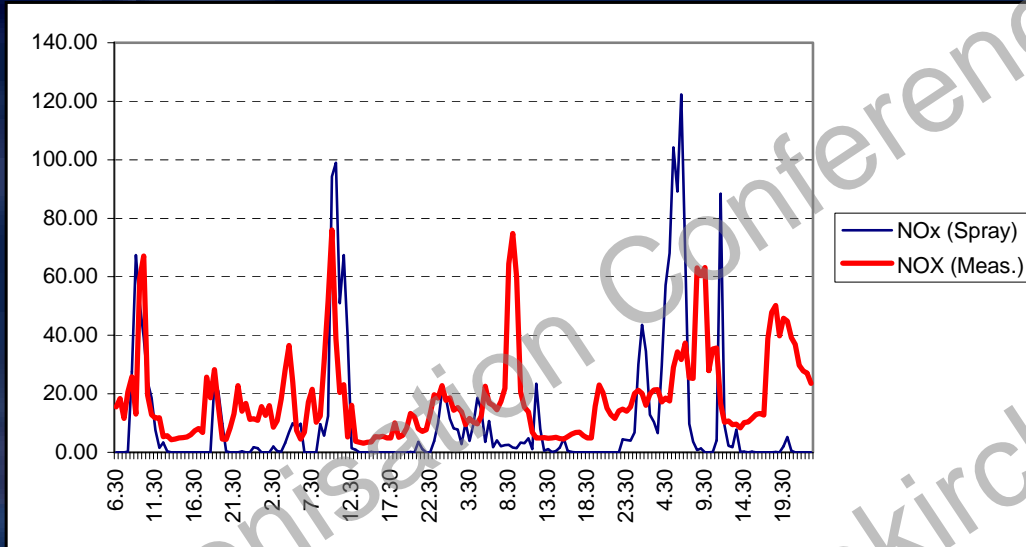
# Main results of Spray-NN model (Simulation with CLPDM) and NN alone (without Nox(Spray)).

5 Hidden Neurons	Percent of data during the training phase								
Spray-NN	40%	50%	60%	70%	80%	85%	90%	95%	100%
Correlation ( R )	0.47	0.48	0.59	0.70	0.67	0.73	0.69	0.75	0.73
Percent of Negative Concentrations (%)	8.0	4.3	3.4	1.2	3.1	1.5	1.2	0.3	3.4
NN alone	40%	50%	60%	70%	80%	85%	90%	95%	100%
Correlation ( R )	0.48	0.55	0.56	0.64	0.64	0.64	0.68	0.64	0.69
Percent of Negative Concentrations (%)	5.8	3.4	6.5	1.5	1.5	0.0	3.1	0.0	0.9

8 Hidden Neurons	Percent of data during the training phase								
Spray-NN	40%	50%	60%	70%	80%	85%	90%	95%	100%
Correlation ( R )	0.44	0.57	0.61	0.72	0.77	0.77	0.80	0.81	<b>0.86</b>
Percent of Negative Concentrations (%)	11.4	10.2	8.0	3.7	6.2	4.0	2.8	2.8	0.9
NN alone	40%	50%	60%	70%	80%	85%	90%	95%	100%
Correlation ( R )	0.55	0.59	0.68	0.70	0.65	0.75	0.76	0.76	0.76
Percent of Negative Concentrations (%)	8.0	7.1	4.3	3.4	1.5	2.2	2.8	3.1	3.1

