Ozone modeling over Italy: a sensitivity analysis to precursors using BOLCHEM air quality model

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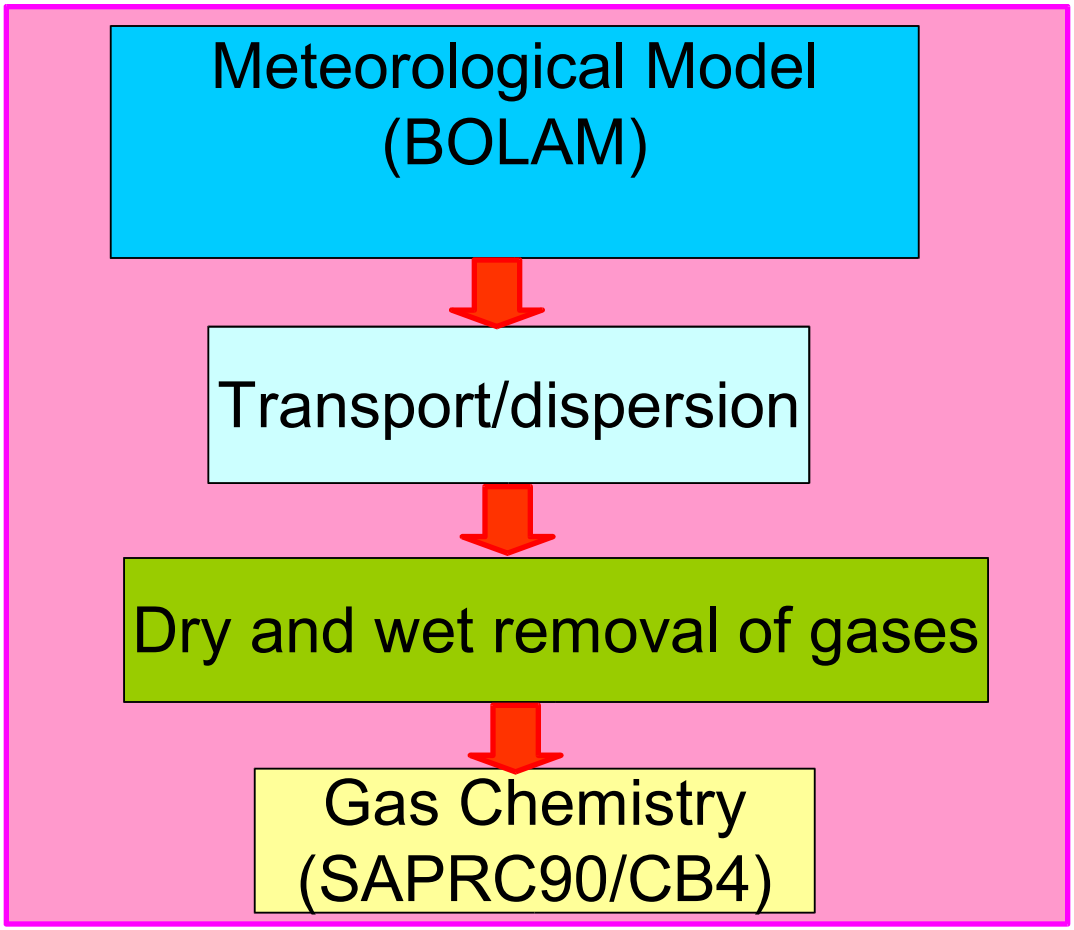
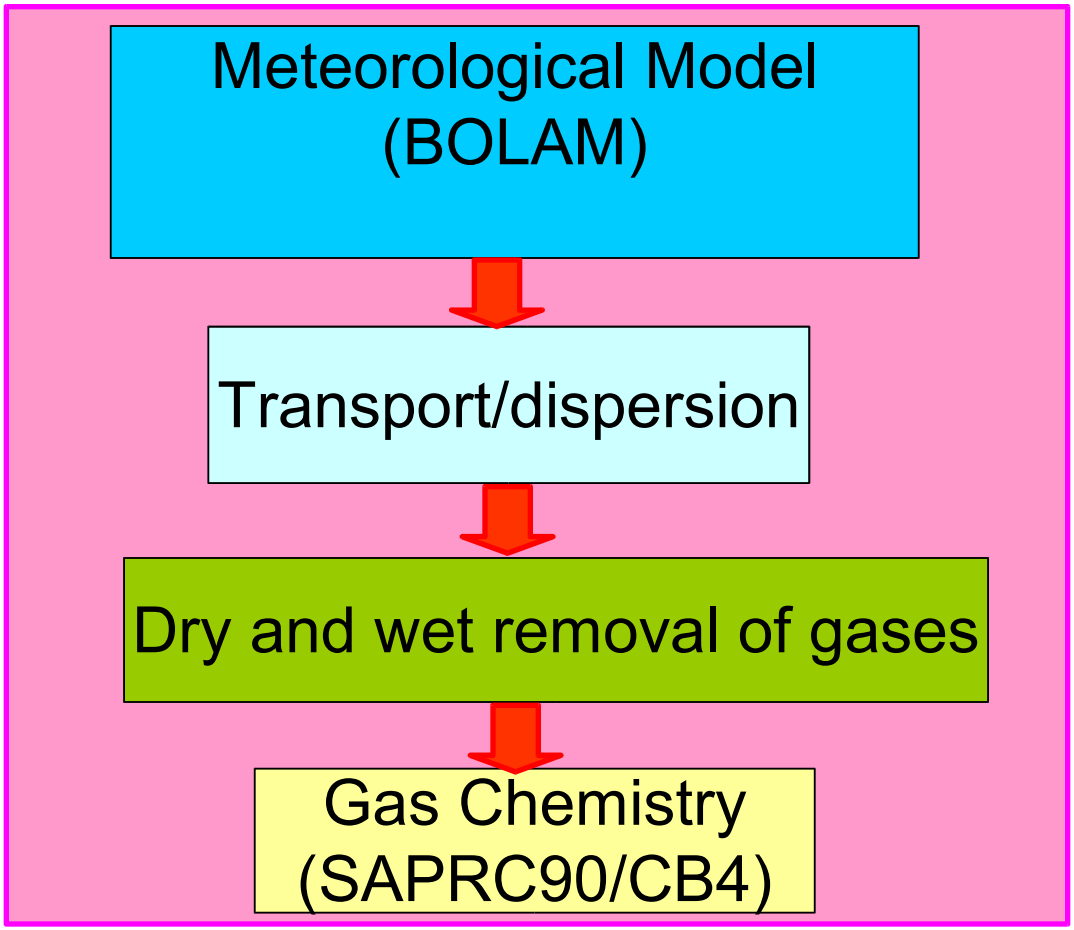
BOLCHEM flow chart



