A Comprehensive Modelling System for Ozone Exposure Assessment

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Abstract

Since high concentrations of tropospheric ozone are quite usual in Mediterranean areas and cause adverse effects on human health, materials and ecosystems, an integrated modelling system has been developed in order to perform a climatological simulation on photochemical pollution and allow estimating AOT indexes, useful indicators of ozone exposure.

The modelling system, including 3D meteorological model CALMET, a flexible emission evaluation model POEM and photochemical transport model CALGRID, has been applied to a Northern Italy domain, including the whole of Regione Lombardia, characterised by complex terrain, high urban and industrial emissions and a close road network.

Initial and boundary conditions for the domain under study are obtained by means of a nesting procedure from the EMEP Lagrangian Photoxidant Model. Since the long-term simulation presented some critical issues, as the run time and the resources management, a time splitting procedure has been developed to allow the use of a PC computing platform.

The model has been run for the period April-September 1996 to perform and compare simulation results and monitored critical levels; some reference stations have been selected from the Regione Lombardia monitoring network by using a clustering analysis technique to characterise their representativeness in the area, in correspondence to different peculiar features of pollutant concentrations.

Introduction

Ozone is considered one of the most significant pollutants with respect to the potential impact to human health and natural ecosystems, both in terms of critical episodes and as long-term exposures. Consequently, in order to assess the comprehensive effects of photochemical pollution, not only ozone peak concentrations need to be examined, but also ozone exposures on "seasonal" scale need to be quantified. Recent works (Hogrefe *et al*., 2001, Tarasson *et al*., 2001) point out the importance to perform policies analysis on a "climatological" basis rather than focusing on a single critical episode, allowing to better evaluate model performances (Hogrefe *et al*., 2001) and also to quantify policies effects with respect to long-term air quality standards.

Modelling systems can represent suitable tools for this purpose, allowing both to study photochemical pollution and to analyse and assess appropriate emission reduction strategies.
For assessment of ozone effects, monitored concentrations sites are surely of interest, but even more important is the knowledge of the spatial distribution in the area. In fact, the spatial and temporal variation is a crucial factor to evaluate the impact of photochemical pollution on natural ecosystems.

In order to assess the long-term impact of ozone concentrations, a cumulative approach may be applied to calculate the number of exceedances of a threshold, defined with respect to the objective, either health, crops or ecosystems protection; critical levels for ozone effects on vegetation are defined using the AOT40 index (i.e. the cumulative exposure over 40 ppb for daylight hours during a growing season), while as for the health protection, according to the WHO guidelines, the main concern is the peak concentrations, well represented by the AOT60.

The photochemical modelling system

An integrated modelling system has been designed and implemented, including 3D meteorological pre-processor CALMET (Scire *et al.*, 1999, Silibello *et al.*, 2001), a flexible emission inventory module POEM (Gabusi, 1998, Catenacci *et al.*, 1999) and the photochemical transport model CALGRID (Yamartino *et al.*, 1992, Silibello *et al.*, 1998).

