6.25 A MODELLING SYSTEM FOR THE TRANSPORT AND DISPERSION OF PHOTOCHEMICAL POLLUTANTS : AN APPLICATION OVER A MEDITERRANEAN AREA

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INTRODUCTION

High ground-level ozone (O_3) concentrations are frequently reached during summer period in the Mediterranean area, characterized by meteorological typical conditions that make possible the creation and persistence of photochemical pollution. Photochemical pollution is influenced by meteorology, physical and chemical processes and emissions. Therefore a combined modelling system that couples meteorological models, emissions pre-processors and dispersions models is needed. The modelling system used for this study consists of two meteorological models, the prognostic model RAMS and the diagnostic model CALMET, and the photochemical grid model CALGRID. The emission data have been obtained through disaggregation, modulation and splitting of national emission inventory CORINAIR and by direct estimation of road transport, agriculture and biogenic emissions. The system has been used to simulate summer photochemical smog episodes over the Salento Peninsula, in the Apulia region (South-Eastern Italy). An analysis of simulation results versus local network monitoring data has been performed.

The modelling system

RAMS (Pielke et al., 1992) is a three dimensional, primitive equation atmospheric mesoscale model that uses a terrain following coordinate system. CALMET (Scire et al., 1992) is a 3-D meteorological model which includes a diagnostic wind field generator and a micrometeorological model for overland and over water boundary layers. RAMS/CALMET meteorological fields have been used as input for the CALGRID model (Yamartino et al., 1992). CALGRID is an Eulerian photochemical three-dimensional model which includes accurate modules for horizontal and vertical advection/diffusion. The model is based on the SAPRC-90 chemical mechanism, which contains 54 chemical species and 129 reactions and it requires emission data in the modelling domain and initial and boundary conditions. It produces a 3D hourly concentrations field of emitted species.

Simulation domain and episode selection

The modelling system has been applied over the Salento Peninsula (Figure 1). The Salento Peninsula is located in the South Eastern part of Italy, and it is surrounded by two different seas, the Southern Adriatic and the Northern Ionian Sea, connected by the Otranto Strait. The Peninsula is quite narrow and the topography is mainly flat with small hills: the maximum altitude (less than 200 m) is along the central axis of the southern part. During Summer, the area is normally affected by warm and dry weather. Just a few frontal systems affect the region in that period and the circulation is governed by local sea-breeze systems. Three chemical monitoring stations (C1, C2, C3) are present in the area. General information regarding the location and characteristics of the stations are summarised in Table 1.

Table 1. Locations of the chemical and meteorological stations

STATION	LAT	LONG	Measured quantities	Measurement heights (m)
Station C1	40.40	18.019	O_3, NO_x	10
Station C2	40.358	18.17	O_3, NO_x	10
Station C3	40.119	18.29	O_3, NO_x	10

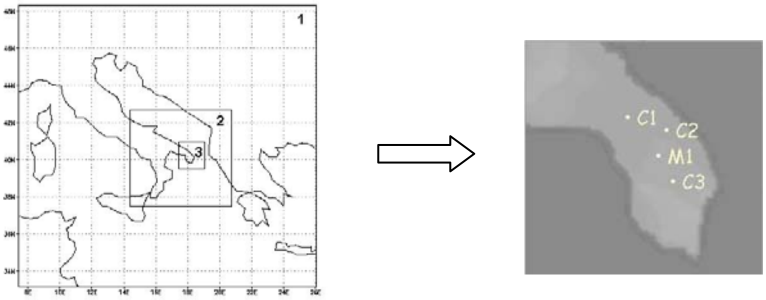

Figure 1. The modeling domain and the three simulation nested grids

Two cases have been simulated, both characterised by high amount of measured ozone ground level concentration but with different meteorological conditions (Schipa I., Phd. Thesis, 2004).

The first case is 1-3 July 2003. During the first day a wide ridge affected the western Mediterranean regions at 500hPa. In the following days, the high pressure centre moved toward the south-southeast at the end of the period, allowing a slightly cyclonic circulation to affect the Mediterranean regions; however, a very weak sea level pressure gradient was still present at the end of the period. These conditions favour the persistence of local sea breeze circulations over Salento.