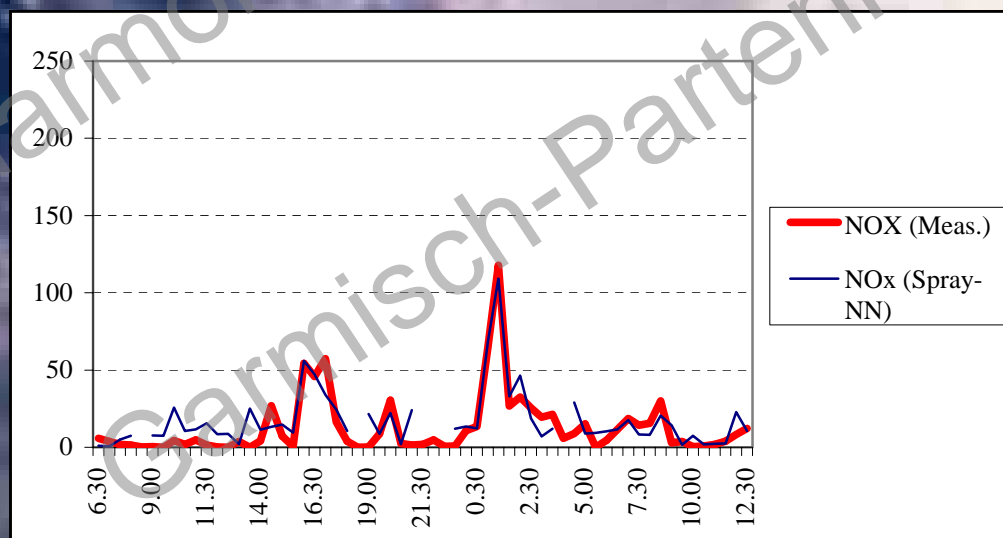
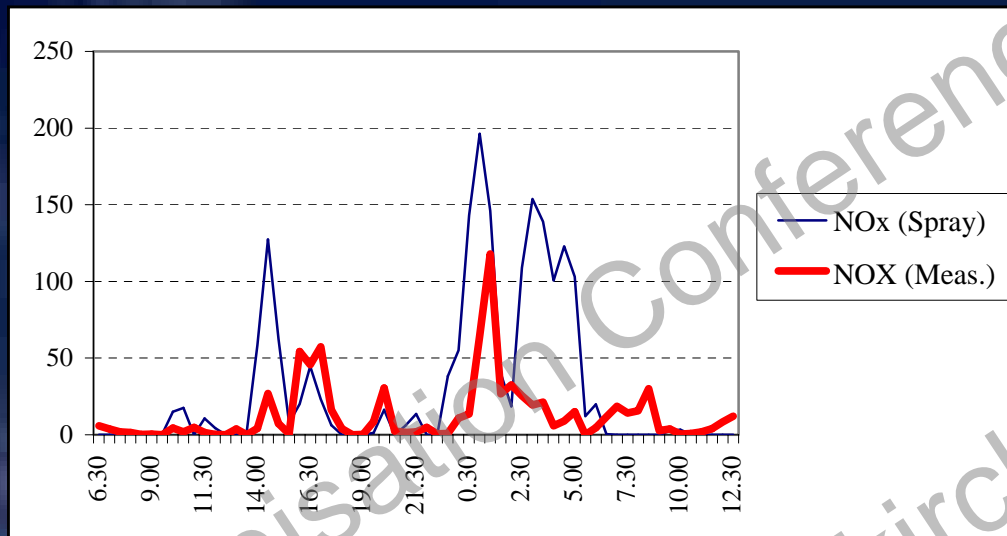
10 Hidden Neurons	Percent of data during the training phase								
Spray-NN	40%	50%	60%	70%	80%	85%	90%	95%	100%
Correlation ( R )	0.56	0.62	0.77	0.75	0.80	0.78	0.83	0.83	0.84
Percent of Negative Concentrations (%)	5.5	10.5	8.6	5.2	4.6	6.8	4.0	2.8	4.3
NN alone	40%	50%	60%	70%	80%	85%	90%	95%	100%
Correlation ( R )	0.49	0.66	0.61	0.68	0.76	0.79	0.75	0.80	0.83
Percent of Negative Concentrations (%)	13.2	11.4	10.8	4.6	8.6	8.6	5.8	8.6	4.6

