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A multiscale modelling approach putting special emphasis on the efficient treatment of urban plumes

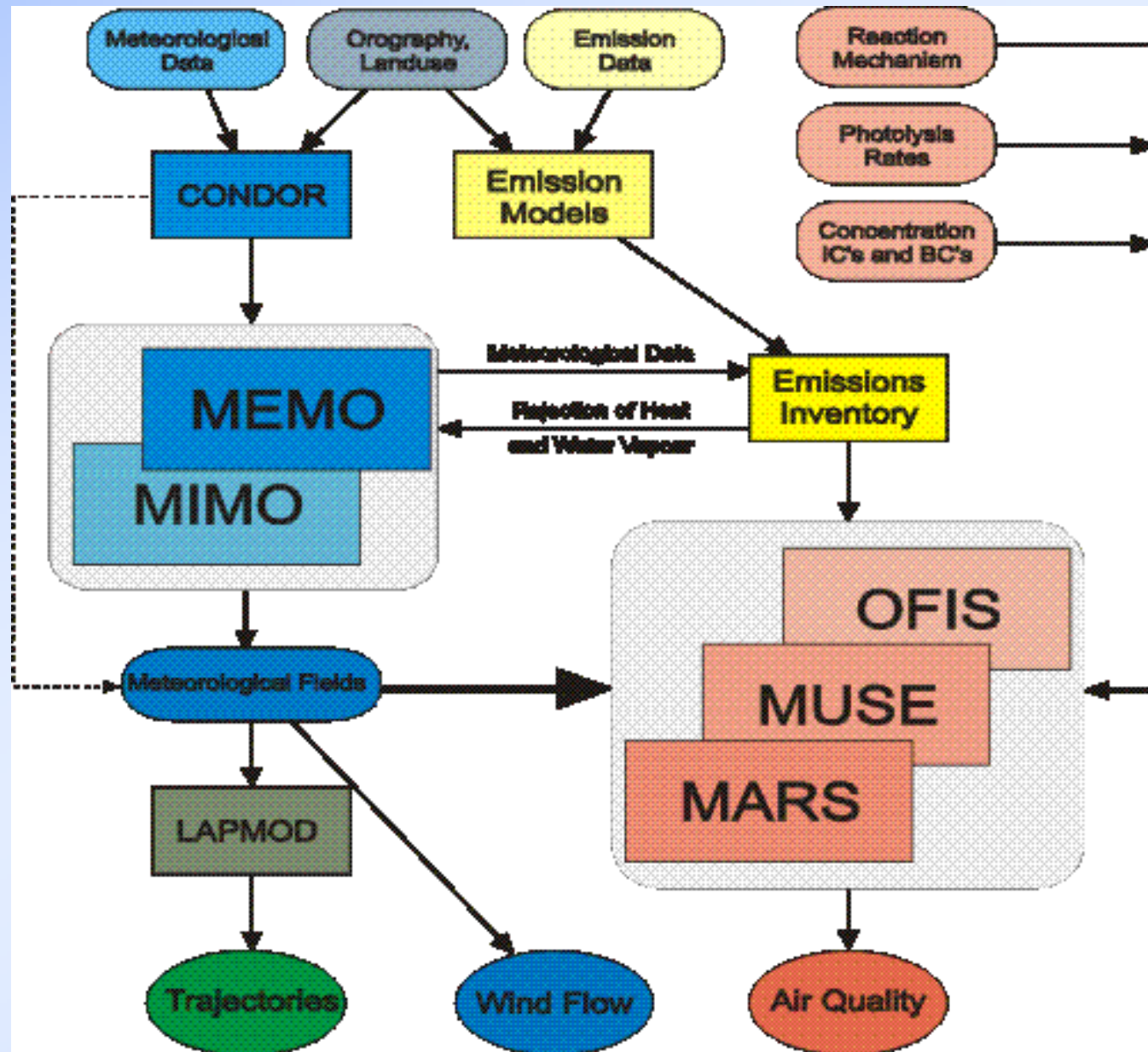
John Douros and Nicolas Moussiopoulos

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European Zooming Model (EZM) system





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Motivation

“...For zones and agglomerations within which information from fixed measurement stations is supplemented by information from other sources, such as emission inventories, indicative measurement methods and air-quality modelling,...”

Article 7, p. 3,
COUNCIL DIRECTIVE 1999/30/EC,
Official Journal of the European Communities

The directions within the Directives rise a twofold challenge for the modelling research community;

- (i) estimating spatial distributions of pollutant concentrations and
- (ii) doing so for at least one year

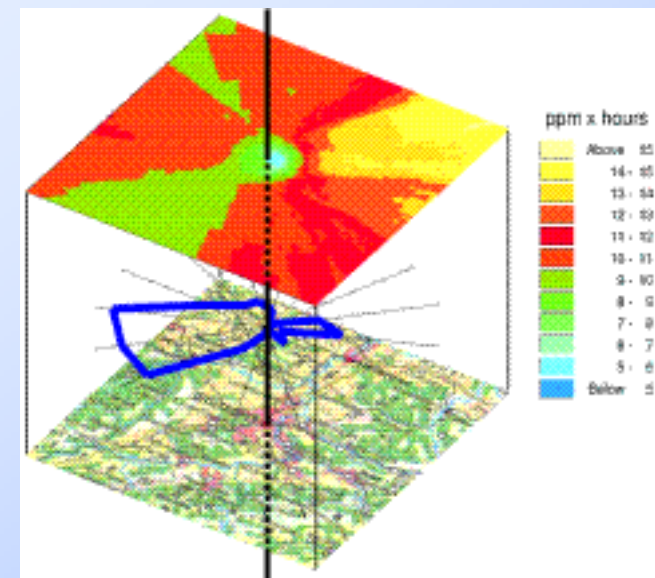


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The Ozone Fine Structure (OFIS) model - Model concept

The OFIS model was developed in order to

- (i) allow authorities to assess urban air quality by means of a fast, simple and still reliable model
- (ii) refine a regional model simulation by estimating the urban subgrid effect on pollution levels



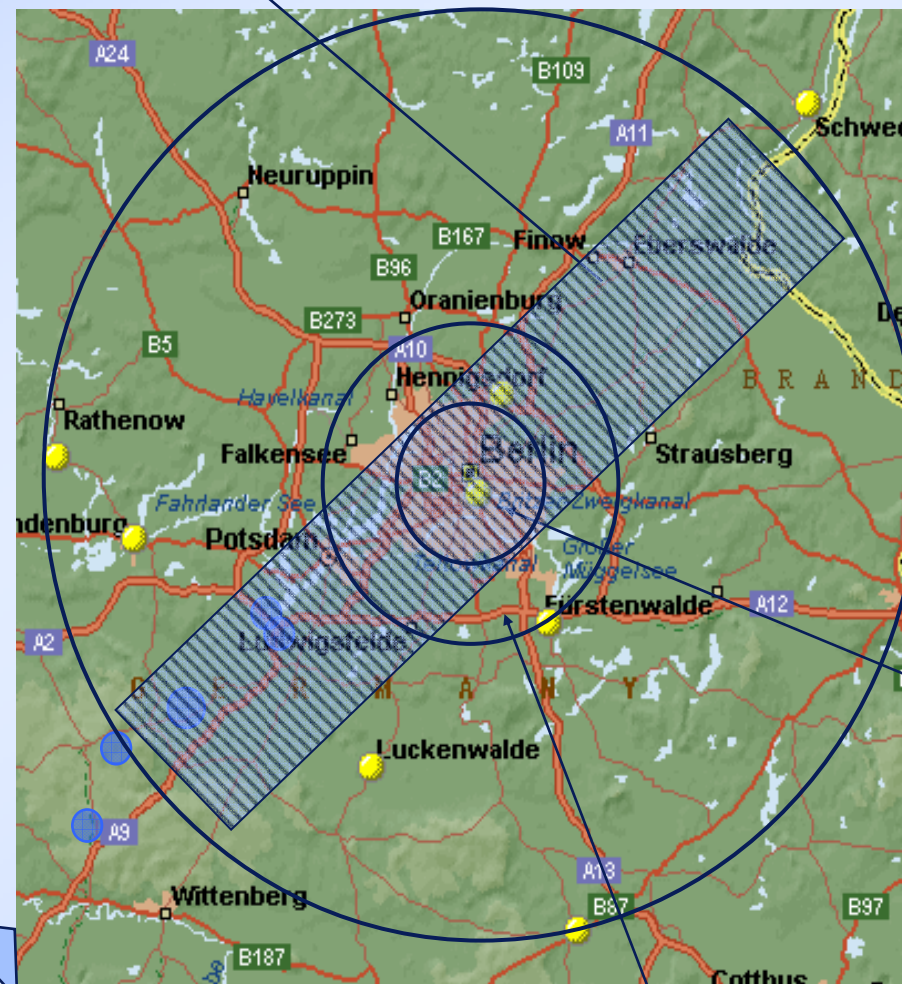


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OFIS - Sample of horizontal grid layout

2D multibox model

- 2-layer gridded strip, length of 240 km
- Width defined by city size
- Prevailing wind from NE
- Altering direction when the meteorological input is modified (every 3 hours)
- First vertical layer extends up to 90m (in accordance with the EMEP model)
- Second one extends up to the mixing height



Wind direction

suburban

urban



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OFIS model - Model description

Pollutant transport and transformation downwind the city (along the prevailing wind direction) calculated with a 2-layer model.

$$\Delta c_i^1 / \Delta t = K_z(c_i^2 - c_i^1) / dz_1^2 + q_i / dz_1 + R_i(c_1^1, \dots, c_n^1) + u(c_i^{u1} - c_i^1) / \Delta x$$

$$\Delta c_i^2 / \Delta t = K_z(c_i^1 - c_i^2) / (dz_2 dz_1) + R_i(c_1^2, \dots, c_n^2) + u(c_i^{u2} - c_i^2) / \Delta x + (c_i^{bc} - c_i^2) \max[0, \Delta H_t / (\Delta t \cdot H_t)]$$