The second period is 19-22 august 2003. In this period the prevalent wind direction was north, north-east. In fact, in the upper level, a north-western wind component was prevalent, due to the presence of a wide ridge over the Central Europe, and a weak, north-eastern circulation, associated with an almost stationary low pressure over the Aegean Sea, affected Apulia region.

Models setup

To improve spatial resolution, a two-way nested grid configuration is employed in RAMS with three horizontal grids, each grid covering a different domain size (Figure 1). The model was initialised and driven using the data from the European Centre for Medium-Range Weather Forecasts (ECMWF), updating fields every six hours. In the vertical, the atmosphere is divided into 25 levels with different thicknesses, from 100-m starting near the surface, and then gradually stretched with a fixed ratio of 1.2 up to the 13th level, to a maximum of 1000m at the top. In the coarsest grid domain, a nudging toward the data is applied in the 3 grid points closest to the lateral boundaries and in the upper 5 grid levels. CALMET and CALGRID have been run on the inner grid of RAMS (Table 2).

Table 2. Specification of domain size and grid spacing used by the system model

Grid	Lx(km)	Ly(km)	Lz (km)	Nx	Ny	Nz	$\Delta x, \Delta y$(km)
1 RAMS	1800	1800	14	60	60	25	30
2 RAMS	570	660	14	38	44	25	15
3 RAMS	108.75	108.75	14	58	58	25	1.875
3 CALMET-CALGRID	108.75	108.75	3	58	58	10	1.875

Figure 2 show the wind field simulated by using RAMS/CALMET meteorological models for the first and the second case study.

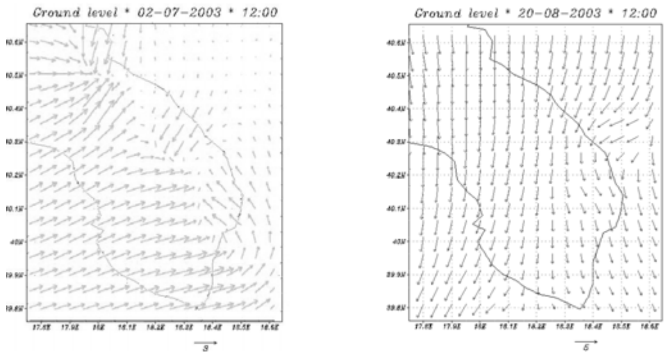

Figure 2. Wind field at ground level for the first and the second case study respectively

Emission data

The emissions have been estimated using two different approaches, the bottom up and the top-down. A direct estimation was utilized for the road transport, agriculture and biogenic emissions. The industrial emissions were determined from the companies' declarations. For all the others emission the national emissions inventory CORINAIR '90-94 was utilized.

The road transport has been obtained from an analysis of mobility and circulation characteristics on every road network arch (Romanini et al., 2001). The biogenic emissions, consisting mainly in VOC emissions, have been directly estimated on the basis of Apulia area vegetation data and calculated by using appropriate algorithms (Schipa I. et al, 2003).

For the other sectors the emission inventory CORINAIR has been adapted spatially and temporally for the species required by the CALGRID. The approach has been based on two main steps:

1. Spatial disaggregation: starting from the province level to gridded domain by using proper surrogate variables highly correlated with emissions and defined by means of national and local statistical sources.
2. Time modulation: starting from the annual to hourly data, by using as much as possible local information about the time behaviour of the activities responsible for the emissions, and considering for each of them monthly, hourly and working days/holidays factors.

The total amount of VOC emitted by different activity sectors has been split into individual organic compounds, according to proper speciation profiles, by using SPECIATE program; then VOC split have been lumped into the emission classes needed by CALGRID.

The boundary and initial conditions of the CALGRID simulations have been obtained using hourly averaged measured data of the monitoring network, in the previous day the simulation started. Figure 3 shows the NO_x emissions distribution over the area. The largest contribution is due to the big industrial sites located in the North Eastern part of the Salento Peninsula.