## •Ispesl station: Spray-NN model results



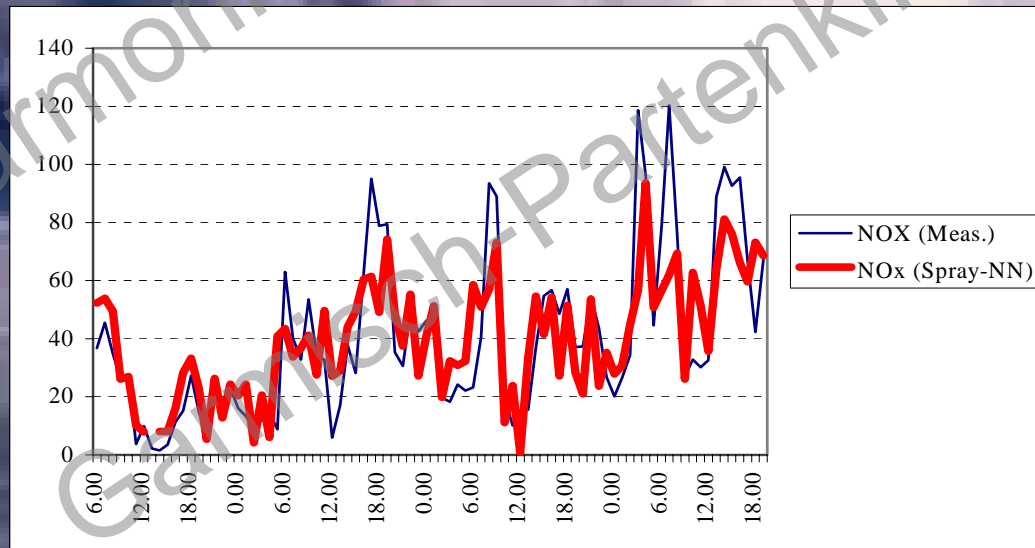
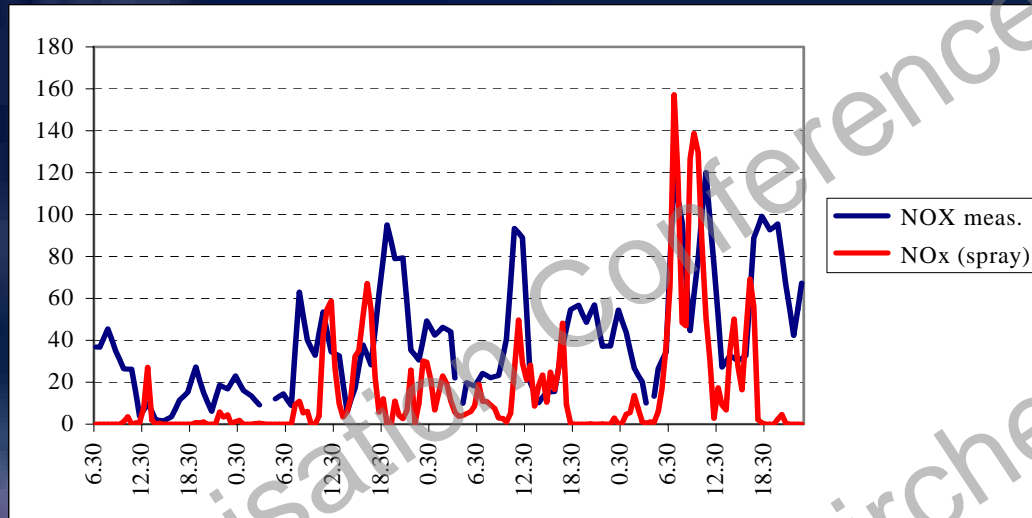
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## Unicem station: Spray-NN model results





## •Guidonia station: Spray-NN model results



# Conclusions I

- Short term Spray results sometimes missed the observed values due to other emission sources (eg. traffic) not included in that study or to an incorrect reproduction of the actual wind field
- The net succeeds in adjusting the Spray results operating on two main factors.
  - The first factor attempt to adjust the peaks of the maximum plume impact (to certainly be ascribed to the cement factory) and to fix the temporal shift produced by the Lagrangian model.
  - The second factor operates on situation where observed values are mainly produced by other emissions sources different from the stack, which was the only one considered in the Spray simulations.
- This has particular relevance in the Guidonia monitoring station, where traffic emissions are, at rush hours, the main contributors to the measured pollutants concentrations.