Ongoing work and future plans

- aerosol process emissions:
  - dust
  - sea-salt
  - SOA
- aerosol sedimentation and dry deposition
- aerosol wet removal in-cloud and below-cloud
- dynamic aerosol model
- in-cloud aerosol processing
- gas and aerosol assimilation for operational forecast
- Aerosol-radiation interaction
- Aerosol-cloud interaction
- Aerosol-gas interaction

BOLCHEM flow chart



Chemistry is coupled on-line, one-way with meteorology

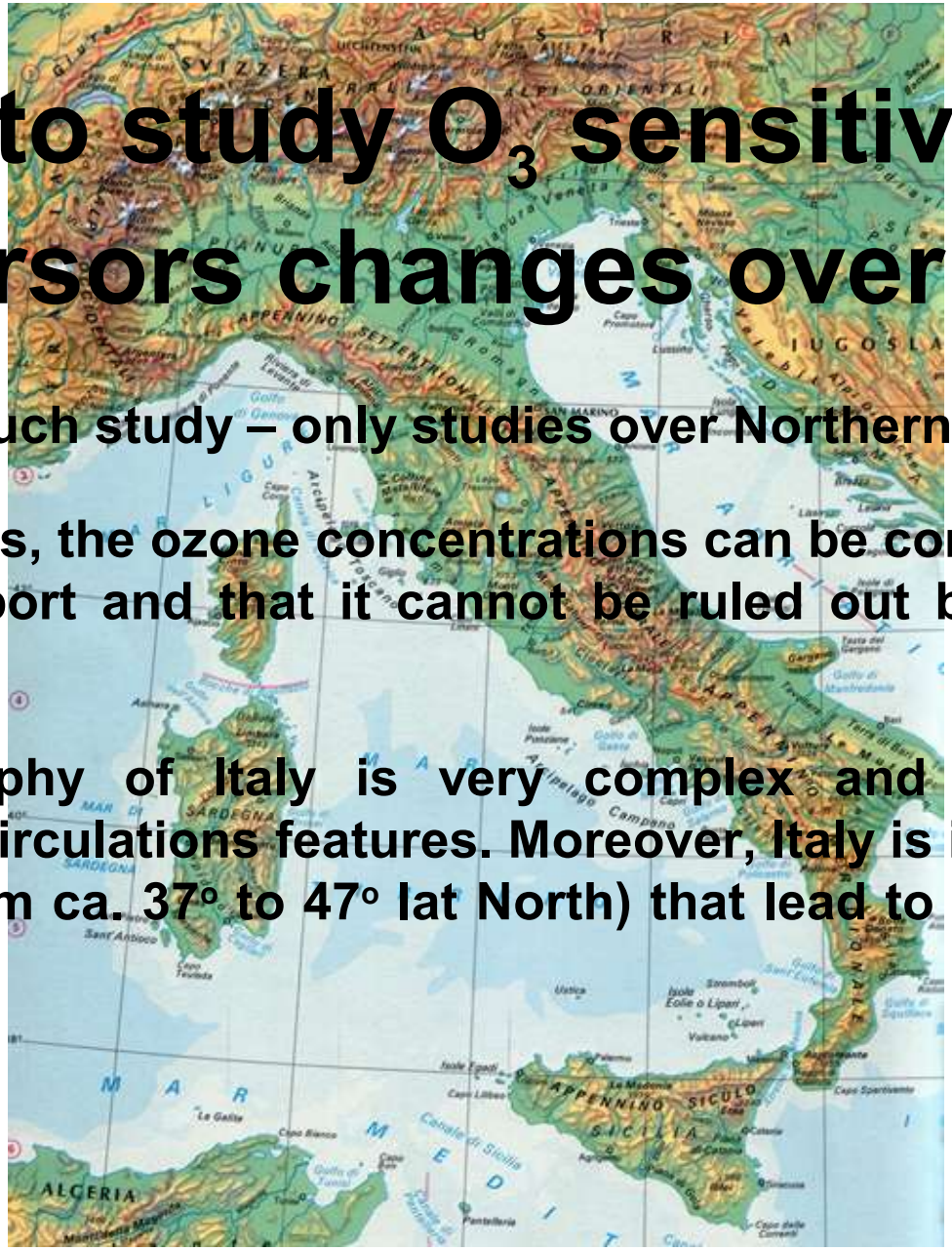
Meteorology and chemistry use:

- **same transport scheme** (WAF (Weighted Average Flux) 3-d advection scheme)
- **same grid: horizontal and vertical components** (the vertical coordinate system is terrain-following (σ), with variables distributed on a non-uniformly spaced staggered Lorenz grid. the horizontal discretization uses geographical coordinates on an Arakawa C-grid)
- **same physics for the subgrid-scale transport** (for example vertical diffusion in surface layer and PBL parameterization depend on the Richardson number)
- **same time step**

More details about model and its validation can be found in Maurizi et al. (Poster 4.5) and in Mircea et al. submitted to Atmospheric Environment

BOLCHEM participates at model intercomparison in GEMS-RAQ EU project and COST 728.

Why to study O_3 sensitivity to precursors changes over Italy?



- there is no such study – only studies over Northern Italy
- in some areas, the ozone concentrations can be controlled by long range transport and that it cannot be ruled out by simulating a small area.
- the topography of Italy is very complex and leads to very complicate circulations features. Moreover, Italy is in a geographic position (from ca. 37° to 47° lat North) that lead to various climate features.

…more motivations…

Investigation of the ozone sensitivity to precursors reduction (NOx and VOC) allows estimations of photochemical indicators. These can be easily compared to measurements and serves both **to reduce the impact of model uncertainty on ozone sensitivity predictions and to verify the efficiency of the emission reduction strategy.**

Simulations setup

- **Simulations with NOx and VOC reduced by 35% with respect to the initial emissions inventory. The simulations were performed for 3 periods during the summer of 1999 (1-3 June, 1-5 July, 5-8 August) and one period during the summer of 2003 (11-15 June).**

  1999 is a reference year in meteorological studies and for the summer 2003 was characterized by very high temperatures for a many days.

- **Simulations with isoprene emissions increased 300%.**

Model configuration and inputs

- **The model domain extends between: NW (20.77, 47.55); NE (4.82 - 47.55); SW (6.17 - 35.79); SE (19.42 – 35.79).**

- **The horizontal resolution used in the simulations is of 20 km. The vertical resolution includes 33 sigma vertical layers from surface to the thropopause. The lower layer is approximately 20m thick above the surface.**

CHEM

The chemical fields are driven by hourly surface emissions and 3 hourly lateral boundary conditions after the initialisation. Emissions, initial and boundary conditions were produced by Thoscane model (Zanini et al., 2004) based on EMEP inventory and a national inventory, which includes ship and point source emissions.