C_i : concentration of chemical species i

K_z : Vertical turbulent exchange coeff.

q_i : emission rate for species i

R_i : Chemical formation or destruction rate for species i

H_t : mixing height

Top of 1st layer = 90 m

2nd layer = mixing height

cell width = city diameter

cell length (Δx) = ~5 km



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The Ozone Fine Structure (OFIS) model - Model features

- Equation system solved with an iterative Gauss-Seidel applied on 2nd order BDF integrator.
- EMEP MSC-W and CBM-IV chemical mechanisms currently available in the model.
- An aerosol module of two modes of log-normal distribution assuming inorganics equilibrium between phases is included.
- Advection is discretised using an upwind scheme.
- Mixing height and turbulent diffusivity estimated in a vertical column atmosphere/soil radiation budget model.
- Requires less than 4 hours of computation time for a full calendar year simulation on a P4 2.0 GHz CPU



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Recent OFIS improvements

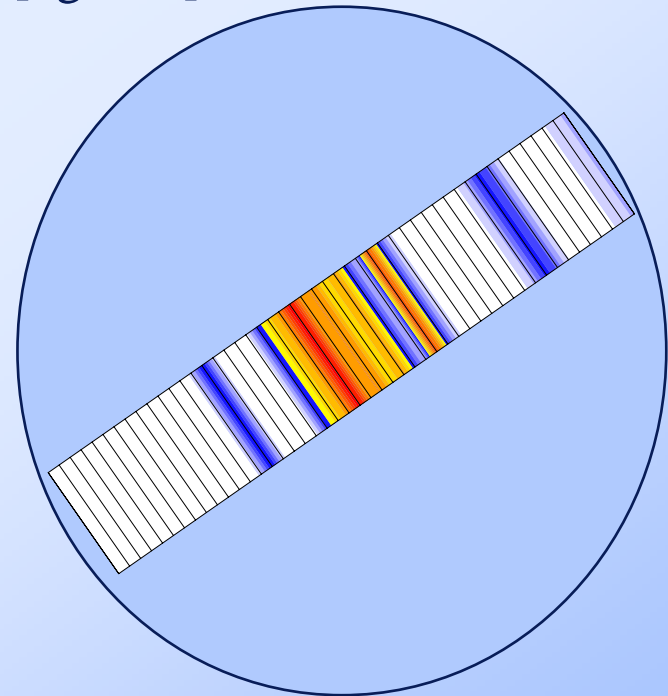
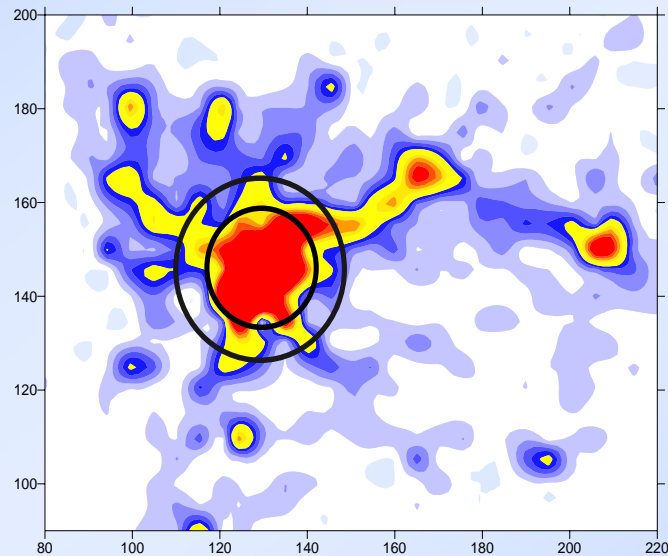
- Capability for use of gridded emissions inventories, besides the default disaggregated ones
- 3-hourly values are used for the meteorological and boundary conditions input,
- Dry deposition parameterised using the aerodynamic resistance approach for gases and particles
- Use of an appropriate parameterisation for wet removal of gases and particles
- Vertical stratification expanded to 5 layers



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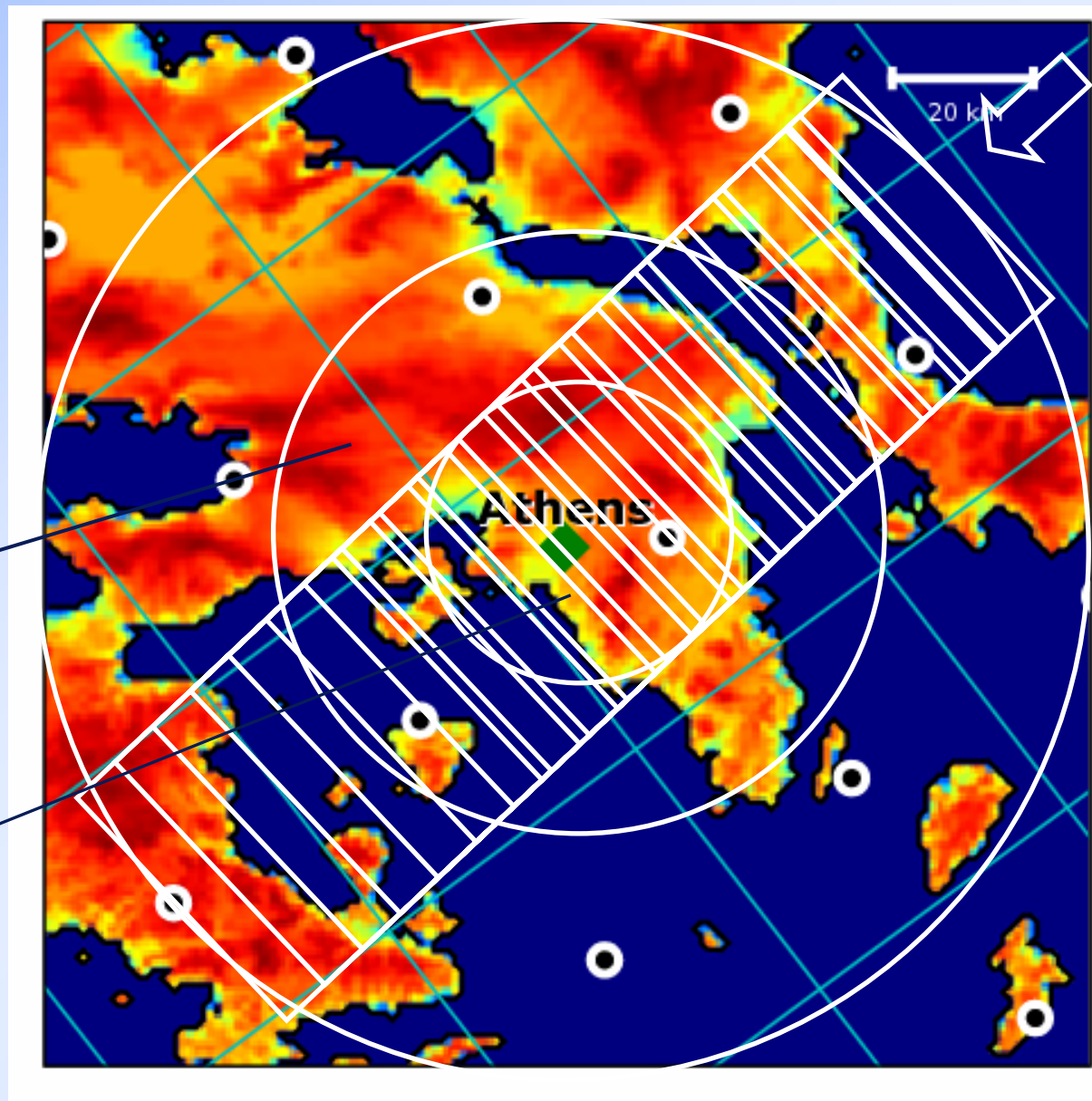
OFIS – Geographical emission distribution as arranged for use in OFIS for Milan

NO_x emissions for 5th of May, 8:00 am, [kg/km²]





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Wind
direction

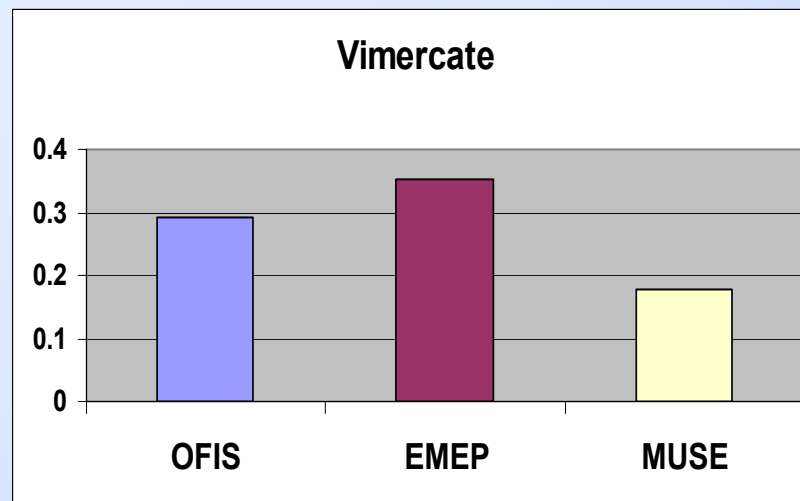
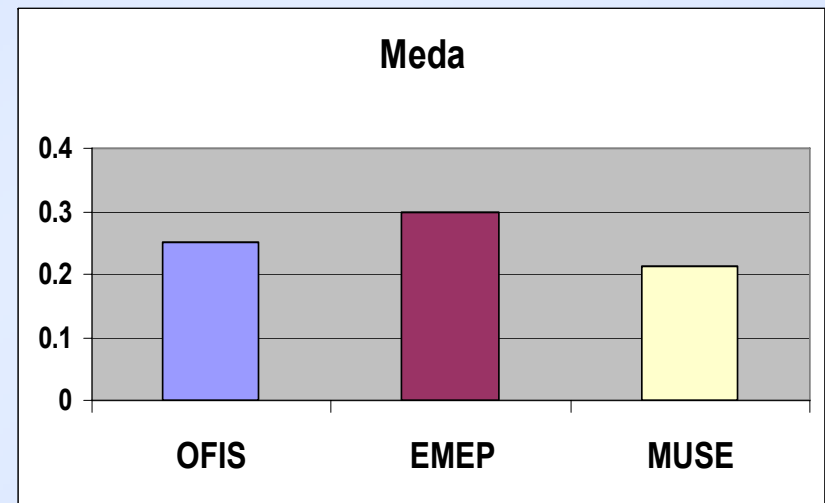
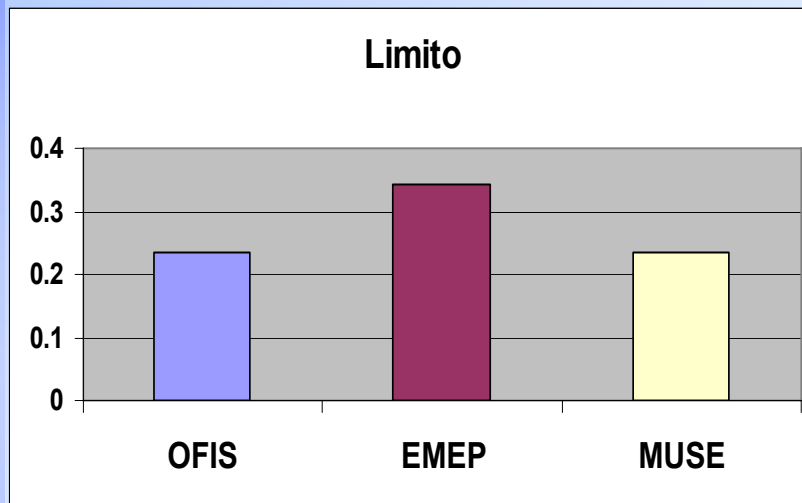
Sub-urban