# Conclusions II

- The comparison of simulation results with the observations collected at selected monitoring stations have shown good agreement for  $\text{NO}_x$ .
- The net improvement in the overall models accuracy is observed when the Neural network was applied downstream to the particle model.
- The introduction of the new spatial coordinates in the NN input variables, allows to extend the spatial estimation of ground concentrations

# The Modeling approach

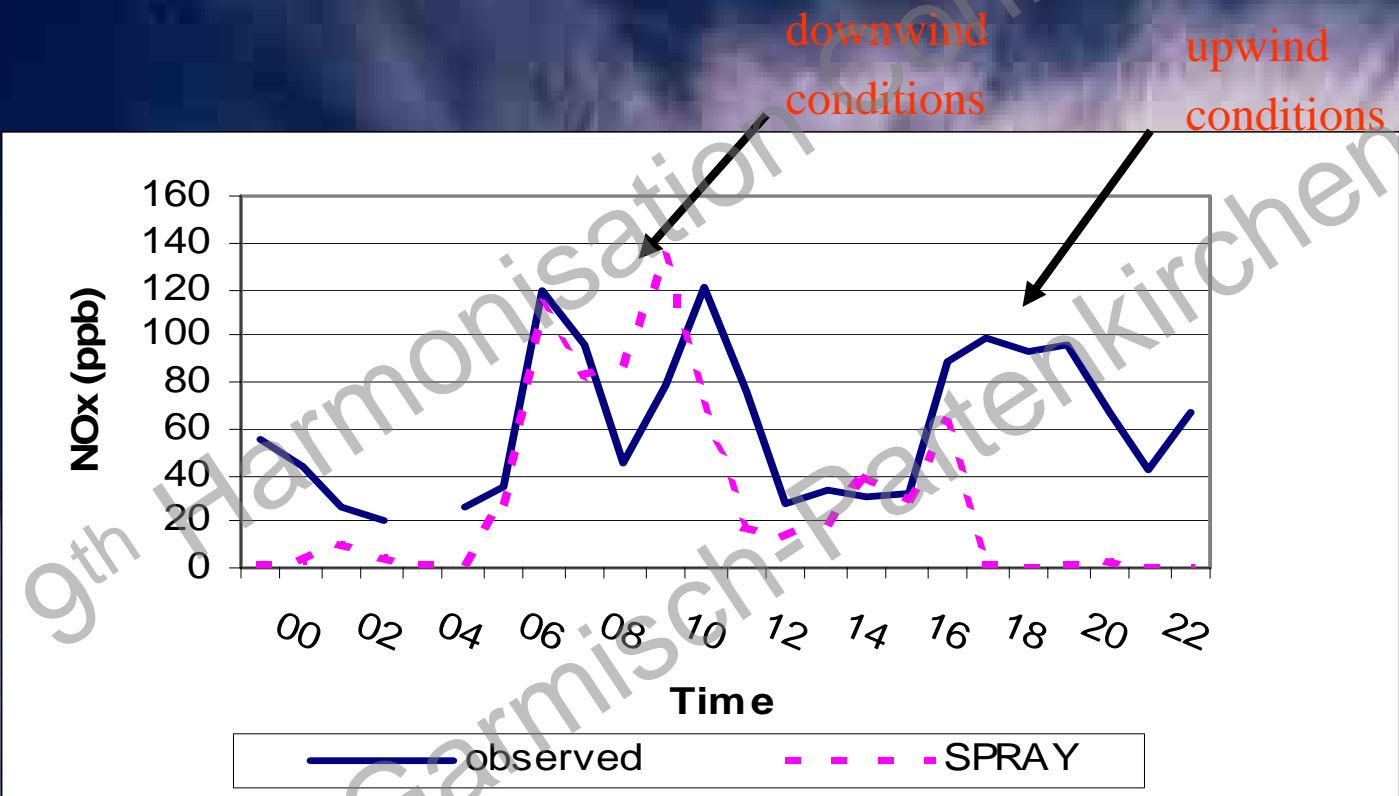
- A combined meteorological-dispersion models approach has been used to achieve better accuracy on pollution ground concentrations estimation.
- Such modeling system is recommended in complex conditions where land/sea interface and topography give rise to complex circulation patterns.
- These atmospheric circulation cannot be reproduced by stationary and homogeneous dispersion models (Gaussian) which produce wrong concentration fields and consequence analysis evaluation with dramatic effects in case of accidental releases of dangerous substances.