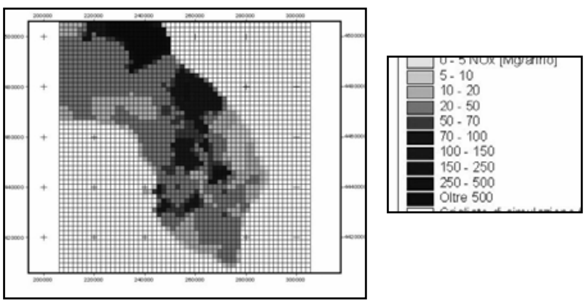

Figure 3. Distribution of total NO_x emissions

Simulation results

Figure 4 and Figure 5 show the comparison between observed and modelled O_3 ground concentration for the two periods considered.

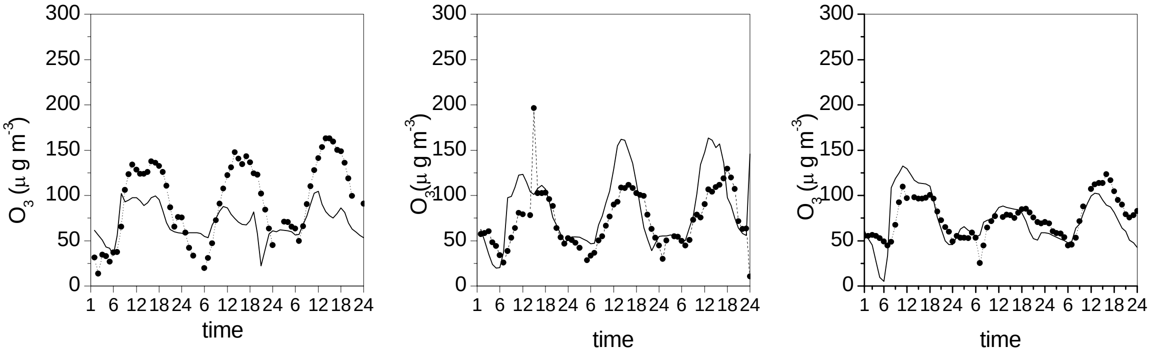

Figure 4. Comparison between observed (dashed line) and modelled (solid line) O_3 ground concentration at station C1, C2 and C3 respectively for the first period considered

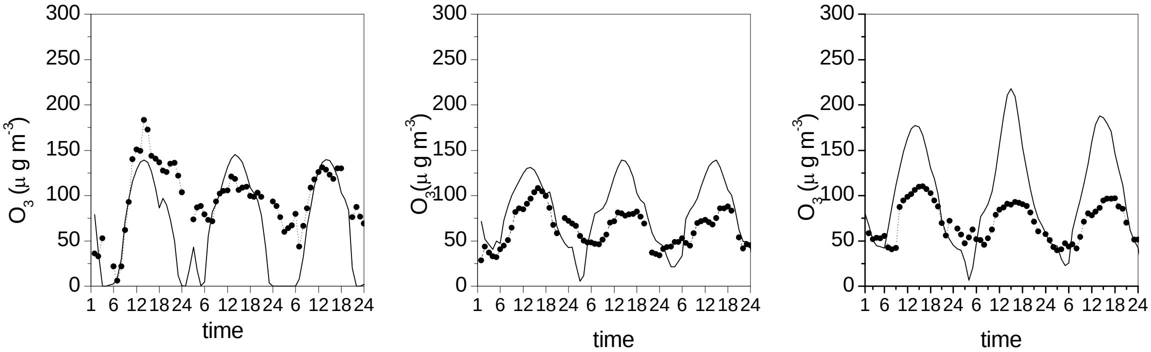

Figure 5. Comparison between observed (dashed line) and modelled (solid line) O_3 ground concentration at station C1, C2 and C3 respectively for the second period considered

From figure 4 and Figure 5 it emerges that the simulated ground level O_3 concentration reproduces the diurnal cycle, but there is a tendency to over-predict the measurements in particular in Station C2 and C3 in the case 2, when the monitoring network is downwind the big industrial sites. By analysing the time evolution of NO_x in this stations (Figure 6) it is evident a tendency of the model to overestimate the NO_x accumulation during the night. This could be due both to uncertainties related to the estimation of the industrial emissions (in particular the time modulation), and the incorrect parameterisation of nocturnal mixing height.