Urban



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Milan – Comparing OFIS to EMEP and MUSE for O₃ *NMSE*

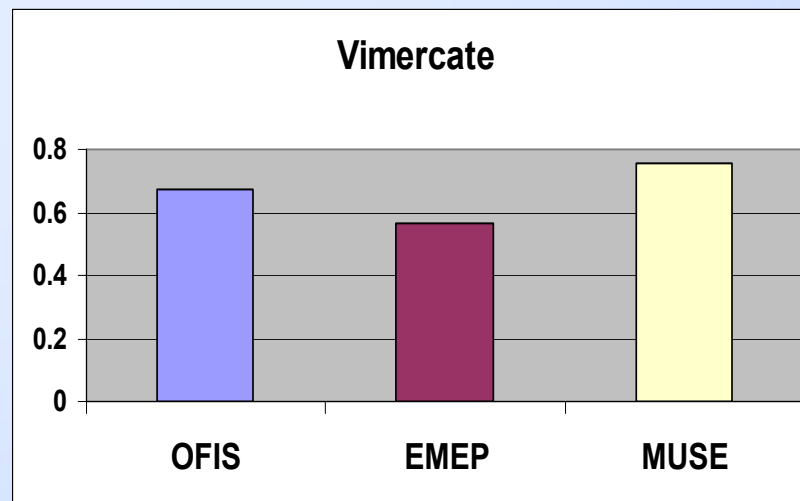
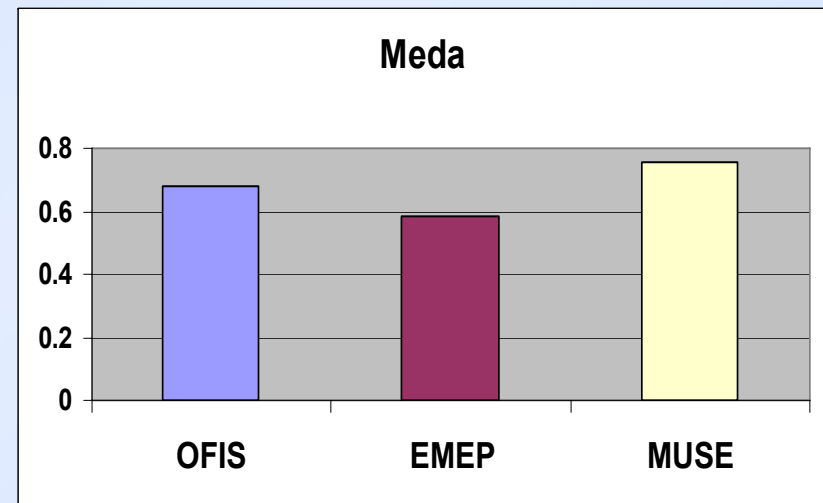
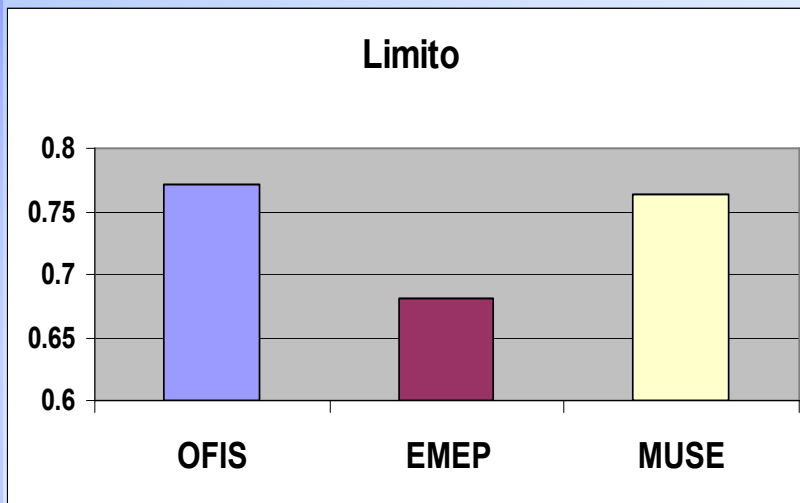




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Milan – Comparing OFIS to EMEP and MUSE for O₃

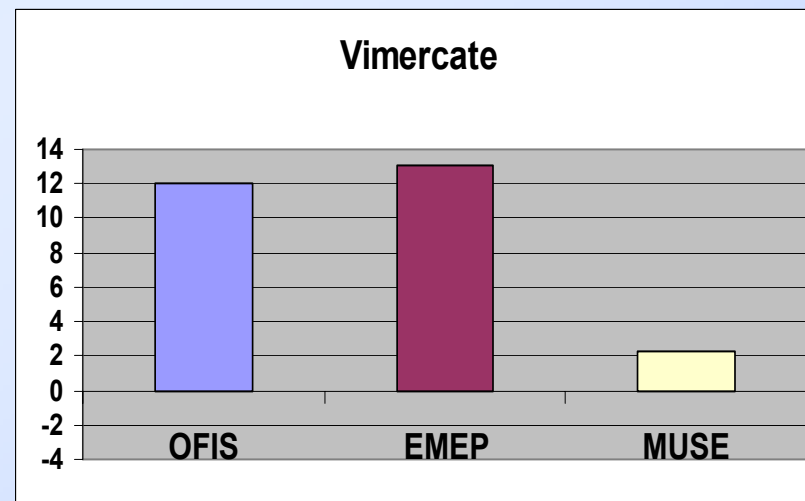
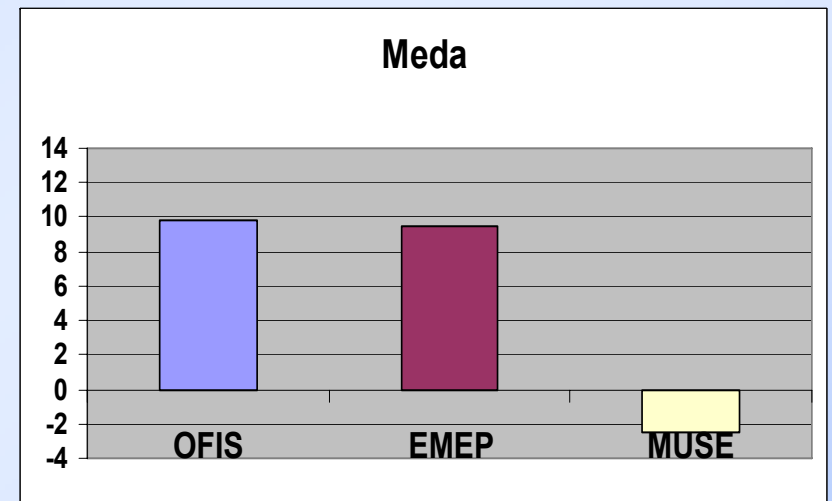
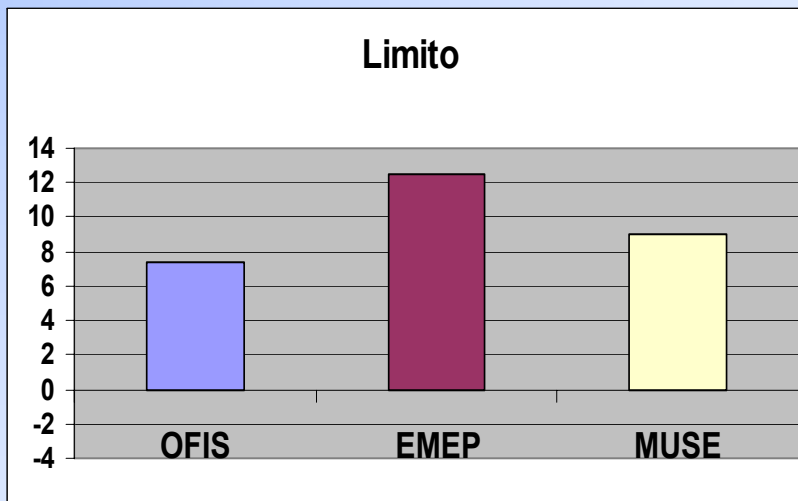
Correlation coefficient