longitudine	311735.3	311036.7	311650.08
latitudine	4653732.15	4652861.8	4651773.19
X-COORDIN	715.88	17.28	630.66
Y-COORDIN	171.69	-698.66	-1787.27
	Ispesl	Unicem	Guidonia

date	Dir Vento	90 Cartesian Angle	CROSSWIND	UPWIND	CROSSWIND	UPWIND	CROSSWIND	UPWIND
			X WIND	Y WIND	X WIND	Y WIND	X WIND	Y WIND
22/10/2001	<b>130</b>	<b>-40</b>	-438.04	<b>591.68</b>	-462.33	-524.10	-1631.95	-963.75
22/10/2001	<b>115</b>	<b>-25</b>	-576.25	<b>458.15</b>	-310.93	-625.90	-1326.91	-1353.29
22/10/2001	<b>125</b>	<b>-35</b>	-487.94	<b>551.25</b>	-414.89	-562.40	-1541.74	-1102.31
22/10/2001	<b>140</b>	<b>-50</b>	-328.64	<b>658.76</b>	-546.31	-435.85	-1774.51	-665.72
22/10/2001	<b>138</b>	<b>-48</b>	-351.43	<b>646.89</b>	-530.77	-454.65	-1750.19	-727.25
22/10/2001	<b>131</b>	<b>-41</b>	-427.64	<b>599.24</b>	-471.40	-515.95	-1648.52	-935.12
22/10/2001	<b>128</b>	<b>-38</b>	-458.42	<b>576.03</b>	-443.75	-539.91	-1597.32	-1020.11
22/10/2001	<b>132</b>	<b>-42</b>	-417.12	<b>606.61</b>	-480.34	-507.64	-1664.59	-906.21
22/10/2001	<b>280</b>	<b>-190</b>	675.19	-293.39	138.34	<b>685.05</b>	931.44	<b>1650.60</b>
22/10/2001	<b>234</b>	<b>-144</b>	680.08	<b>281.88</b>	-396.68	<b>575.38</b>	-540.32	<b>1816.62</b>
22/10/2001	<b>268</b>	<b>-178</b>	721.44	-146.60	-7.11	<b>698.84</b>	567.90	<b>1808.19</b>
22/10/2001	<b>296</b>	<b>-206</b>	568.16	-468.14	321.80	<b>620.38</b>	1350.32	<b>1329.92</b>
22/10/2001	<b>289</b>	<b>-199</b>	620.98	-395.40	243.80	<b>654.97</b>	1178.18	<b>1484.57</b>
22/10/2001	<b>297</b>	<b>-207</b>	559.91	-477.98	332.58	<b>614.67</b>	1373.33	<b>1306.16</b>
22/10/2001	<b>266</b>	<b>-176</b>	726.11	-121.33	-31.50	<b>698.16</b>	504.45	<b>1826.91</b>
22/10/2001	<b>233</b>	<b>-143</b>	675.05	<b>293.71</b>	-406.66	<b>568.37</b>	-571.94	<b>1806.92</b>
22/10/2001	<b>283</b>	<b>-193</b>	658.91	-328.33	174.00	<b>676.87</b>	1016.54	<b>1599.59</b>
22/10/2001	<b>316</b>	<b>-226</b>	373.79	-634.23	514.58	<b>472.90</b>	1723.75	<b>787.88</b>
22/10/2001	<b>238</b>	<b>-148</b>	698.08	<b>233.76</b>	-355.58	<b>601.65</b>	-412.28	<b>1849.89</b>
22/10/2001	<b>222</b>	<b>-132</b>	606.61	<b>417.12</b>	-507.64	<b>480.34</b>	-906.21	<b>1664.59</b>
22/10/2001	<b>213</b>	<b>-123</b>	533.89	<b>506.88</b>	-576.53	<b>395.01</b>	-1155.45	<b>1502.33</b>
22/10/2001	<b>229</b>	<b>-139</b>	652.92	<b>340.08</b>	-445.32	<b>538.62</b>	-696.59	<b>1762.62</b>
22/10/2001	<b>236</b>	<b>-146</b>	689.50	<b>257.98</b>	-376.36	<b>588.88</b>	-476.59	<b>1834.37</b>
22/10/2001	<b>222</b>	<b>-132</b>	606.61	<b>417.12</b>	-507.64	<b>480.34</b>	-906.21	<b>1664.59</b>