METEO

The meteorological fields were supplied by ECMWF. The lateral boundary conditions are updated every 6 hours. The weather fields were re-initialized every 48 hours with the analyses in order to avoid an excessive error growth in the meteorological forecast.

Photochemical mechanisms

CB-IV (Gery et al., 1989) : lumped-structure condensed mechanism

-85 reactions and 30 chemical species

-organics are grouped according to bond type (for example, as carbon single bonds, carbon double bounds or carbonyl bounds)

-organic species are treated explicitly (e.g. formaldehyde, ethene, isoprene), represented by carbon bond (PAR – single bonded one carbon atom, OLE –two carbon atoms) or molecular (TOL and XYL aromatic hydrocarbons) surrogates according with their chemistry or importance in the environment.

SAPRC90 (Carter, 1990) : lumped-molecular condensed mechanism

-131 reactions with 35 chemical species

-calculate the kinetic and mechanistic parameters for lumped species in the mechanism created for representative emissions profile (mole-weighted approach)

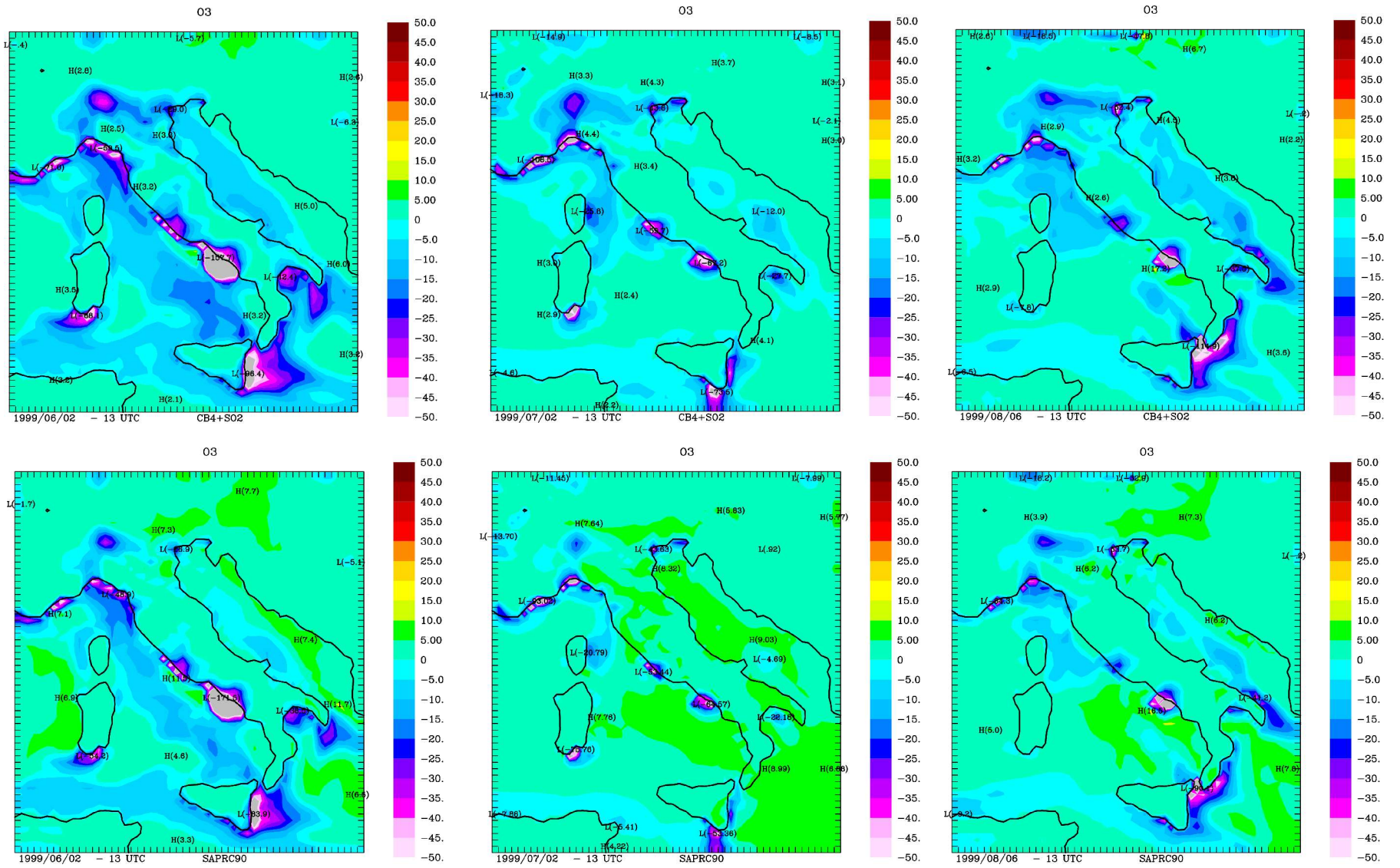
-organics species are treated explicitly (e.g. formaldehyde, acetaldehyde, etc) or represented by molecules as alkane, alkenes, aromatics, etc.

Results of NOx/VOC sensitivity study

- Distribution of the chemical regimes
- Temporal variation of NOx and VOC limited areas
- Distribution of photochemical indicator transition values

Chemical regimes over Italy:1999

ΔO3 > 0 NOx limited area
ΔO3 <0 VOC limited area



Differences in ozone concentrations: ΔO3=O3(65%VOC)-O3(65%NOx)