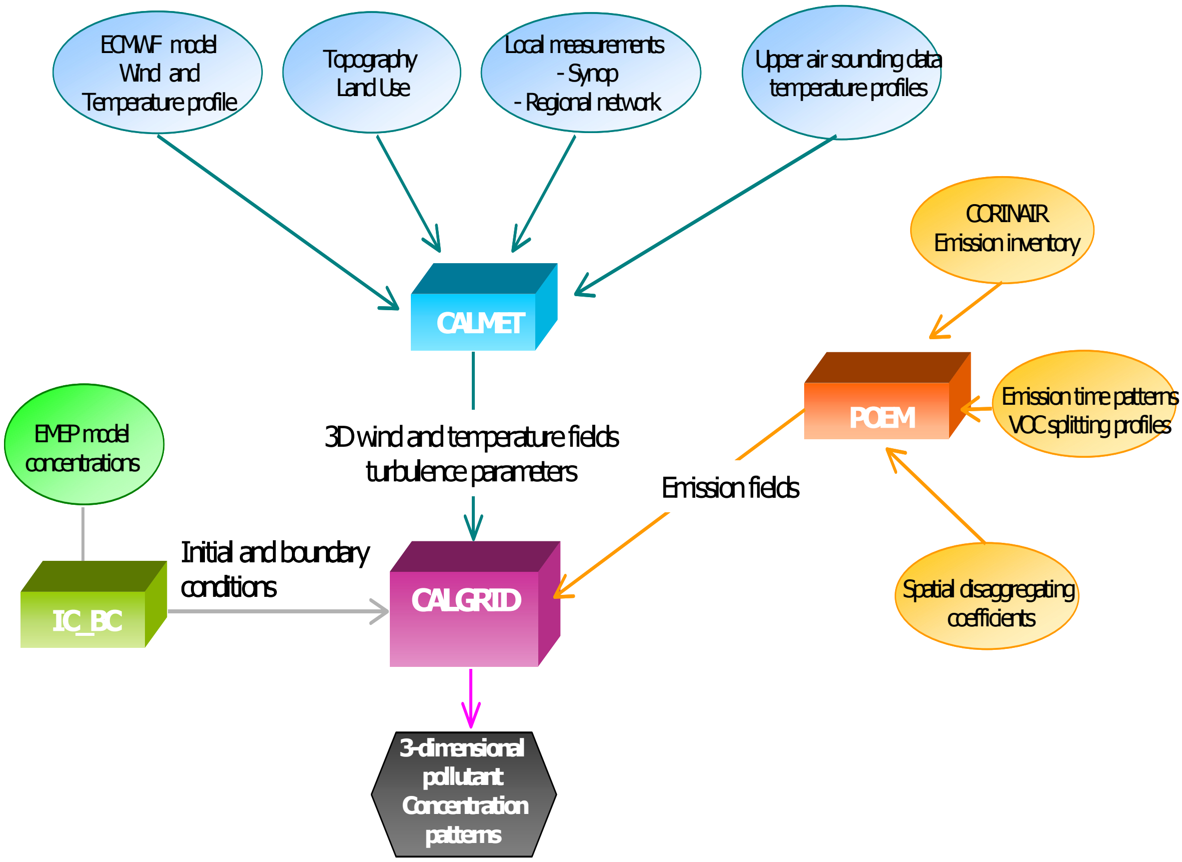

Figure 1. The modelling system.

Meteorological fields have been provided starting from topography information and both ground-based and upper-level meteorological data. Land-use information has been used to define some geophysical parameters needed by turbulence and deposition modules. As for meteorological data, hourly ground level measurements have been monitored in 31 stations. Information about the vertical structure of wind and temperature fields has been provided by two radio-sounding stations and by the ECMWF (European Centre for Medium range Weather Forecast, Reading, UK) model 6-hourly analyses. The data sets describe different aspects of the atmospheric circulation over the studied area: synoptic features are outlined by ECMWF fields, while local effects are accounted for by ground measurements. To better harmonise the available data, the initial guess fields for the CALMET diagnostic wind module have been defined only employing the ECMWF model output. Then, the measured data have been introduced on the obtained wind field, in order to account for local effects.

The emission processor POEM (POllutant Emission Model) has been specifically designed to produce present and alternative emission field estimates by means of an integrated top-down and bottom-up approach. POEM can be applied in particular starting from Italian CORINAIR data and integrates diffuse and main point sources estimates based on different activity sectors. The road transport, agriculture and biogenic emissions are estimated by means of a bottom-up approach, while the emissions due to other source categories are computed disaggregating the CORINAIR90 data set, updated on the last available Italian CORINAIR report (1994). The road traffic emissions are estimated up to 1996.

The photochemical module CALGRID is an Eulerian three-dimensional model. It implements an accurate advection-diffusion scheme in terrain-following coordinates with vertical variable spacing; a resistance-based dry deposition algorithm takes into account pollutant properties, local meteorology and terrain features. The CALGRID chemical module uses SAPRC-90 mechanism (Carter, 1990), including 54 chemical species with 129 reactions and the QSSA (Quasy Steady State Approximations) solver for the integration of kinetic equations.

The modelling application

The modelling domain

The selected simulation domain is 240×232 km^2 wide and includes the whole Lombardia Region, with several cities as well as rural areas. It is a complex terrain region located in the Po Valley and it is one of the most industrialised and populated areas of Northern Italy. Industries and a close road network are the most relevant sources in the basin. The critical anthropogenic emissions, the frequent stagnating meteorological conditions and the Mediterranean solar radiation regularly cause high ozone level episodes, especially during summer months.

The area has been subdivided according to a grid system having 60 per 58 horizontal cells, with 4 km step size and 11 vertical layers of variable thickness (20, 45, 80, 130, 230, 400, 650, 1000, 1700, 2800 and 3900 m).

Boundary conditions have been defined on the basis of EMEP model; the model is one-layer Lagrangian trajectory model covering the whole Europe, with a resolution of 150x150 km^2 and providing 6-hourly boundary layer mean concentrations. Fields provided by the EMEP model have been interpolated in time and extrapolated above PBL height, according to mixing-height estimations provided by CALMET model. Concentrations have been assumed to be well-mixed in the PBL and exponentially decreasing with height for all species except for ozone where a free atmosphere (3000 m a.s.l.) background level of 60 ppb have been assumed.