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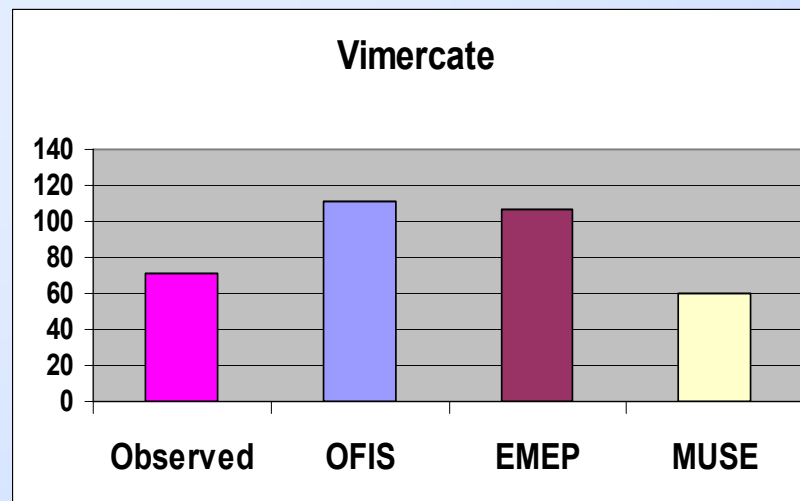
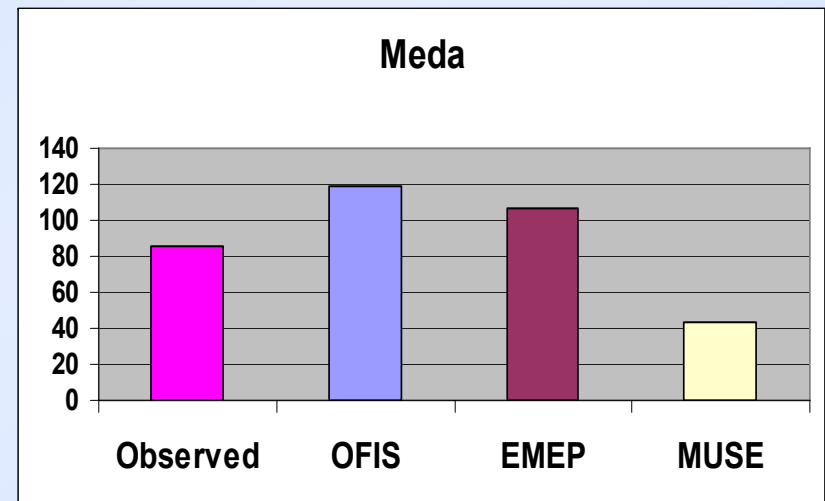
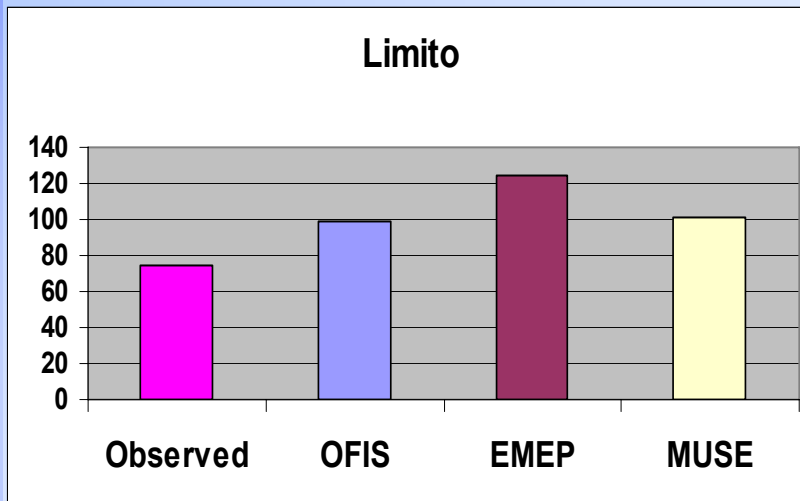
Milan – Comparing OFIS to EMEP and MUSE for O₃ *Bias*





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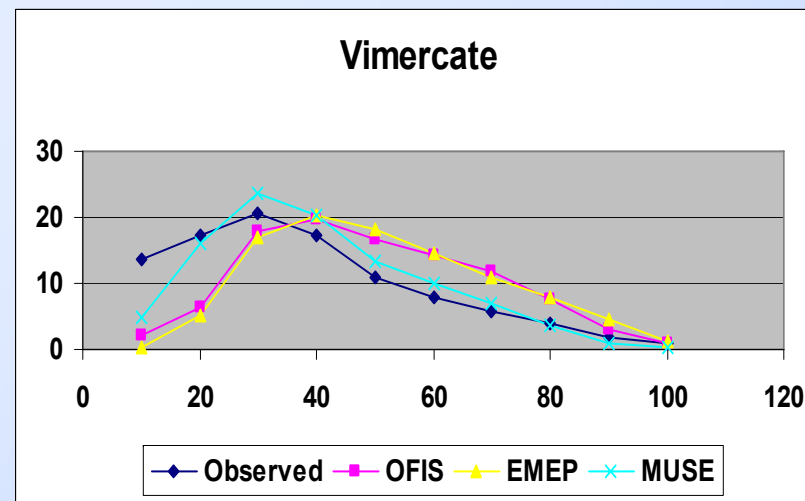
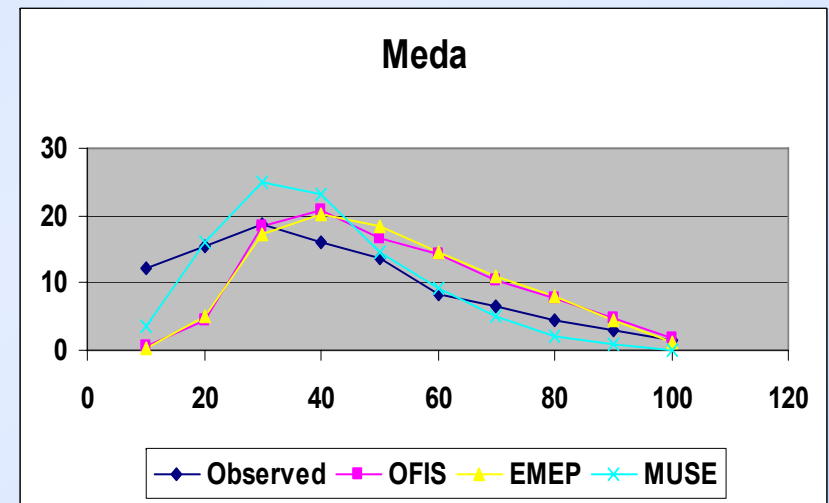
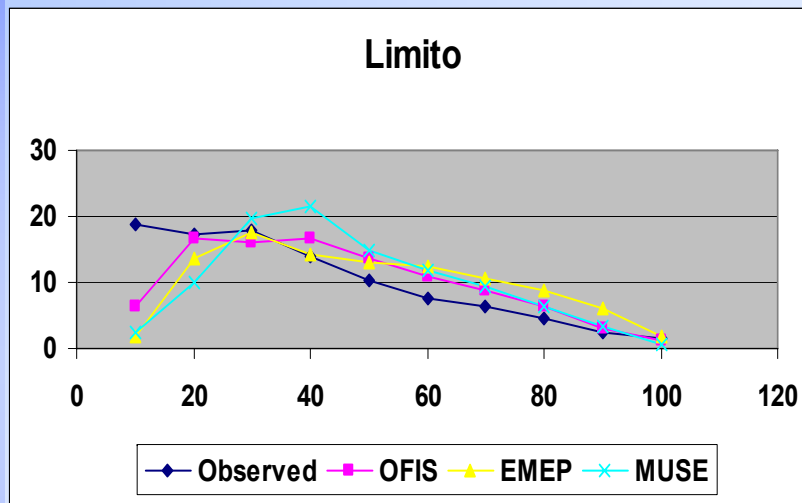
Milan – Comparing OFIS to EMEP and MUSE for O₃ *Exceedance days (120 µg/m³)*





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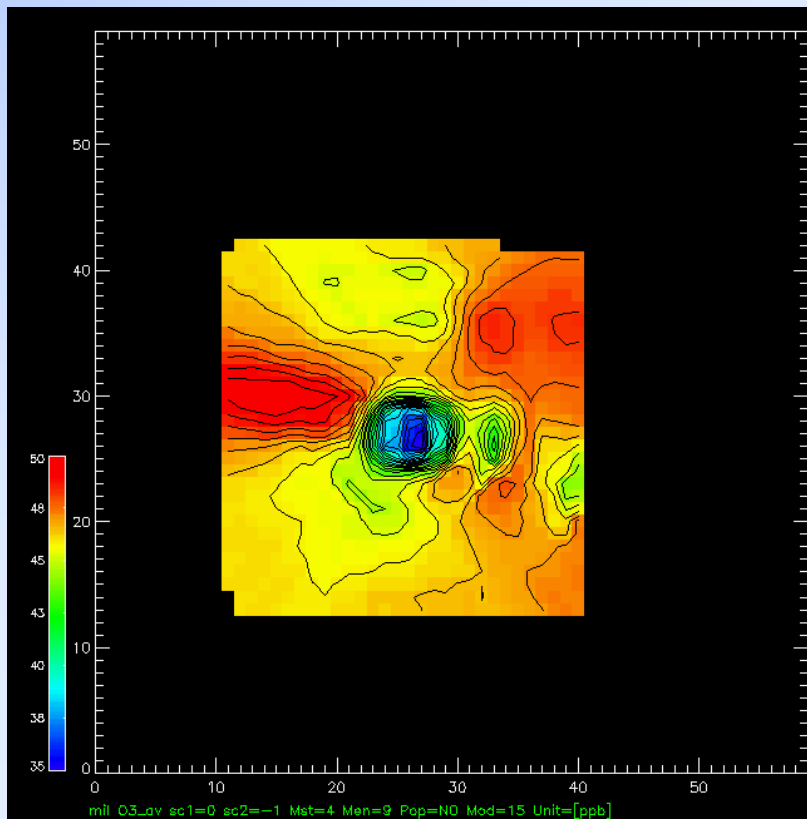
Milan – Comparing OFIS to EMEP and MUSE for O₃ *Frequencies diagram*