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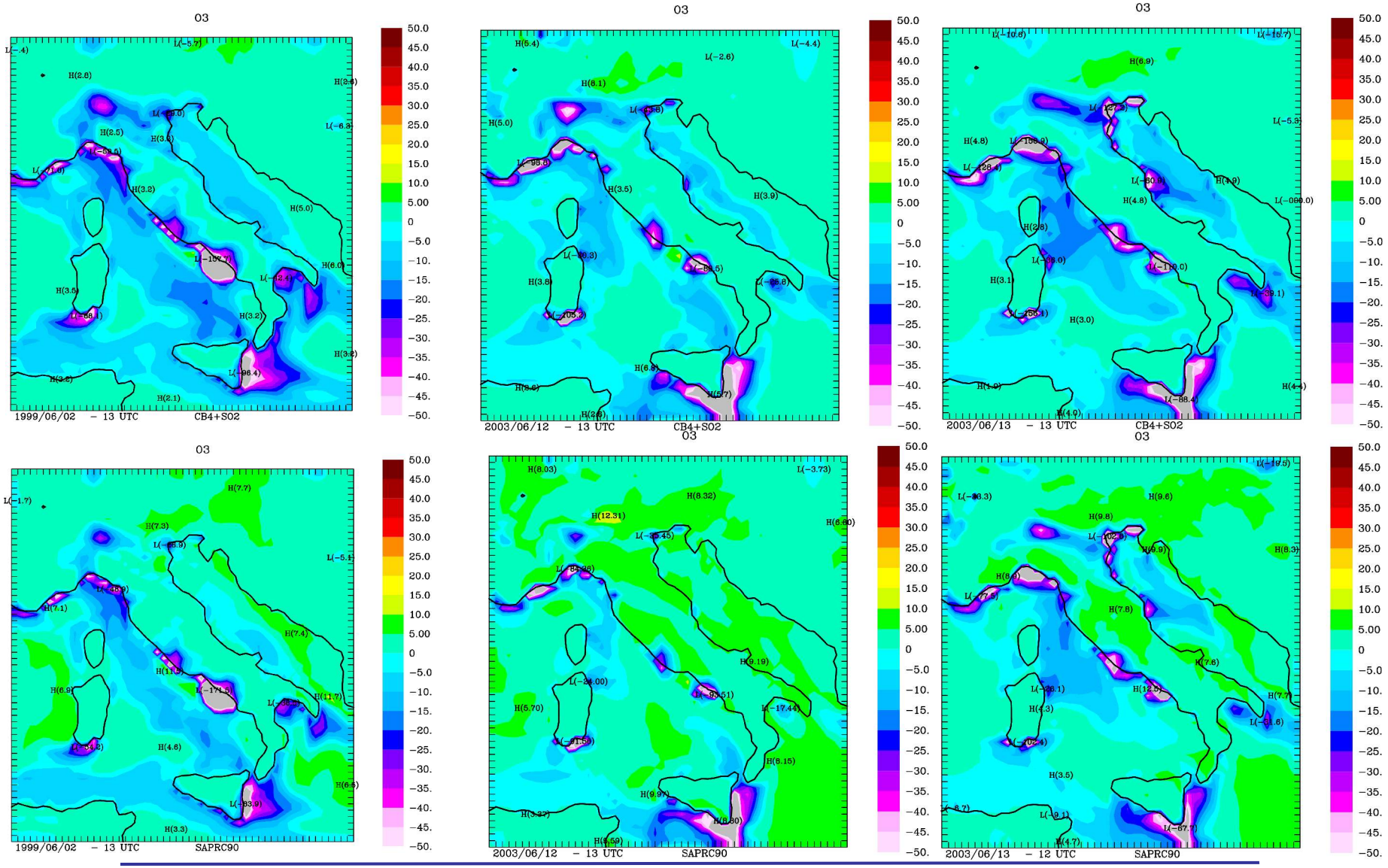
Chemical regimes over Italy:June 1999 vs 2003



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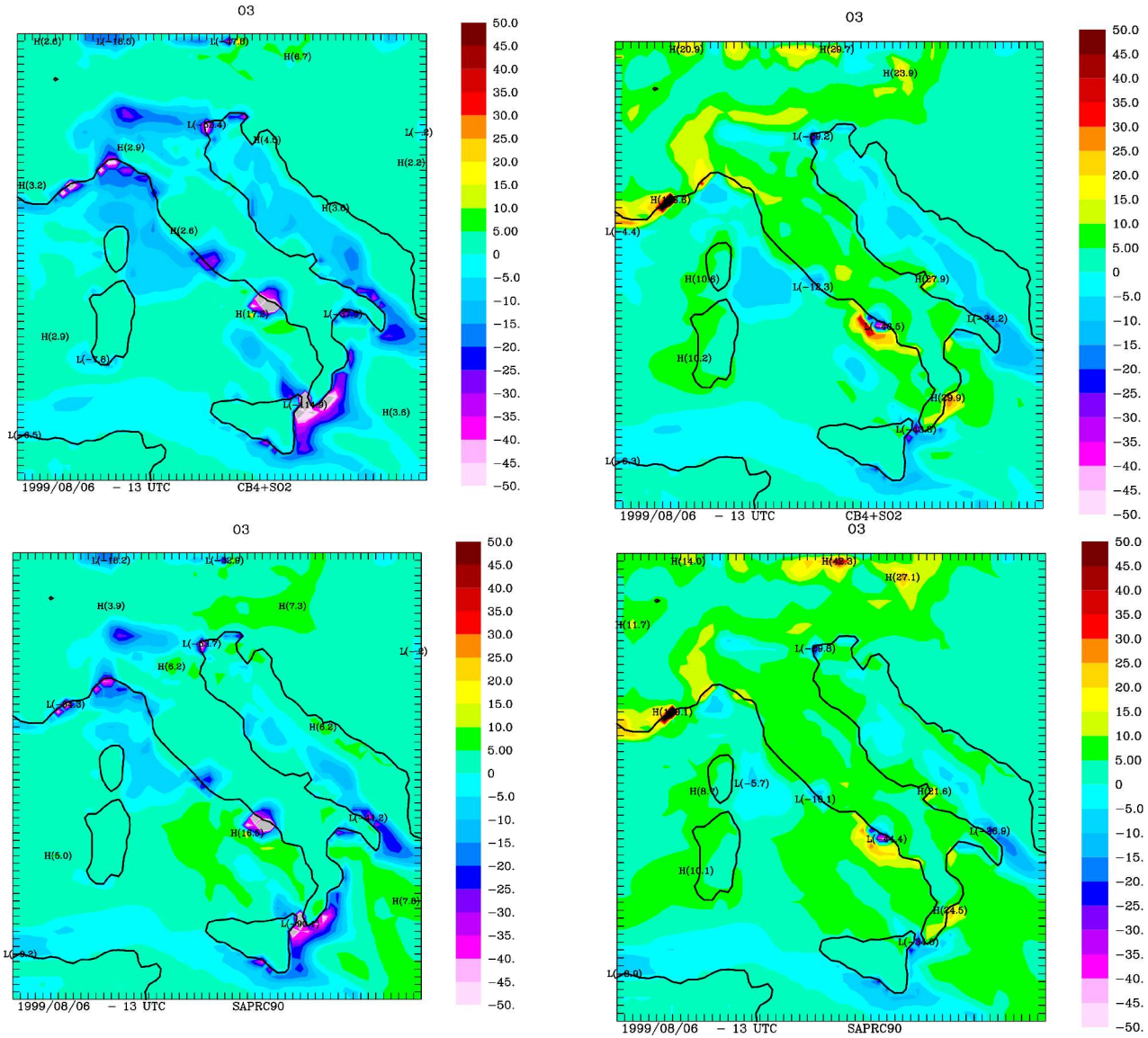
Chemical regimes over Italy: August 1999 vs more isoprene