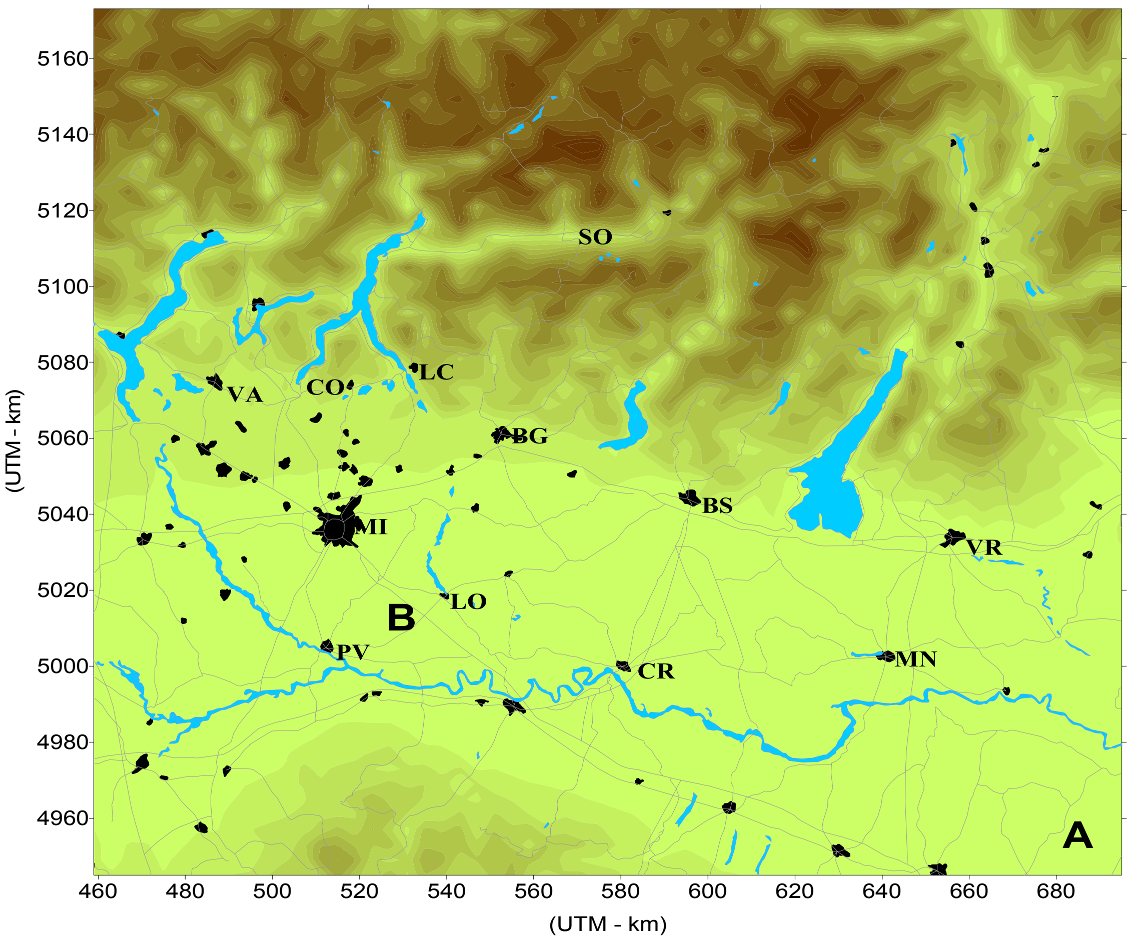

Figure 2. The selected domain.

Ozone pattern analysis

Ozone time series from the air quality networks have been analysed by means of a clustering analysis technique, to evaluate similarity in terms of levels and temporal variability (frequency and peak distribution, daily feature).

Cluster analysis is a statistical multivariate procedure for detecting natural groupings in data; in this study, the variables considered are the observed hourly concentrations and the similarity is established on the Euclidean distance function and correlation factor. In fact, the Euclidean distance pointing out the similarities from a quantitative point of view, while the correlation factor allows to focus similarities among temporal trend phases (Lavecchia *et al.*, 1996).

The analysis has been applied to ozone data provided by regional air quality network and two other remote measurement sites owned by ENEL (National Electricity Board) and Bolzano Province, considering only the stations with minimum 75% reliable data available over the 6-months period. Starting from results, a reduced set of 8 representative monitoring stations has been selected to compare estimated concentrations with measurements (see Figure 3). In Figure 4 is reported the ozone mean day features for the selected stations.