# Results of lagrangian model. Comparison with monitoring data



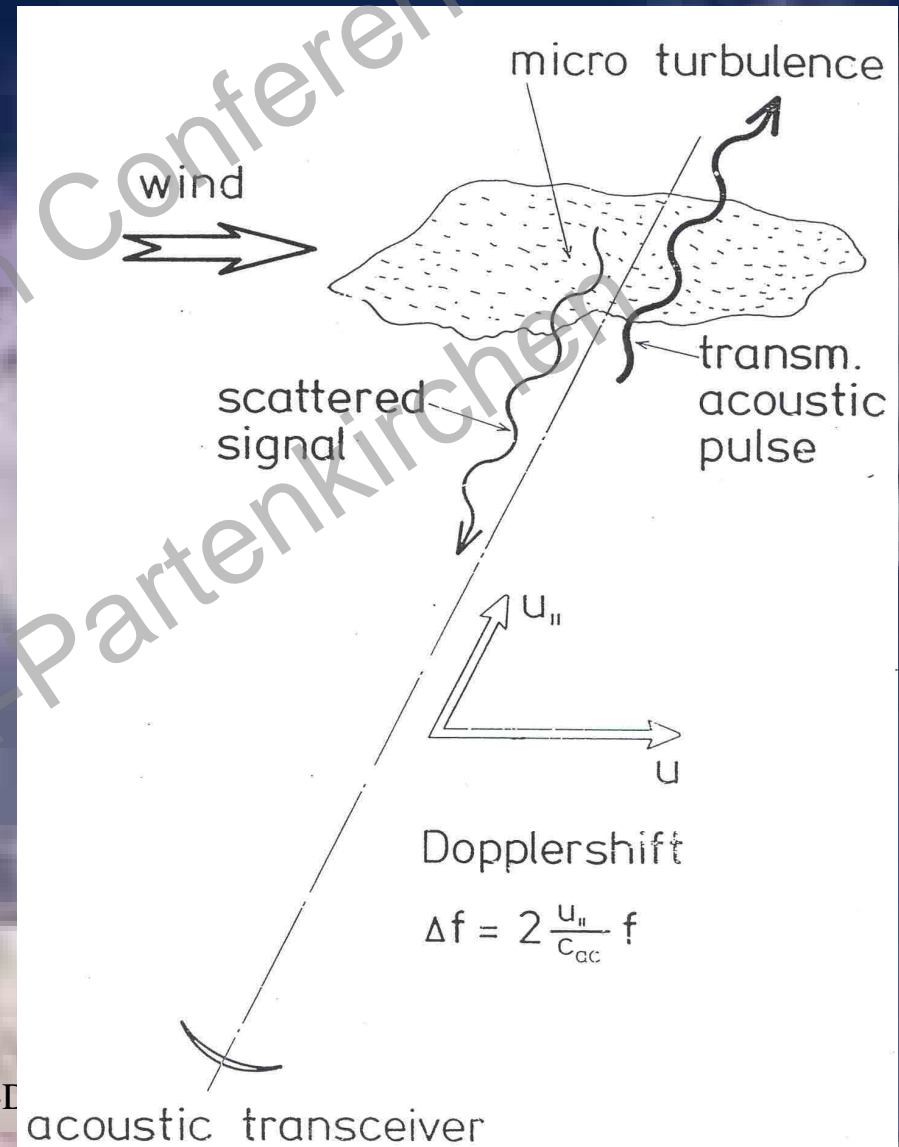
Guidonia monitoring station on November 5<sup>th</sup>

# Acoustic remote sensing

A SODAR (Sound Detection And Ranging) is a system able to measure Planet Boundary Layer (PBL) parameters such as wind and turbulence profiles, which have a great influence on air pollution dispersion.

# SODAR Measuring Principle

The SODAR transmits short and high powered acoustic pulses. A fraction of the acoustic energy is scattered back from atmosphere fluctuations. Its frequency is shifted according to the wind component parallel to the beam axis (Doppler effect). Height range can be evaluated from the pulse propagation time. Three orthogonal acoustic beams are used to reconstruct the three Cartesian wind components.





# The ISPESEL Mini-SODAR

- Vertical profile of:
  - Cartesian wind components
  - Horizontal wind components
  - Vertical wind speed
  - Reflectivity
  - Standard deviation of wind direction
  - Wind inclination angle
- Maximum height 400 m
- Vertical resolution 2 m