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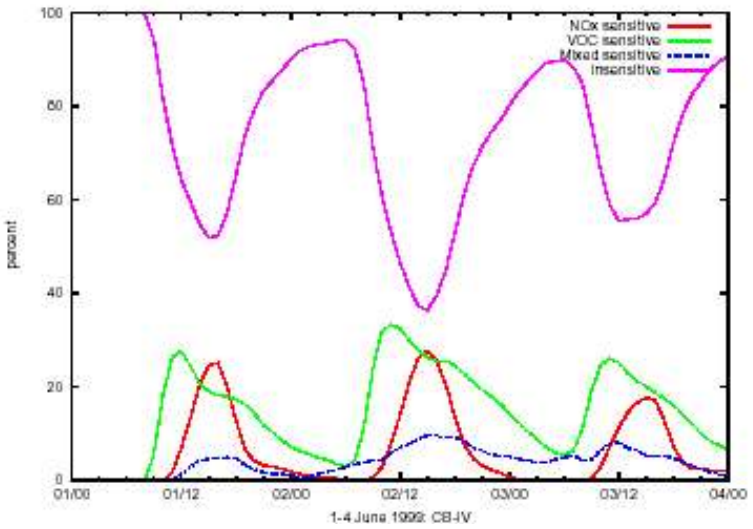
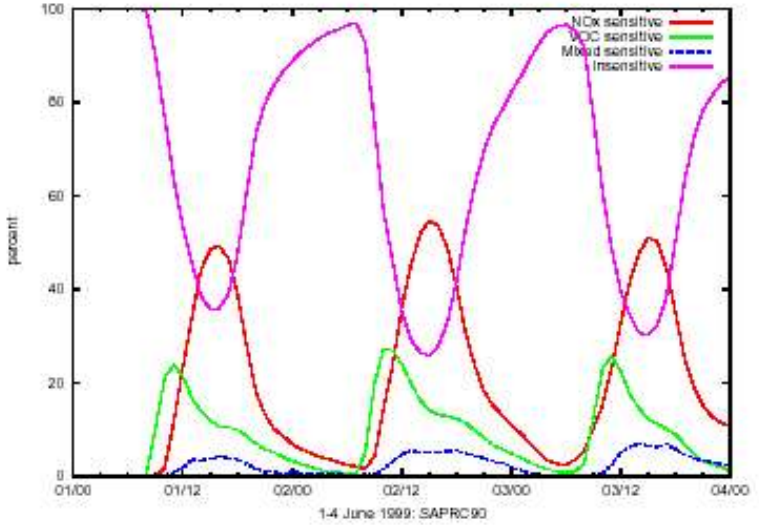
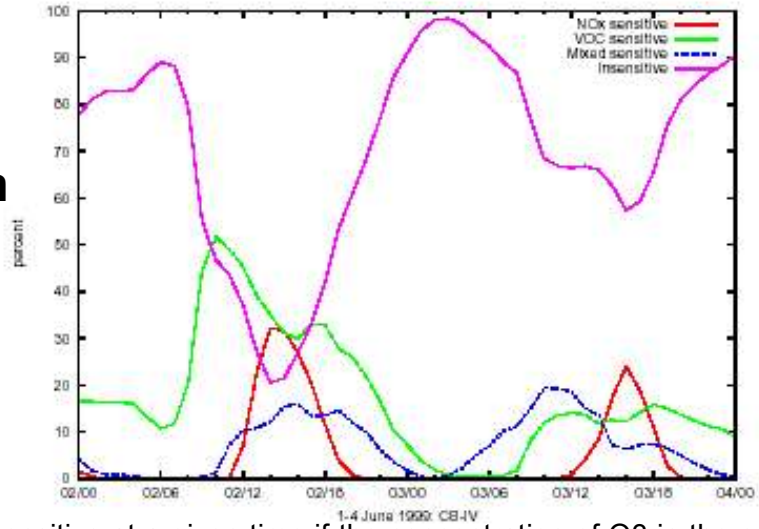
Temporal variation of NOx and VOC sensitive areas: June 1999

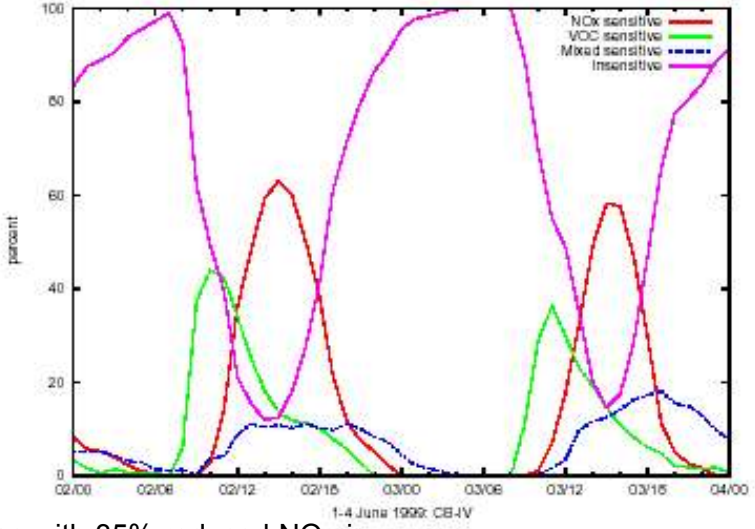
Italy





Milano 400kmX400km





Sillman et al. (2003): NOx-sensitive at a given time if the concentration of O3 in the case with 35% reduced NOx is lower then the concentration of O3 in both the base case and in the case with 35% reduced VOC by at least 2ppb. VOC-sensitive similar. Mixed- the concentration of O3 in the cases with reduced NOx and VOC is lower than the concentration of O3 in the base case by at least 2 ppb. Insensitive -the rest of the grid cells.