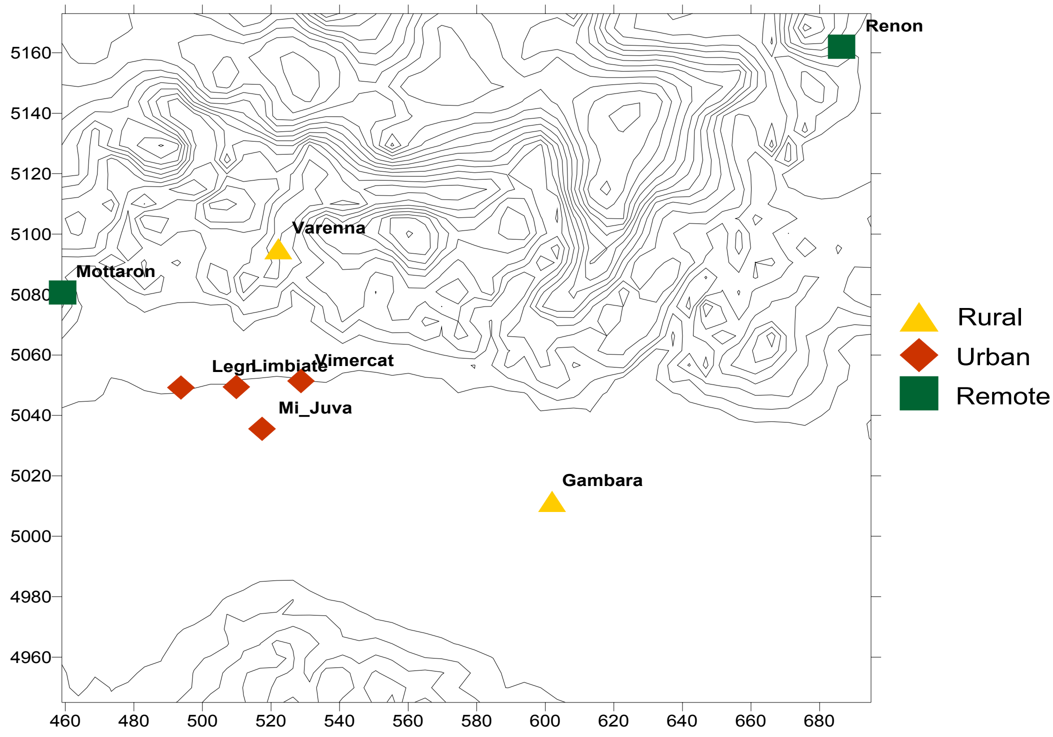

Figure 3. The representative classified stations.

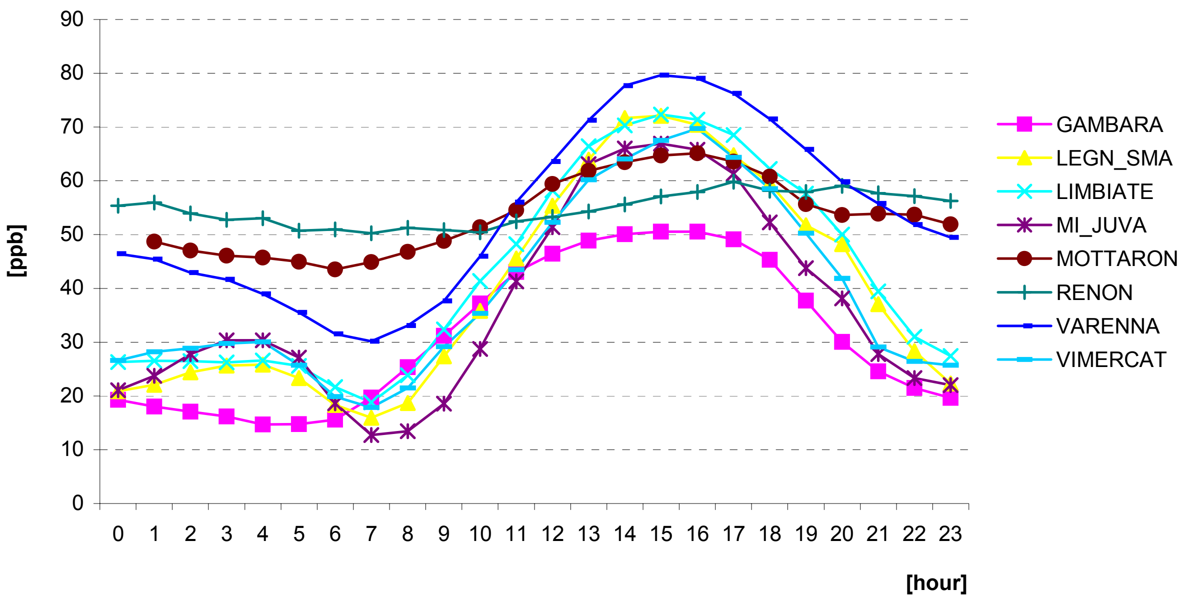

Figure 4. Mean ozone day features for the considered stations.

Air quality simulations

Air quality impact simulations have been performed for the summer period April – September 1996 (Gabusi *et al.*, 2002).

Figure 5 reports the comparison between observed and simulated 6-months average concentration, while Figure 6 shows a similar comparison between day features. The largest differences with respect to measured data are evidenced from an overestimation of the mean value at Gambara station, probably descending from an inadequate temporal modulation of boundary concentration in SE part of the domain. The mean day features evidence a peak underestimation for the urban sites and a quite constant overestimation for the rural ones.

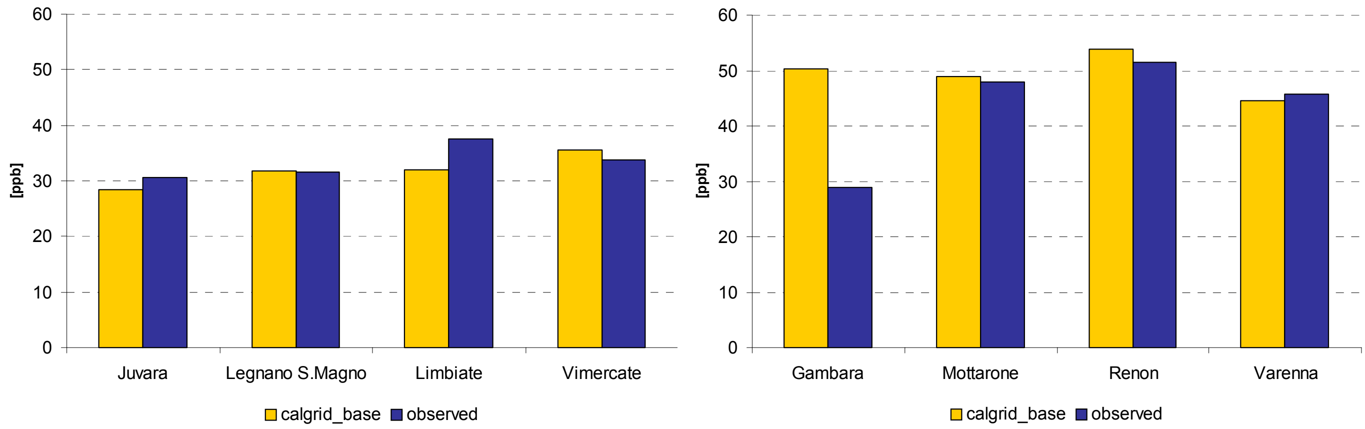

Figure 5. 6- months mean value at urban sites (left); rural sites (right).