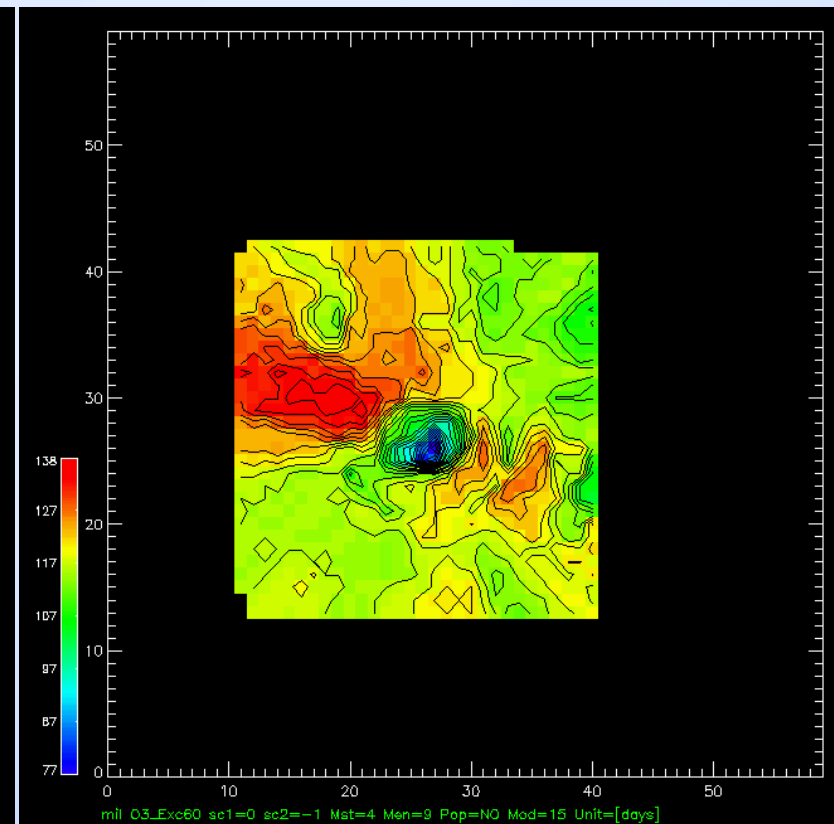


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Milan – Spatial distribution of O₃



6-month average

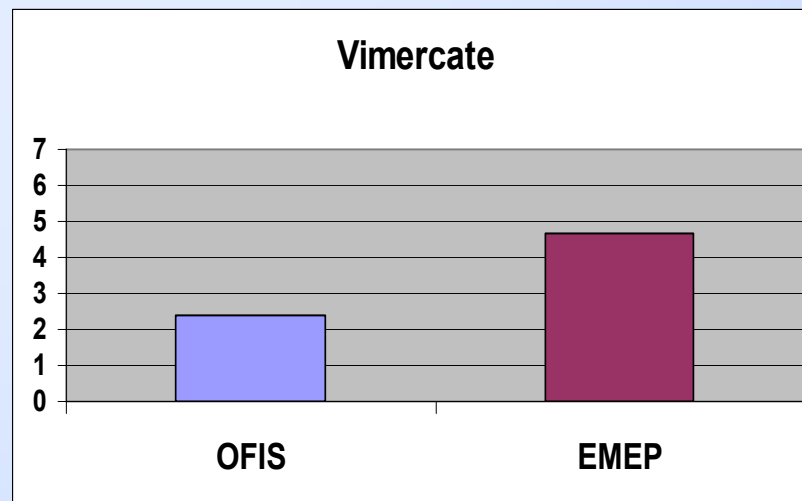
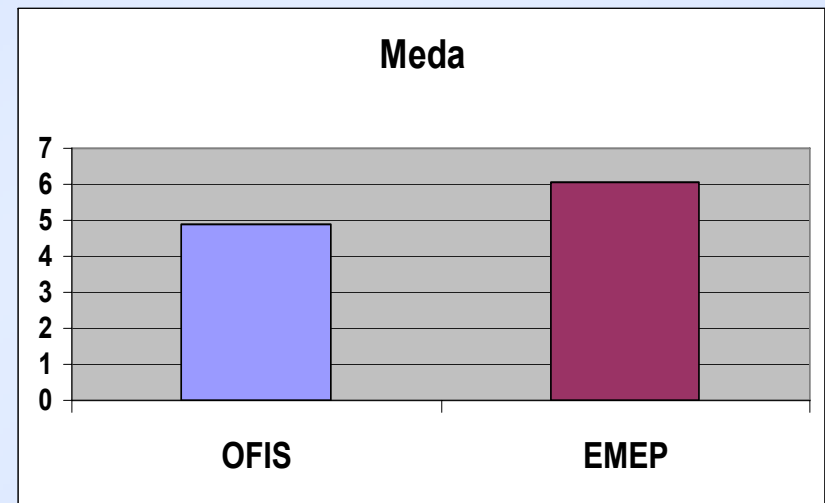
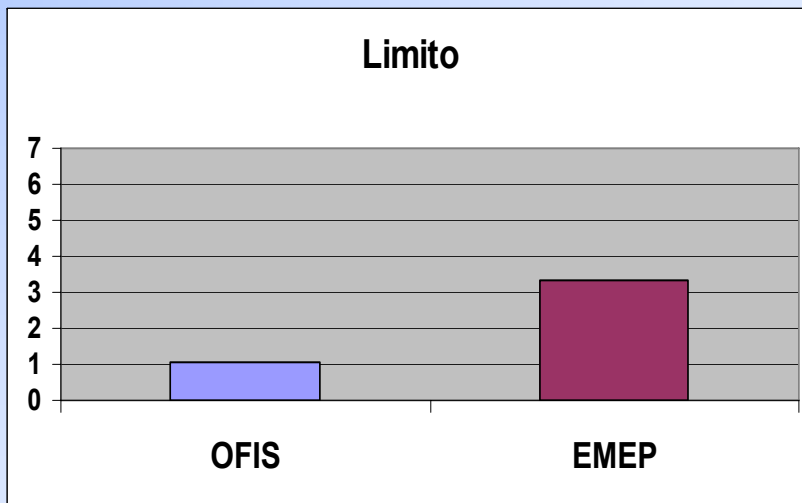


Exceedance days



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Milan – Comparing OFIS to EMEP for PM₁₀ *NMSE*

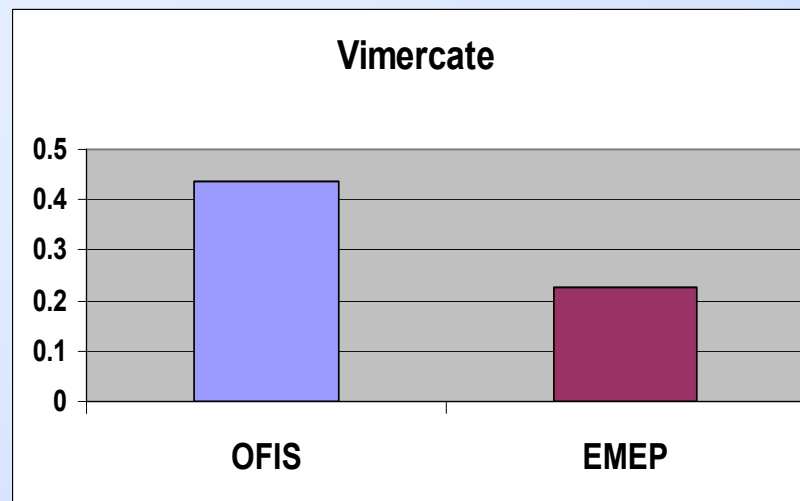
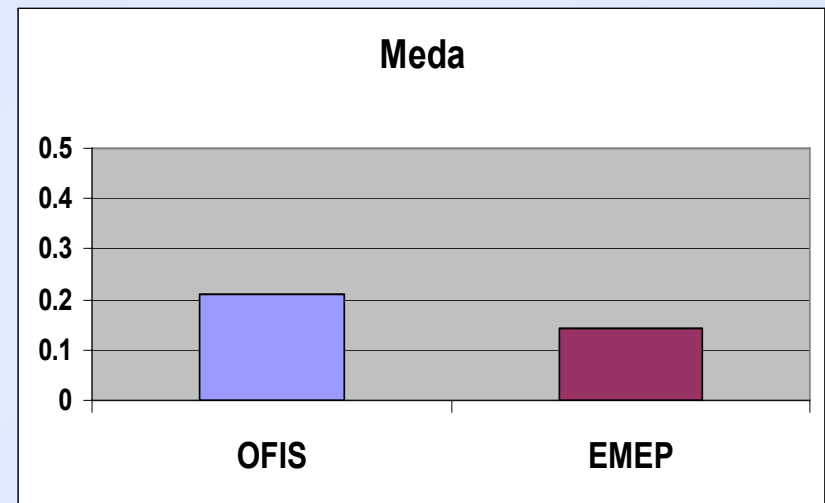
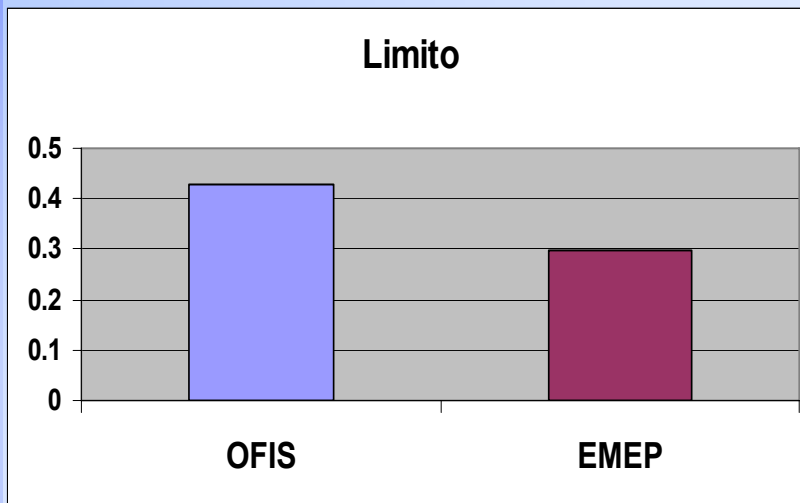