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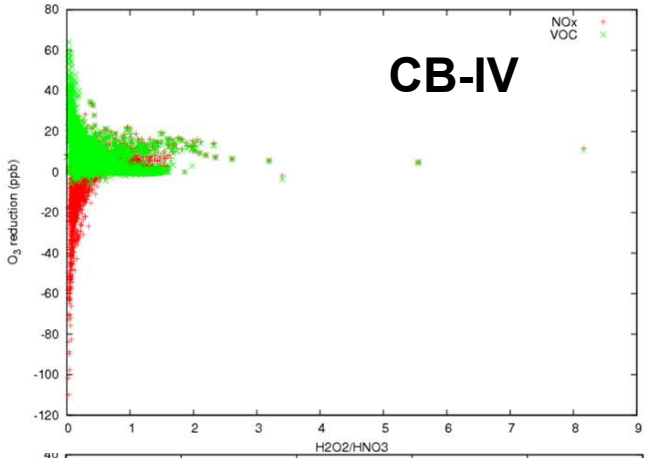
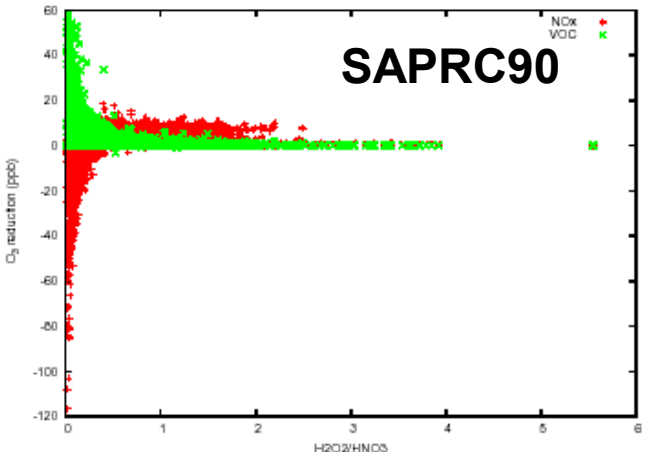
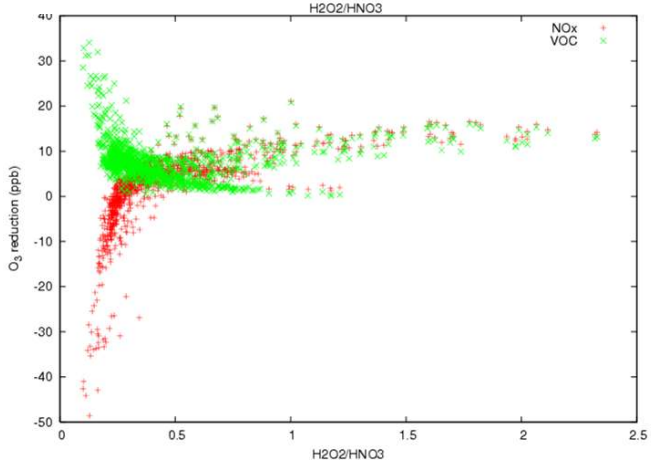
Photochemical indicators

- Photochemical indicators are individual species or species ratio that consistently assume different values under conditions of NOx –sensitive and VOC-sensitive ozone (Sillman, 1995). Most used indicators are: NOx, NOy, NOz, HCHO/NOy, H2O2/NOy, H2O2/NOz, O3/NOz, O3/NOy, O3/HNO3, H2O2/HNO3, extent-of-reaction parameter(EOR).
- Indicator transition values represent the values when O3 sensitivity transfers from VOC sensitivity to NOx sensitivity conditions. Quantitatively, they represents the 95th percentile of VOC-sensitive areas along with the 5th percentile of NOx-sensitive areas.

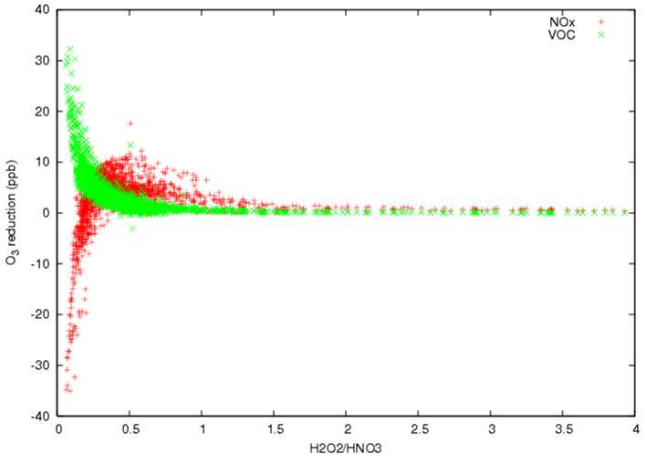


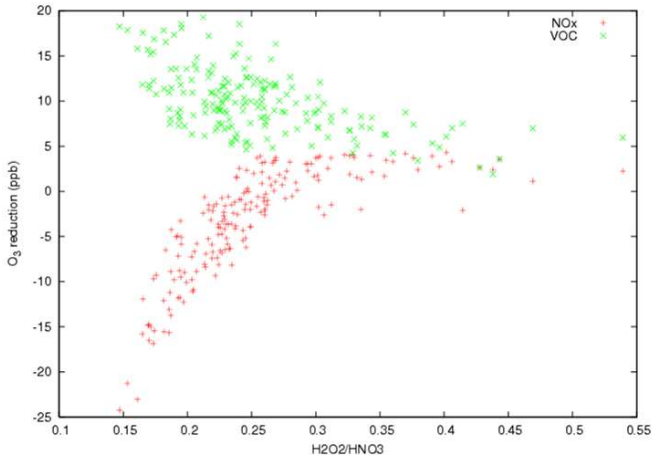
Italy



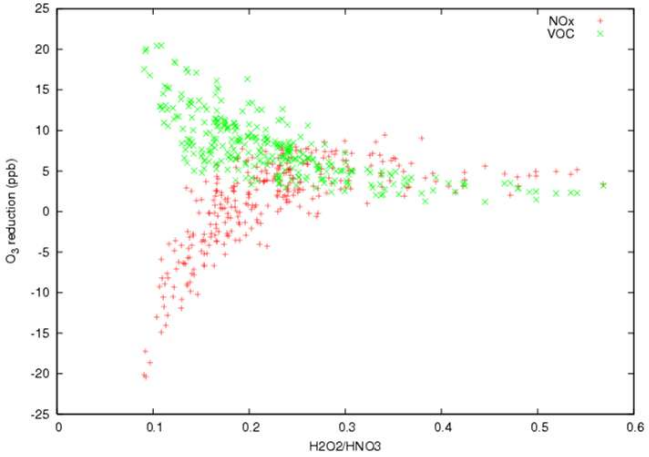


Milano
400kmX400km





Milano
100kmX100km



Distribution of photochemical indicator values for NOx- and VOC-sensitive chemistry