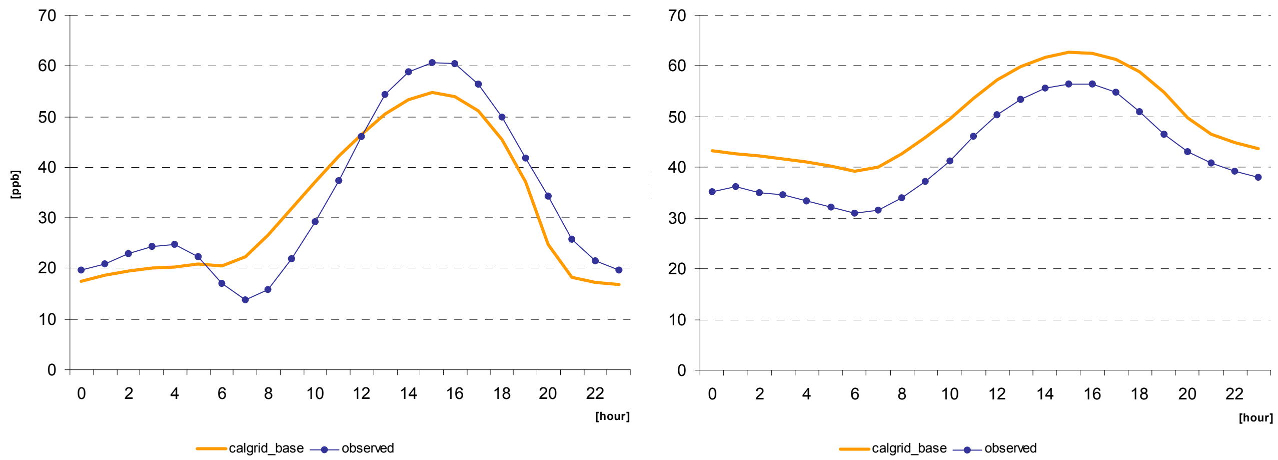

Figure 6. The mean day features for the urban (left) and rural (right) sites.

The 6-months simulated daylight concentrations scatter plots (Figure 7) points out a quite satisfying agreement with the respect to observed data. The model mostly simulates the overall temporal behaviour of the measured ozone concentrations, but in some days and episodes the estimates differ significantly from the measured concentration levels. Because of the complex interactions between transport, removal and physical-chemical processes, it is difficult to relate such discrepancies to specific model lacks without detailed process-analysis studies. A more comprehensive process-analysis of the discrepancies is planned for the future.

