

B.C. nesting approach harmonisation: UAM-V/CALGRID model exercise on Northern Italy

A contribution to subproject SATURN

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Summary

The ozone episode occurred in the first ten days of June 1998, was monitored by second Intensive Observation Period of LOOP campaign, and has been simulated by means of an integrated modelling system over the entire Lombardia region.

Ozone concentrations at selected monitoring stations were compared with three simulation results: the CALGRID regional simulation; the UAM-V simulation with nested boundary conditions; the UAM-V simulation with constant flux from the surroundings.

Introduction

The Milan metropolitan area is regularly affected by intense photochemical pollution episodes. Three-dimensional photochemical models are useful tools in understanding the causes of these levels because of their capability to consider the influence of emissions, transport and chemistry on pollutant behaviour at different spatial scales. Such models have been extensively applied to the Milan metropolitan area in order to develop a comprehensive modelling system designed to analyse and select possible air quality strategies (Silibello *et al.* 1998, Volta *et al.* 1999, Finzi *et al.* 2000).

Objectives

One of the most critical points related to the improvement of air quality management is the comprehension of the model limits, in particular the influence of the boundary conditions. This work investigates the improvement of a nesting procedure in modelling simulation.

Activities

An integrated modelling system has been designed and implemented, including 3D meteorological pre-processor (CALMET), a flexible emission inventory module (POEM) and photochemical transport models (CALGRID, UAM-V).

3D wind fields have been reconstructed by CALMET, merging background field with measurements, introducing mesoscale features (mountain-valley breezes and local effects) revealed by ground-level measurements and estimating temperature fields as well as turbulence parameters. The emission model POEM (Pollutant Emission Model) is specifically designed to produce present and alternative emission fields estimated by means of an integrated top-down and bottom-up approach. 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, modulating and splitting the CORINAIR90 data set, updated by the last available Italian CORINAIR report (1994). The road traffic emissions are estimated up to 1998.

Model outputs can be the results of all possible combinations of the following three steps:

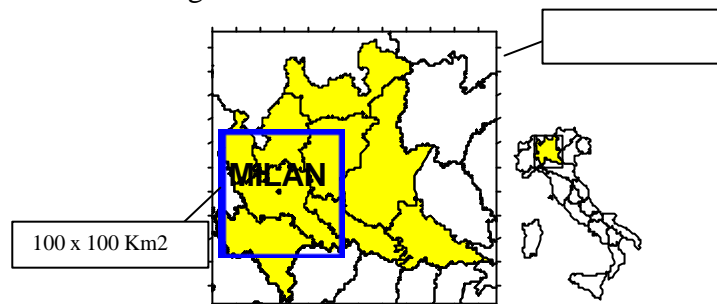
1. *spatial disaggregation*: starting from the province level, the model estimates municipality emissions; then it is possible to distribute emissions on a gridded domain by using proper

surrogate variables highly correlated with emissions and defined by means of national and local statistical sources, GIS and land-use information.

2. *time modulation*: starting from the annual data base, the model can provide emission fields for any assigned time interval on a daily or hourly basis. Fuel use, temperature, degree-days, working time, production cycle, traffic counts and road statistics are the main indicators that have been used for the temporal modulation of emission activities;
3. *VOC splitting*: the total amount of VOC emitted by different activity sectors is split into individual organic compounds according to proper speciation profiles and then lumped into the emission classes needed by the photochemical transport model.

Both CALGRID and UAM-V are photochemical Eulerian three-dimensional models implementing accurate advection-diffusion schemes in terrain-following co-ordinates with vertical variable spacing. The CALGRID model includes the SAPRC-90 mechanism, comprising a lumping scheme for hydrocarbons, 54 chemical species with 129 reactions and the QSSA (Quasi Steady State Approximations) solver for the integration of kinetic equations. The UAM-V model (Urban Airshed Model Variable) uses an extended version of the Carbon Bond IV mechanism, in which model species represent different types of carbon bonds in hydrocarbons. The reactions included in the two mechanisms for inorganic species are nearly identical while organic species cannot directly be compared except when treated explicitly. CB-IV adopts 32 species and 81 reactions.

The models have been applied on 2 domains. The larger simulation domain includes the entire area of Lombardia region (Northern Italy), a complex terrain region located in the Po Valley where industrial and urban areas and a close road network are quite relevant pollution sources. The smaller one, enclosed by the regional domain, is centred on the city of Milan. The ozone episode occurred at the beginning of June 1998; 2-5 June simulation days are here compared (PIPAP0 campaign, second Intensive Observation Period).



Results

Meteorology

Linate vertical sounding and many surface stations have been selected for CALMET meteorological pre-processor, within the regional area for CALGRID simulation, and in the inner domain for UAM-V. While the CALMET meteorological output can be directly provided to CALGRID, some calculations have been performed for the UAM-V meteorological input, specifically for the vertical turbulence exchange coefficients (K_v), the 3D humidity and pressure files. The former has been estimated applying a CALGRID algorithm which uses *friction velocity* and *Monin-Obukhov length* calculated by CALMET, as suggested by Hanna (Hanna *et al.*, 1996).

Emissions

The POEM pre-processor has provided the domain emission fields including area and point sources. Spatial disaggregation, time modulation of yearly emissions and VOC splitting have been performed. The last POEM step supplies directly SAPRC90 species, while further work has been carried on in order to relate every compound to CB-IV species.