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Milan – Comparing OFIS to EMEP for PM₁₀

Correlation coefficient

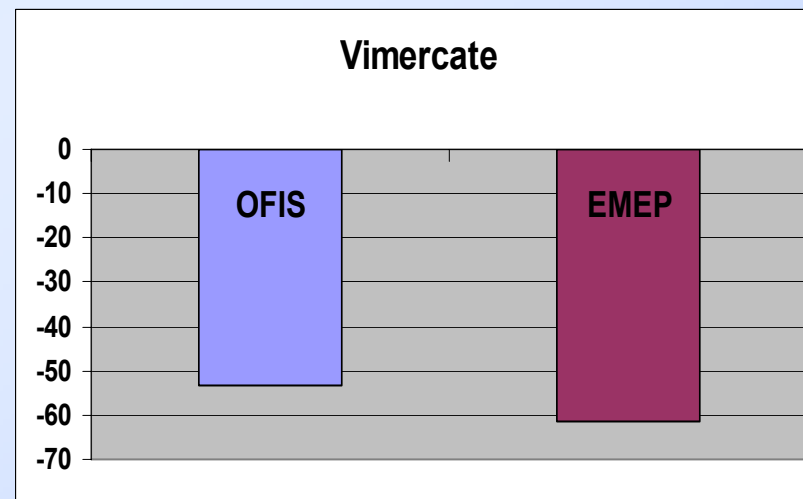
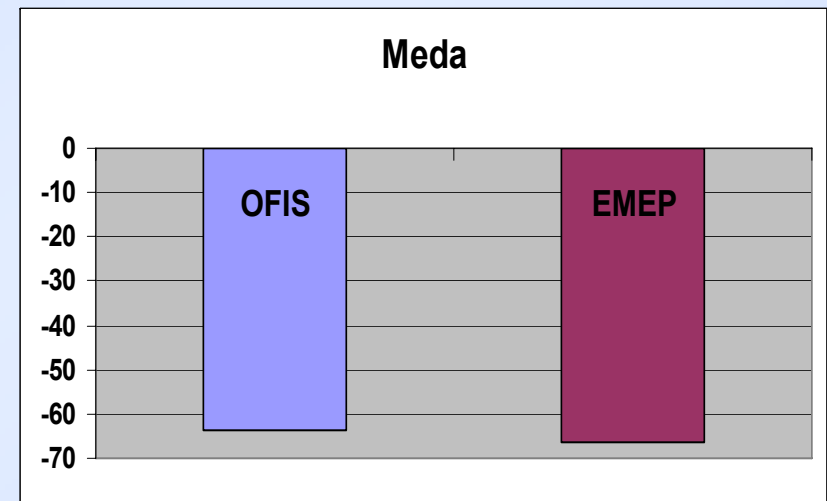
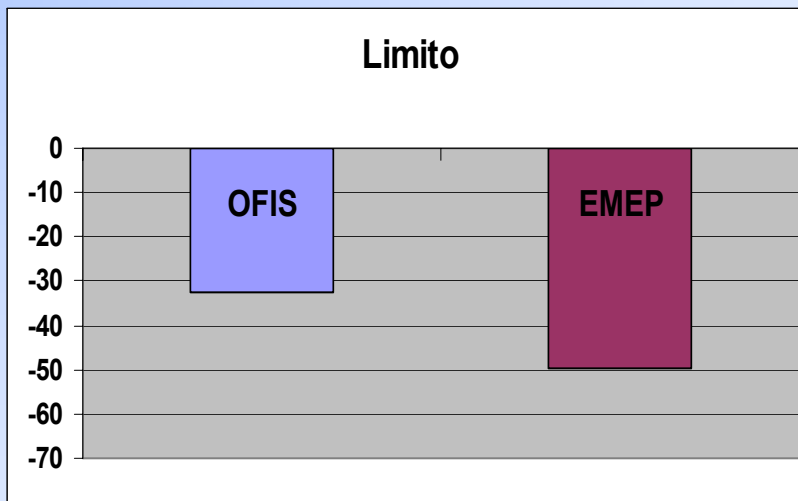




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Milan – Comparing OFIS to EMEP for PM₁₀

Bias

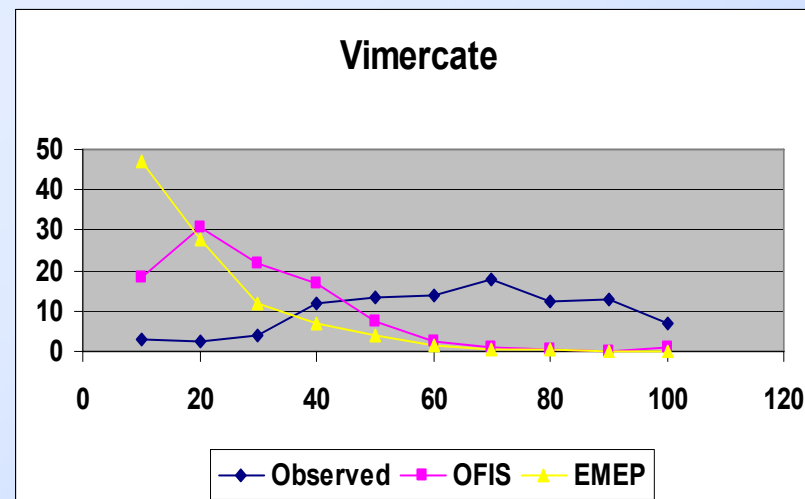
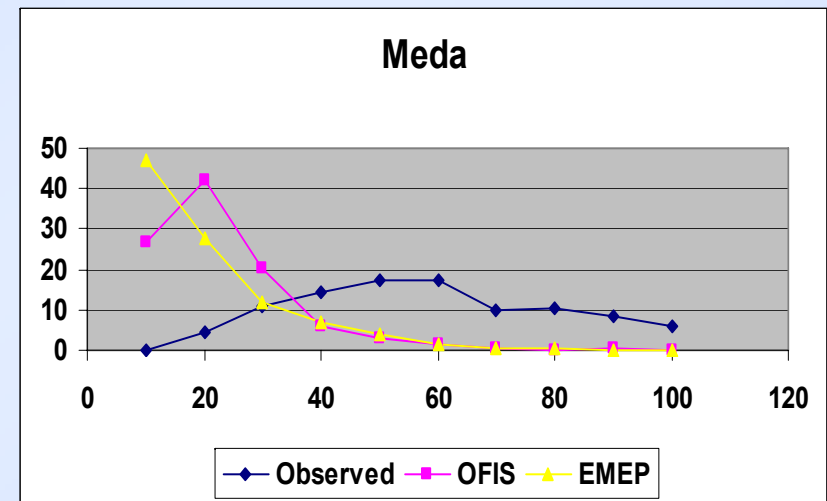
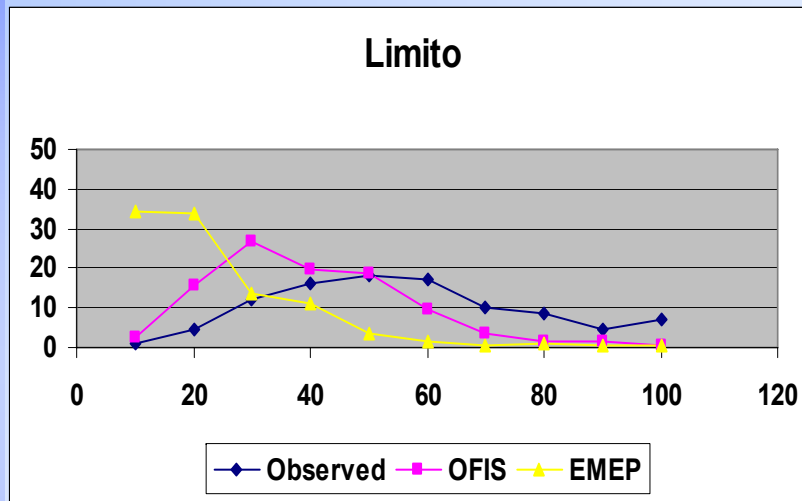




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Milan – Comparing OFIS to EMEP and MUSE for PM₁₀