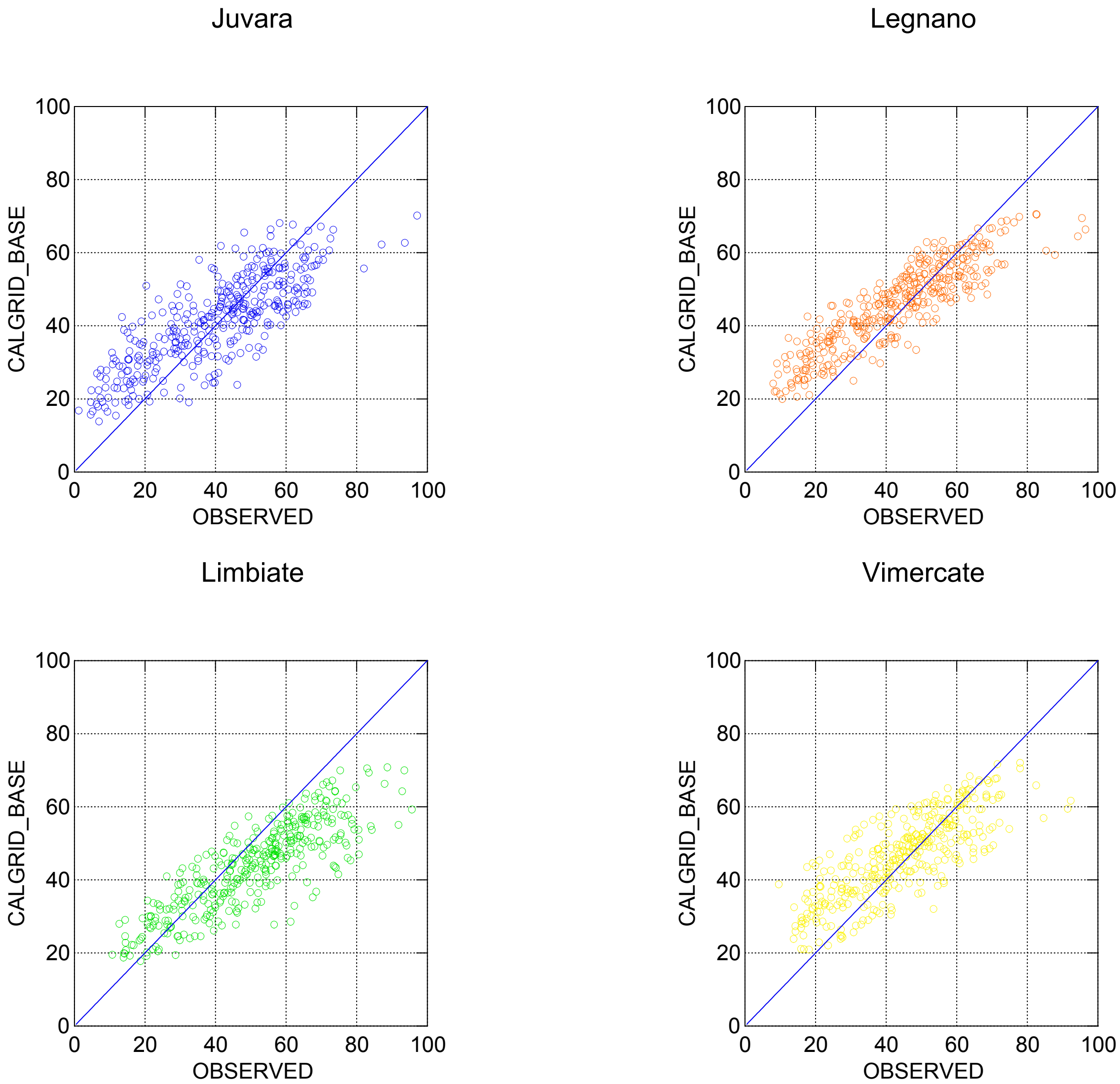

Figure 7. 6-months mean hourly concentrations for daylight hours.

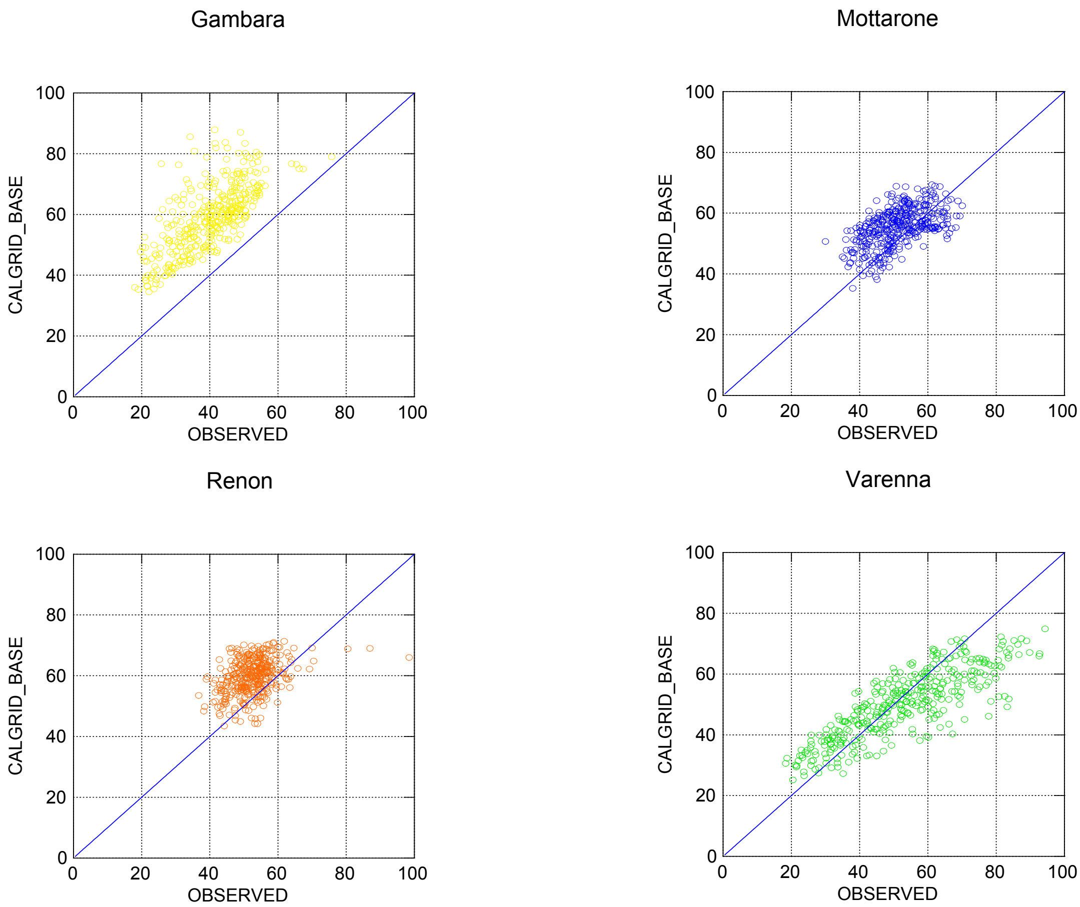

Figure 7 (continued). 6-months mean hourly concentrations for daylight hours.