Boundary conditions

In order to provide boundary and initial concentrations, grid cells have been subdivided into three categories (urban, rural and mountain) on the basis of height and land use cover (Silibello *et al.* 2000). Boundary conditions have been assumed to be constant in time except

for ozone, NO, NO₂. They have been derived from available measurements in the surroundings or from literature values (Sandnes, 1993; Kumar *et al.*, 1994; Fowler *et al.*, 1997). O₃, NO, and NO₂ ground level boundary have been hourly defined on the basis of the available measurements for each cell category. The vertical profile of boundary and initial conditions has also been assigned on the basis of measurements (Pellegrini, 1999). The ozone vertical distribution has been estimated establishing the top value (60 ppb over 2600 m a.s.l.) and defining a sigmoid profile for each ground level value. For all other species a decreasing profile has been assumed reducing progressively ground-level concentrations. Boundary conditions for UAM-V simulation, in the inner domain, have been firstly set to constant values both in time and space, for almost all compounds; only ozone concentrations have been assumed to increase from 30 to 40 ppb in the last two days. A second UAM-V run has been also performed using CALGRID regional simulation results providing temporally and spatially variable boundary conditions. For organic compounds, lumped according to SAPRC scheme, no univocal correspondence to CB-IV is commonly established. In fact species can be assigned according to definition but coefficients are dependent on VOC mixture (ALK1, which in SAPRC represents less reactive alkanes, is related to CBIV PAR species, that identifies C single bond, and in this study ALK1 - 4 PAR).

Conclusions

In order to compare simulated and observed ozone concentrations, stations from the Regione Lombardia monitoring network and the PIPAPO campaign have been selected. Time series in urban and rural stations are depicted in Figure 1 for the three simulations: the CALGRID regional simulation, the UAM-V simulation with nested boundary conditions and the UAM-V simulation with constant flux from the surroundings. The first two series are useful to evaluate model performances and to check the possibility of adopting the proposed nesting technique, while the third simulation is helpful to appreciate the influence of boundary conditions.

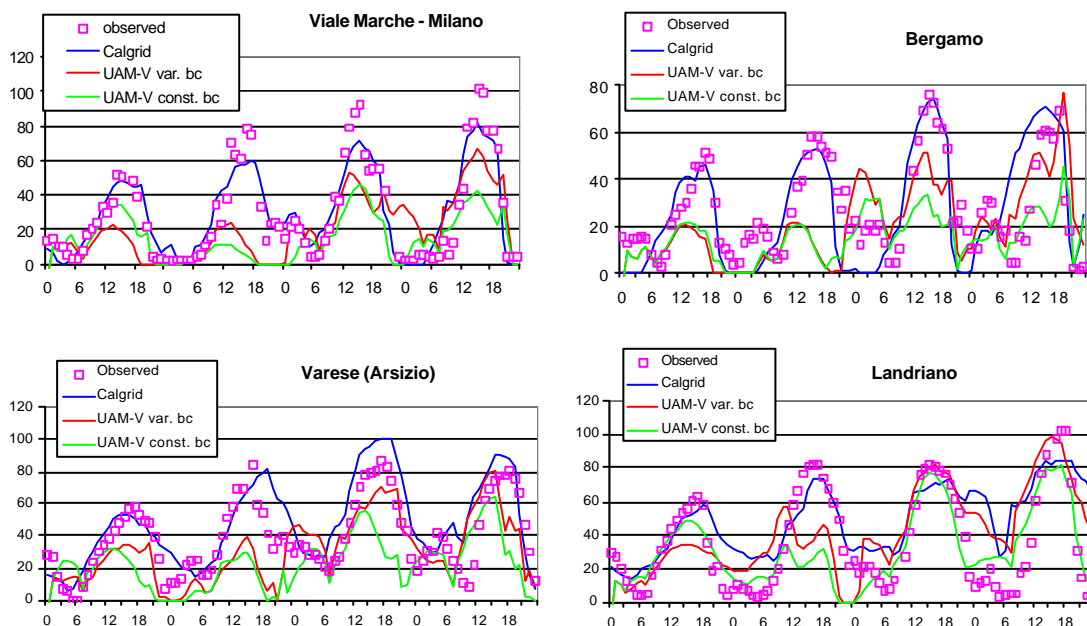


Figure 1: June 2-5 hourly ozone concentration (ppb), in urban (Milano, Bergamo) and rural (Varese-Arsizio, Landriano) sites.

Maximum ozone values were mainly observed on the afternoon of June 4th; this is especially true for the PIPAPO stations located in the north of the city of Milan, while within the city of Milan maximum values were also observed on the last day. The predicted ozone levels underestimate the observed maxima over all the selected stations (unpaired highest prediction

accuracy is about -20% for both CALGRID and UAM-V). CALGRID simulated maxima are mainly on June 4th while UAM-V maxima are shifted towards June 5th. In general better agreement between observed and CALGRID simulation is obtained. When the ozone plume is decreasing, after June 4th, CALGRID is able to follow this trend while the UAM-V simulation is slower and tends to accumulate ozone. This effect is enhanced with variable boundary conditions when ozone transport is almost increasing. UAM-V simulation with nested boundary conditions rather than with constant transport, show ozone levels closer to measured data, confirming that variable boundary conditions are required to properly simulate ozone episodes. CALGRID results usually show higher levels of O₃. Both UAM-V simulations have similar ozone and precursors (not reported here) temporal trends, that are different from the CALGRID ones. UAM-V results have been affected by an incorrect parameterisation of vertical diffusion (K_v) which has not been derived by the dedicated meteorological pre-processor module; this is especially true for night-time concentration predictions. Therefore comparison between UAM-V and CALGRID nocturnal levels cannot be evaluated in terms of model performances. Daytime comparison of O₃ and NO₂ concentrations reveal discrepancies that have been ascribed to the chemical schemes.

The proposed nesting approach seems to be a viable solution, especially when embedded nested models are not available.

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