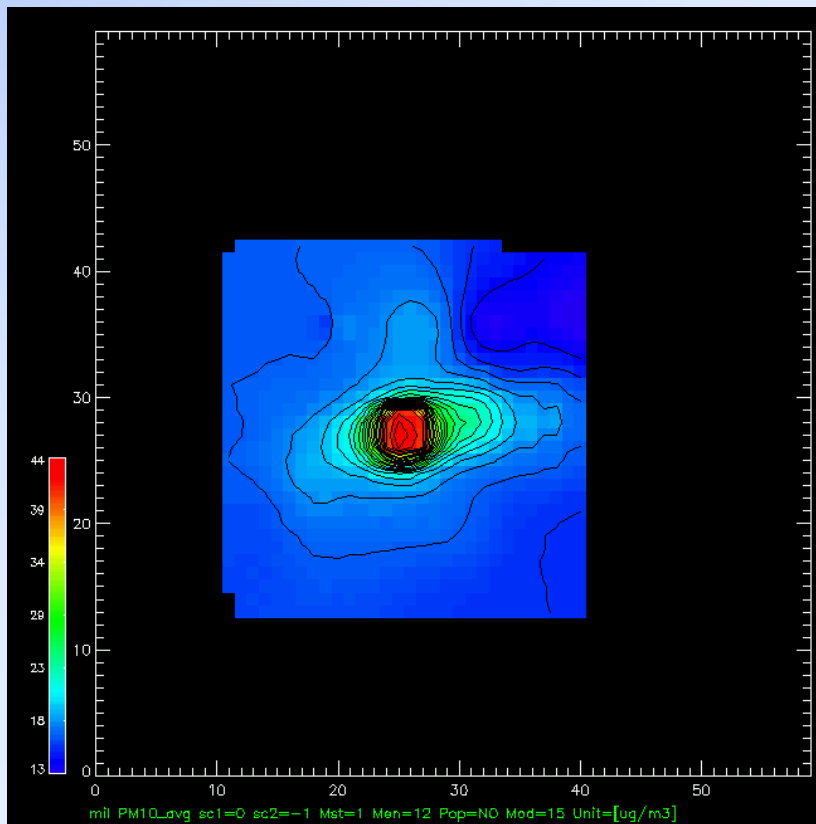
Frequency diagram



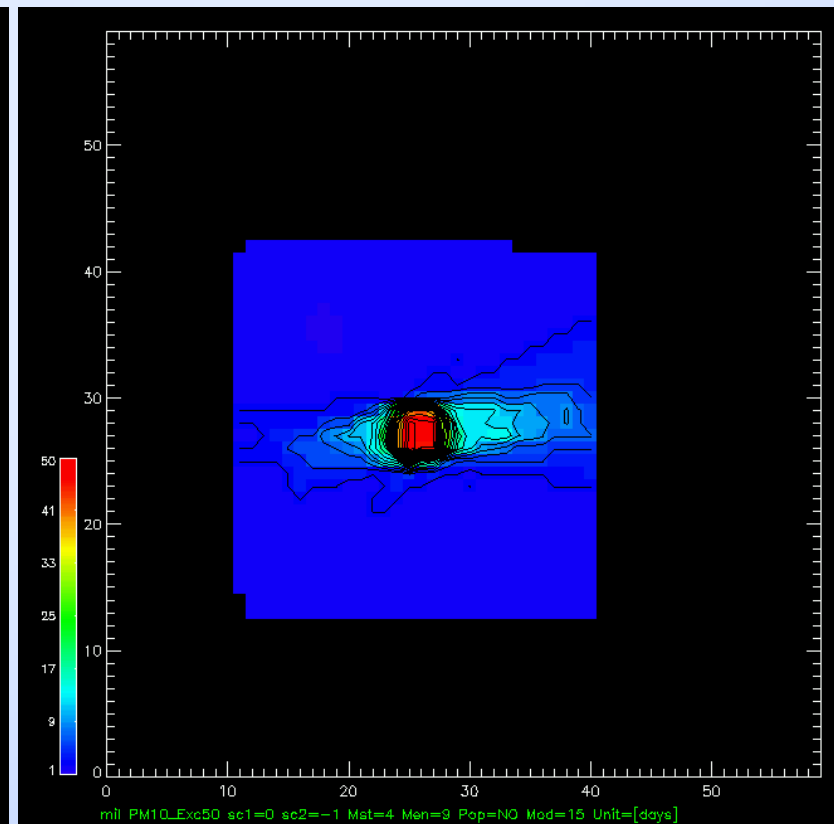


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Milan – Spatial distribution of PM₁₀



1-year average



Exceedance days



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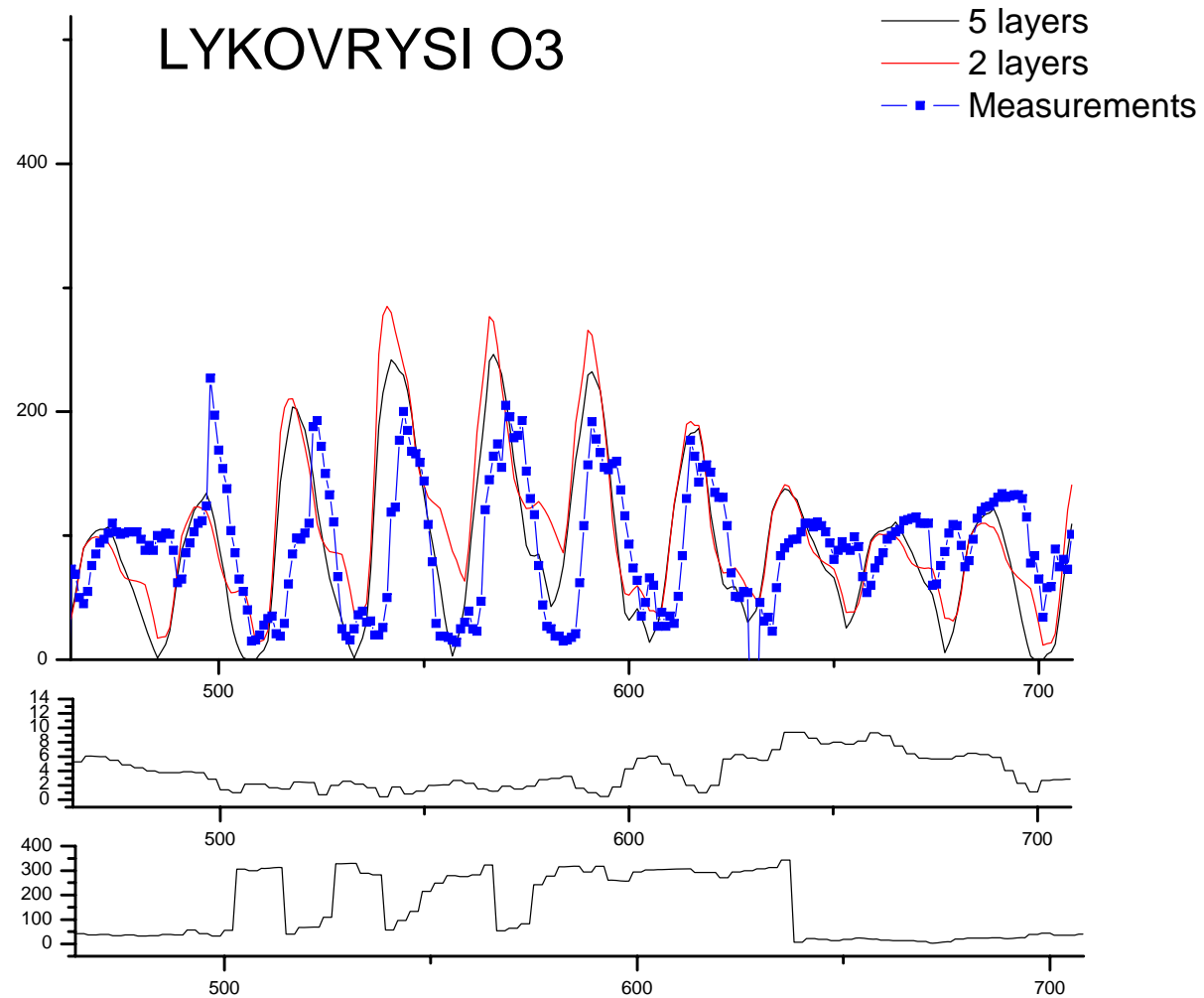
5-layer OFIS version

- 1st layer: 20 m (constant)
- 2nd .. : 1/2 mixing height
- 3rd .. : mixing height
- 4th .. : 5th layer minus entrainment zone
- 5th .. : 3000 m



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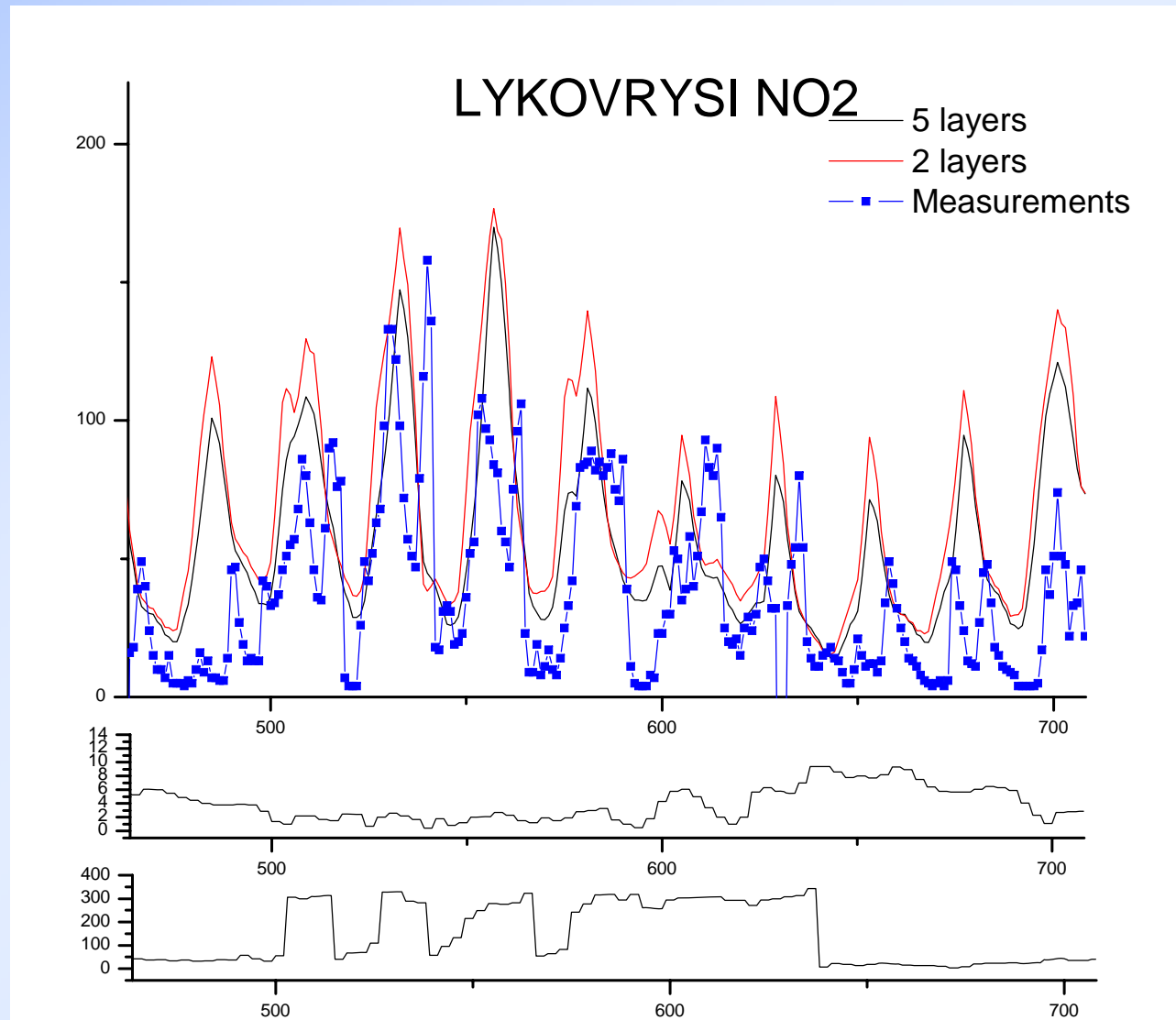
Episodic behaviour