CB-IV

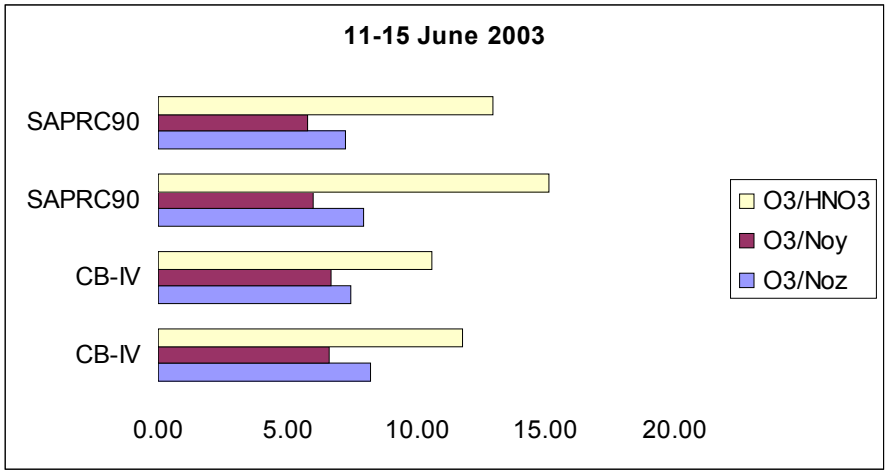
	VOC sensitive regime			NOx sensitive regime		
	5th	50th	95th	5th	50th	95th
NOx	1.69	4.02	17.04	0.71	1.02	2.01
Noy	11.33	16.72	31.51	7.21	9.84	13.57
Noz	8.85	12.44	18.44	6.26	8.63	12.42
HCHO/Noy	0.16	0.21	0.31	0.18	0.24	0.41
H2O2/NOz	0.12	0.22	0.30	0.32	0.42	0.54
H2O2/Noy	0.07	0.16	0.24	0.28	0.36	0.47
O3/Noz	5.01	6.56	8.20	7.47	8.80	10.91
O3/Noy	2.36	4.98	6.61	6.68	7.80	9.53
O3/HNO3	6.50	8.86	11.79	10.58	12.29	16.31
H2O2/HNC	0.16	0.30	0.41	0.49	0.57	0.77
EOR	0.39	0.55	0.61	0.58	0.61	0.64

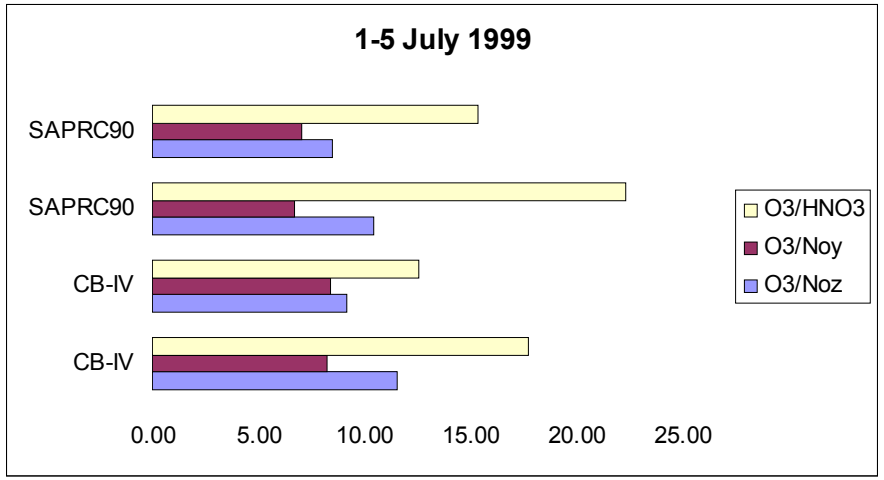
SAPRC90

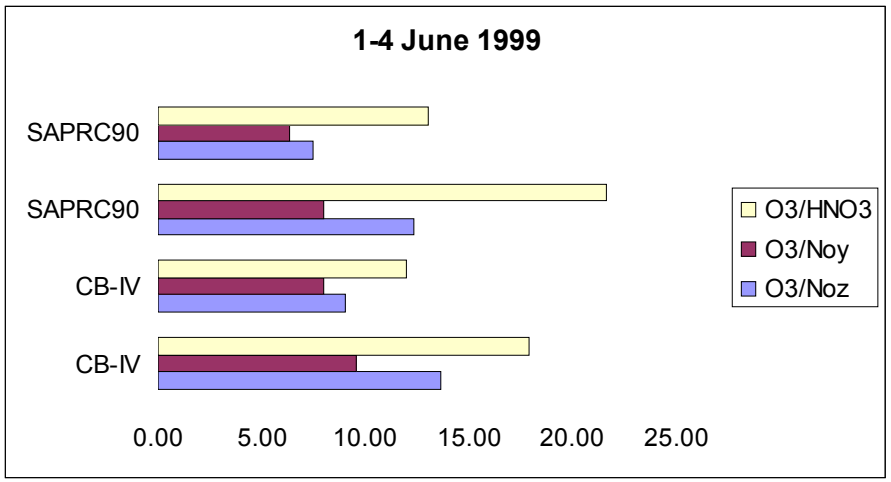
	VOC sensitive regime			NOx sensitive regime		
	5th	50th	95th	5th	50th	95th
NOx	3.36	7.74	27.51	0.84	1.92	4.41
Noy	14.58	22.84	46.06	8.79	12.54	19.71
Noz	9.37	14.31	21.56	7.19	10.45	16.24
HCHO/Noy	0.21	0.28	0.36	0.29	0.33	0.42
H2O2/NOz	0.07	0.14	0.20	0.16	0.26	0.39
H2O2/Noy	0.03	0.08	0.15	0.13	0.22	0.33
O3/Noz	4.68	6.27	7.91	7.26	8.91	11.51
O3/Noy	1.73	3.94	6.01	5.78	7.52	9.37
O3/HNO3	7.96	10.91	15.14	12.93	16.45	24.10
H2O2/HNC	0.13	0.25	0.36	0.31	0.48	0.73
EOR	0.33	0.48	0.57	0.54	0.59	0.63

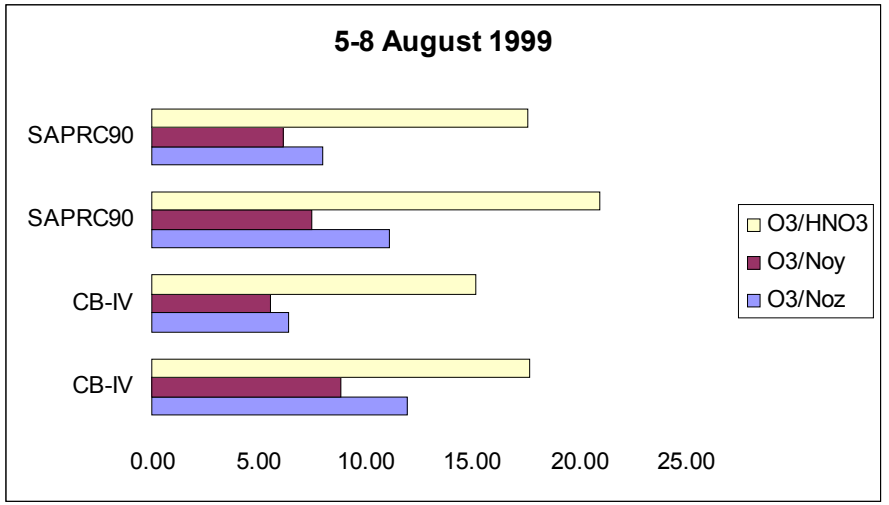
Italy

Distribution of photochemical indicator transition values for NOx- and VOC-sensitive chemistry: Italy