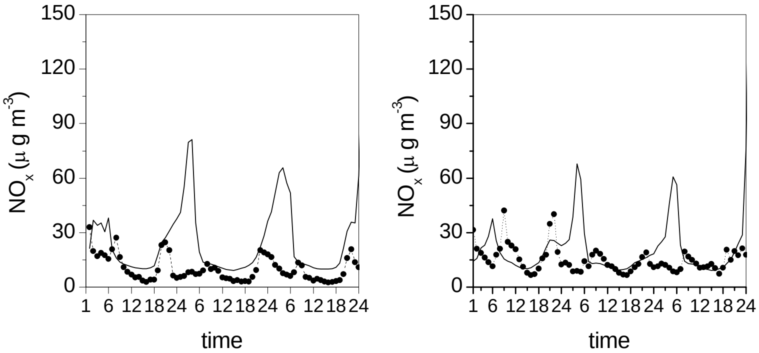

Figure 6. Comparison between observed (dashed line) and modelled (solid line) NO_x ground concentration at station C2 and C3 respectively for the second period considered

CONCLUSIONS

The RAMS/CALMET/CALGRID modelling system has been applied over the Salento Peninsula in South Italy to simulate photochemical smog episodes.

Two cases were analysed characterised by different meteorological conditions. Comparison with measurements shows for both cases a satisfactory reproduction of daytime ozone, with a tendency to over-predict ozone ground level concentration when the monitoring network is downwind the big industrial sites. This tendency seems to be associated with night time primary pollutants accumulation, which could be due to an incorrect estimation of the industrial emissions and/or to the time modulation of the emissions and/or to an incorrect parameterisation of nocturnal mixing height. Further investigation are necessary and will be oriented i) to include a better parameterisation of the mixing regimes, especially during night, ii) to use a larger scale photochemical model to properly assign boundary conditions on the adopted domain.

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REFERENCES

Carter, WPL. 1988: Documentation for the SAPRC Atmospheric Photochemical Mechanism Preparation and Emission Processing Programs for Implementation in Airshed Models, Appendix C, California Air Resource Board.

Pielke, R. A., W. R. Cotton, R. L. Walko, C. J. Tremback, W. A. Lyons, L. D. Grasso, M. E. Nicholls, M. D. Moran, D. A. Wesley, T. J. Lee and J. H. Copeland, 1992: A comprehensive Meteorological Modeling system –RAMS, *Meteor. Atmos. Phys.*, **49**, 69-91.

Romanini, G., and C. Mangia, 2001: An integrated system for estimating and managing road transport emissions, *Air Pollution IX*, 337-342.

Scire, J.S., F. R. Robe, M. E. Fernau and R. J. Yamartino, 2000: A User's Guide for the CALMET meteorological model, Version 5. ,Earth Tech., Inc., Concrd, MA.

Schipa, I., A. Tanzarella, C.Mangia, M. Miglietta, P. Martano, U. Rizza, F. Santese, G.P. Marra, 2003: A modelling system for studying the photochemical pollution: an application over a Mediterranean area, Proceedings of International Workshop On "New Developments On Sensors For Environmental Control (ENVSENS), S. Cesarea Terme (Lecce), Italy, World Scientific, ISBN 981-238-338-7, pp. 229-233.

Schipa, I., 2004: 'Un sistema modellistico per lo studio della dispersione di inquinanti inerti e reattivi dalla scala locale a quella regionale', Phd. Thesis, Messina, Italy.

Yamartino, R. J., J. S. Scir,e, G. R. Carmichael and Y. S. Chang, 1992: CALGRID: A Mesoscale Photochemical Grid Model, Vol. I: Model Formulation Document, *Atmos. Emviron*. **26A**,1493-1512.