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Episodic behaviour





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Sensitivity on the choice of boundary concentrations and meteorology

- Both initial and lateral boundary concentrations as well as the meteorological fields used to drive photochemical dispersion models were considered.
- Data came from the regional scale models: EMEP/PARLAM-PS and LOTOS-EUROS
- Aim: to quantitatively evaluate the relative impact of the aforementioned input on the simulated concentrations.



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OFIS set-up to ensure data compatibility

- A mass-preserving interpolation scheme had to be applied to account for the different horizontal and vertical setup.
- A logarithmic law was applied in view of the different height at which wind speed was provided.
- As the models use different chemical mechanisms, there was a need for a suitable correspondence between the chemical species available.
- A split of the lumped CBM-IV alkanes, alkenes and aldehydes had to be performed, following a statistical evaluation of the relative mixing ratios of the relevant EMEP MSC-W species.



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EMEP configuration

- Eulerian grid model with European coverage, using a polar stereographic projection.
- Horizontal grid cell size of the model is 50×50 km².
- In the vertical the model uses 20 layers, the first of which has a thickness of approximately 90m.
- 3-hourly meteorological data from PARLAM-PS, a dedicated version of HIRLAM.
- EMEP utilises various versions of the EMEP MSC-W chemical mechanism.



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LOTOS-EUROS configuration

- Eulerian grid model covering Europe.
- The model domain is divided into 140×140 grid cells with a size of $0.5^\circ \text{lon.} \times 0.25^\circ \text{lat.}$ ($\sim 25 \times 25 \text{ km}^2$).
- The lowest 3.5 km of the atmosphere are represented by three terrain following prognostic layers for which the continuity equation is solved and an additional (diagnostic) surface layer with a thickness of 25m.
- Driven by 3-hourly meteorological data produced by the Free University of Berlin (ECMWF can also be used).
- Adapted version of the CBM-IV chemical mechanism.
- 28 species and 66 reactions, including 12 photolytic reactions.



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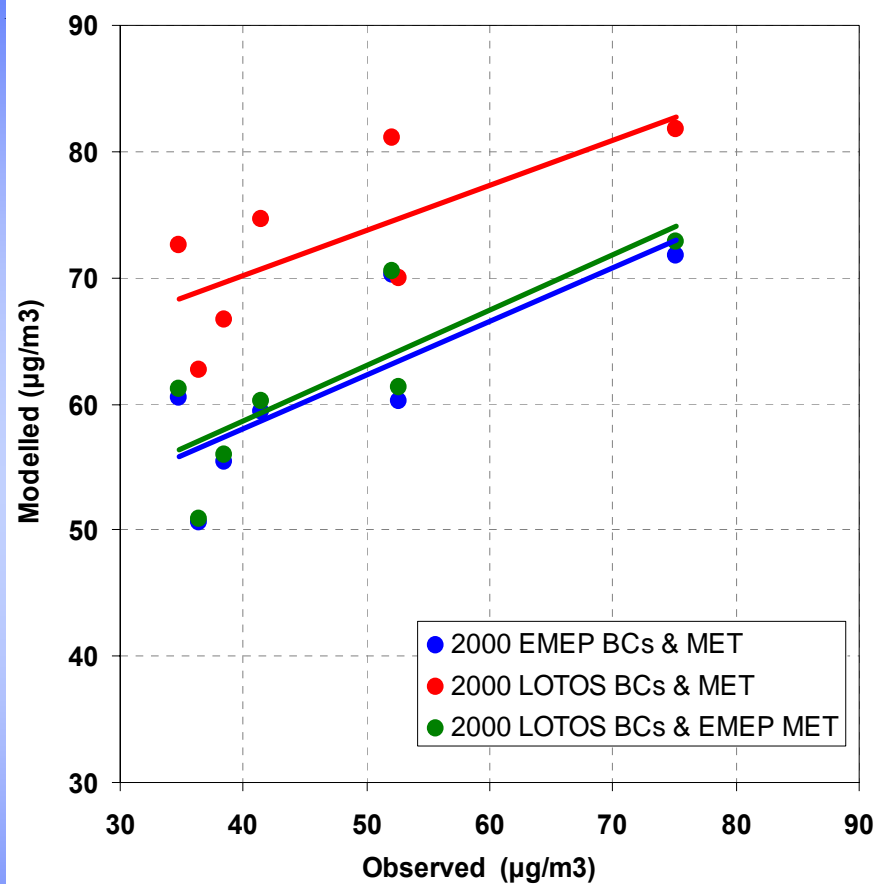
Runs performed

Three sets of runs were performed:

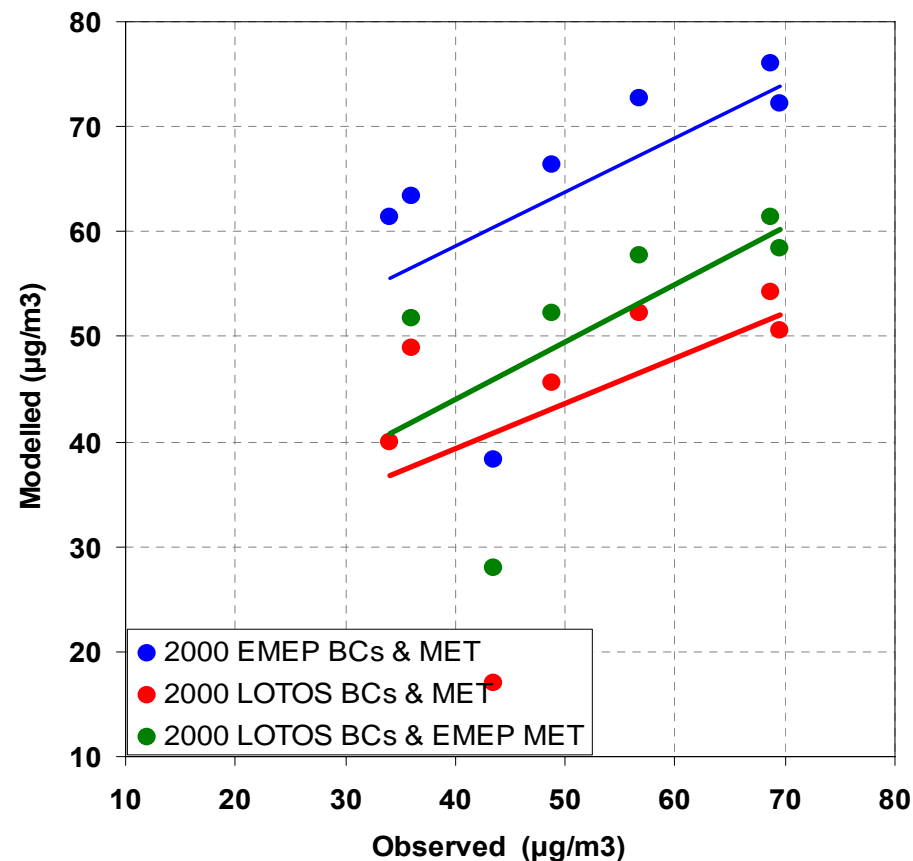
- The first two by using the same source for boundary conditions (regarding concentrations) and meteorology
- Third run where concentration boundary conditions originated from LOTOS-EUROS, while meteorology was from EMEP/PARLAM



Scatter plot for annual mean NO_2 concentrations in Athens



Scatter plot for annual mean O_3 concentrations in Athens



	EMEP BCs & MET	LOTOS BCs & MET	LOTOS BCs & EMEP MET
NO_2	0.64	0.51	0.66
O_3	0.35	0.23	0.57



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Results/Comments (1/2)

- The runs differ substantially, most notably for O_3 , probably due to the steep gradient of O_3 concentrations in the first few layers of each regional model
- Best results in terms of the correlation coefficient are achieved by the “mixed” run for both pollutants.
- Better performance of the “EMEP BCs and met” run compared to the “LOTOS BCs and met” run, which can be attributed to the affinity of EMEP and OFIS (common treatment of vertical layers and chemistry)



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Results/Comments (2/2)

- Importance of scale interactive processes: significant dependence of urban scale model results on the input boundary conditions and meteorology from regional scale models.
- The prospect of even better results with the use of concentration and meteorological fields from different regional models does not certainly comprise a proposed methodology, but rather enhances the notion that careful consideration and selection of all input parameters or use of coupled/integrated models is crucial in the urban and local scales.



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Conclusions

- Simple approaches such as the OFIS model could be complementary to full 3D models especially for users who do not have the infrastructure/expertise
- Although initially conceived for compliance purposes and future assessment (scenario runs), OFIS has exhibited some promising characteristics, most notably a satisfactory performance coupled with a computational speed which is more than 1 order of magnitude greater than the speed of complex 3D fine scale models.
- The model achieves its main goal by refining the results of regional models
- Work is under way to couple OFIS with the meteorological model MEMO in order to take into account the direct effect