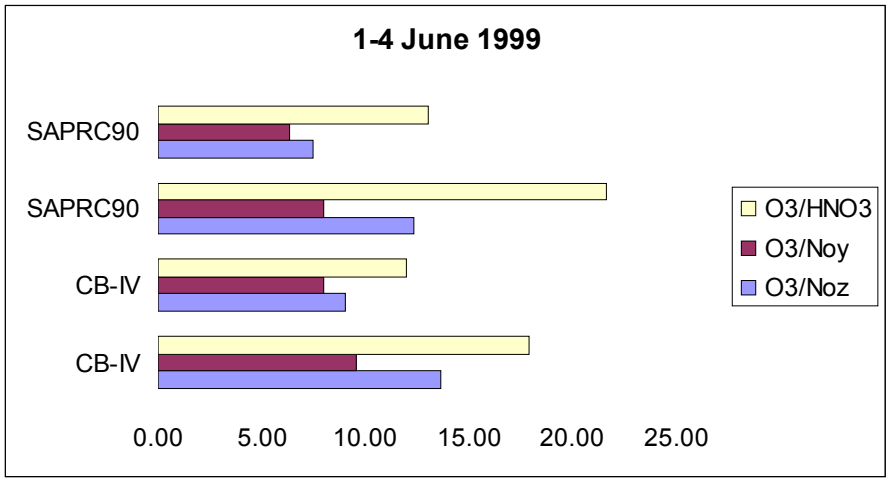


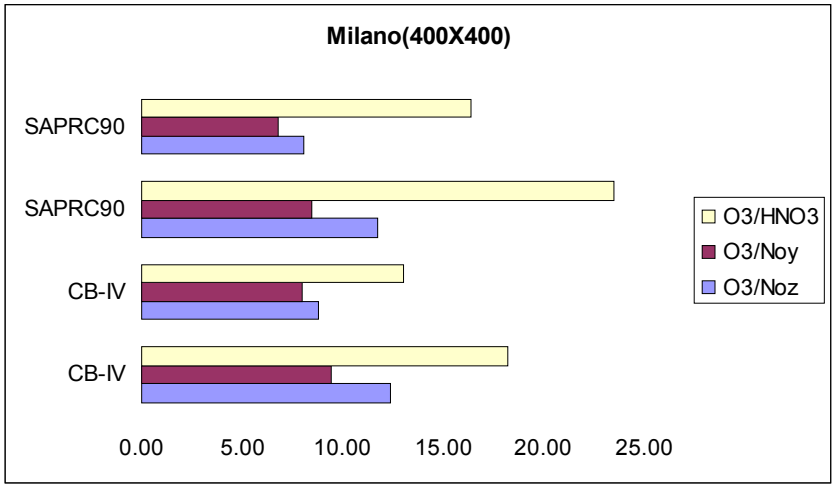


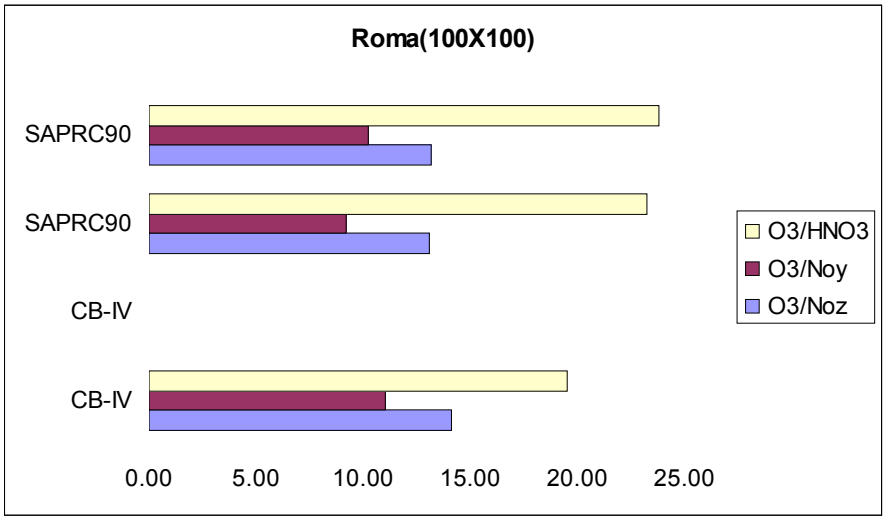


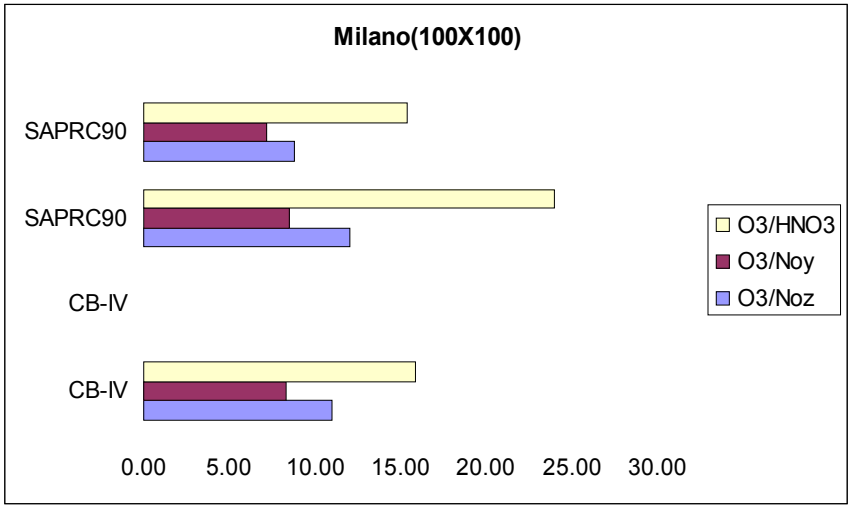


Distribution of photochemical indicator transition values for NOx- and VOC-sensitive chemistry









Conclusions

- Spatial distribution of chemical regimes over Italy is more influenced by the photochemical mechanisms than by the meteorological conditions.

- Both photochemical mechanisms show that Italy is mainly under an NOx chemical regime, but strong VOC areas exist around big cities, harbours and industrial areas.

- The increase of isoprene emissions eliminate the VOC sensitive areas, therefore, the uncertainties in isoprene emissions can strongly bias model results and strategies to improve air quality.

- The indicator transition values vary with meteorological conditions and with the size of the domain analysed.

- The indicator transition values for Milan area are similar with those published by other authors for industrialized areas. A full assessment of the variability of the indicator transition values is in progress.

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