Ozone exposure assessment

The assessment of environmental risk related to long-term ozone exposure is currently based on the “critical levels” concept, defined as the atmospheric concentrations of air pollutants, above which adverse effects on receptors such as plants, ecosystems or materials can be expected according to the state of the art (UNECE 1996).

Critical level for vegetation has been proposed by EC as the seasonal cumulative exposure over the thresholds concentration of 40 ppb, the AOT40 index. For agricultural crops AOT40 is calculated over three months (May to July) while for forest trees over six months (April to September) so covering the periods where the ozone concentrations may have effective adverse effects on plant growth and crop yield. As for health protection, the peak concentrations are evaluated by means of the AOT60 index, calculated over a period of 6 months (from April to September).

The EC 2002/3 Directive in force for air ambient quality defines AOT40 ozone thresholds for vegetation (6000 $\mu g/m^3 \cdot h$ accumulated from May to July) and forests (20000 $\mu g/m^3 \cdot h$ accumulated from April to September) protection. A level of 0 ppb·h for AOT60 corresponds to zero exceedances of the WHO guideline limit of 120 $\mu g/m^3$.

The simulated indexes, both for crops and forest trees, denote an underestimation in the urban sites with respect to the observed value, and an over-estimation for the rural ones, with the exception of Varenna station, located in the North part of Milan metropolitan area.

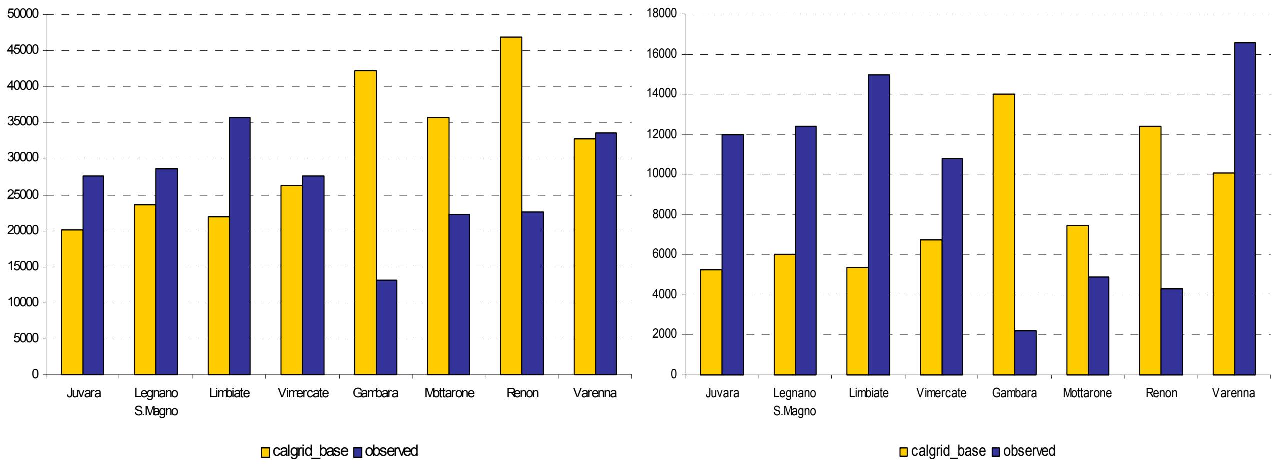

Figure 8. AOT40 (left) and AOT60 (right) for the 6-months period simulated by CALGRID.

Figure 9 reports AOT40 simulated fields for forests. Both in Northern and Southern part of the domain, the model exhibit higher values outside urban areas. Highest values occur in the portion of Prealps placed near urban areas, and, in Southern part, in correspondence of Appennini mountains.

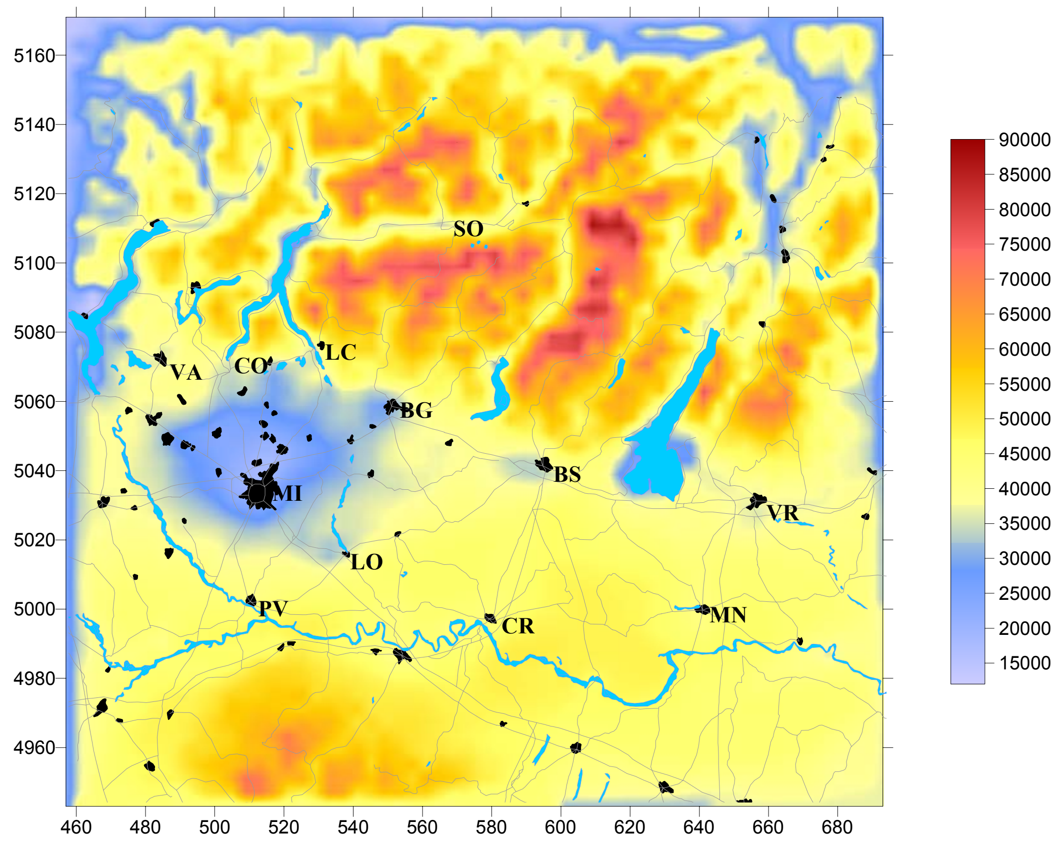

Figure 9. AOT40 (April-September) simulated fields.

Figure 10 reports AOT40 crops estimated for the same domain by EMEP Eulerian model (EMEP, 1999), performing simulation over all Europe with a 50 km grid resolution. As can be noticed AOT patterns are quite similar, with highest values placed in the same areas. Anyway, thanks to a higher horizontal resolution, CALGRID is able to better reproduce AOT40 variations, particularly over complex terrain areas, where wide extensions of vegetation and natural ecosystems are located.

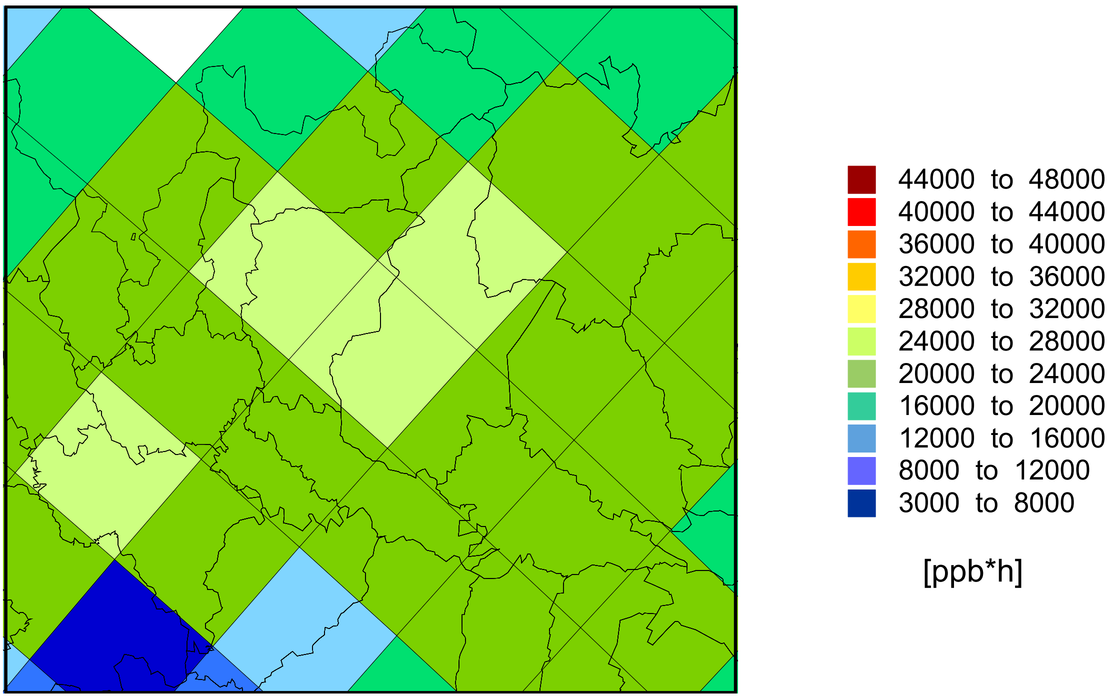

Figure 10. AOT40 (April-September) simulated fields by EMEP model (50X50 km).

Conclusions

A prototype integrated modelling system for the long-term analysis of photochemical pollution has been applied to a seasonal simulation (April-September 1996) over Lombardia Region, in Northern Italy. The system integrates meteorological and emissions pre-processors as well as the transport-chemistry model CALGRID.

In order to compare model outputs and monitored critical levels, some reference stations have been selected from the Regione Lombardia monitoring network by using cluster analysis technique. The preliminary results of the long-term run have been compared with air quality data, in order to assess the model cleverness in describing time and spatial features of pollutant concentrations. The long-term ozone exposure assessment in term of some useful indicators, as the AOT40, has been presented.

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