Air quality modelling system over a central mediterranean region

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ABSTRACT

This work presents a complex modelling system for air quality studies. The system couples meteorological models, emission preprocessors and dispersion models. Two meteorological models have been coupled in cascade: a mesoscale meteorological model and a 3D diagnostic micro-meteorological model, which is able to provide a realistic three-dimensional wind and temperature fields and two dimensional fields of boundary layer parameters. The emission data were obtained trough disaggregation of national emission inventory, by using a database related to all industrial sources, and through direct evaluation of road transport and biogenic emissions. Meteorological fields and emission data have been used by a photochemical model and by a Lagrangian puff dispersion model. The modelling system has been applied over Salento Peninsula, located in the south-east corner of Italy, in the Mediterranean central area in a real typical summer scenario.

RESUMO

Este trabalho apresenta um complexo sitema de modelagem para estudos de qualidade do ar, acoplando modelos meteorológicos, preprocessadores de emissão e modelos de dispersão. Dois modelos meteorológicos foram acoplados em cascata: um modelo meteorológico de mesoescala e um modelo de diagnóstico micrometorólgico 3-D; capaz de gerar campos realísticos e tridimensionais de vento e temperatura e campos bidimensionais de parâmetros da camada limite planetária. Os dados de emissão foram obtidos do inventário nacional de emissão, que consiste em um banco de dados de todas as fontes industriais, e por estimativa direta da emissão de veículos e biogênica. Os campos meteorológicos e dados de emissão foram inseridos em um modelo fotoquímico e um modelo de dispersão puff-Lagrangeano. Todo o sistema foi então aplicado na Península de Salento, localizada no extremo sudeste da Itália, área central do Mar Mediterrâneo, para um cenário típico de verão.

1. INTRODUCTION

When the domain investigated is large and of non-homogeneous nature air quality dispersion modelling needs realistic three-dimensional atmospheric fields as input for transport and dispersion studies of atmospheric pollutants. They need also an efficient emissions inventory, defined as a database of emissions data and descriptive information for sources of air pollutants over the investigated domain.

The modelling system used in this paper consists of:

- two combined meteorological models, the prognostic model RAMS and the boundary layer model CALMET;
- the Lagrangian puff model CALPUFF, to estimate ground concentration level of non-reactive pollutants;
- the photochemical grid model CALGRID, to evaluate the concentration of reactive species.

The emission data for the modelling domain were computed following two approaches:

1. the first is based on disaggregation, modulation and splitting of national emission inventory;

2. the second is based on direct estimation of road transport, agriculture and biogenic emissions .

The systems have been applied to the Salento Peninsula. This area is surrounded by two different seas and is subject in all its coastal perimeter to complex sea-land breeze systems which make simplified models unable to take into account most of needed details.

2. MODELLING SYSTEM

RAMS (Regional Atmospheric Modelling System) (Pielke et al., 1992) is a highly versatile system developed at Colorado State University for simulating and forecasting weather system. It contains an atmospheric model, which performs the actual simulation and a data analysis package, which prepares initial data for the atmospheric model from observed meteorological data. The atmospheric model is constructed around the full set of primitive dynamical equations, which govern atmospheric motions; these equations are supplemented with optional parameterisations for turbulent diffusion, solar and terrestrial radiation, sensible and latent heat, exchange between the atmosphere, kinematic effects of terrain. The equation system is solved on a rectangular grid using terrain following co-ordinates. The RAMS model was initialised and driven using the data from the European Centre for Medium-Range Weather Forecasts (ECMWF), updating fields every six hours.

CALMET (CALifornian METeorological model) (Scire et al., 1990) is a meteorological model which includes a diagnostic wind field generator and a micrometeorological model for overland and overwater boundary layers. Here, it is used in the option which allows to consider as input the wind field produced by the prognostic model.

CALPUFF (CALifornian PUFF model) (Scire et al., 1990) is a non-steady-state Gaussian puff model containing modules for complex terrain effects, overwater transport, coastal interactive effects, building downwash, dry and wet pollutant removal, and simple chemical transformation. It is designed to use the three dimensional meteorological fields provided by CALMET.

CALGRID (CALifornian GRIDded model) (Yamartino et al., 1992) is an Eulerian photochemical three-dimensional model which includes accurate modules for horizontal and vertical advection/diffusion. A resistance-based dry deposition algorithm takes into account pollutant properties, local meteorology and terrain features. The model is based on the SAPRC-90 (Statewide Air Pollution Research Center)(Carter, 1988) chemical mechanism, which contains 54 chemical species and 129 reactions.

Figure 1 shows the modelling system scheme.

The emission data for the modelling domain were obtained trough disaggregation of national inventory data.

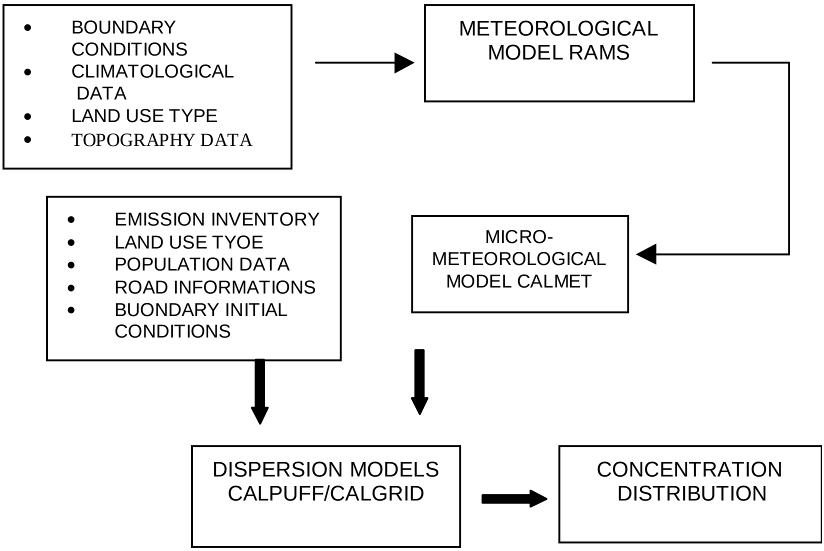

Fig. 1. Modelling system scheme

3. MODELLING DOMAIN

The Salento Peninsula, located in the south-eastern corner of Italy, is surrounded by two different seas, the Southern Adriatic and the Northern Ionian Sea. This area is subject in all coastal perimeter to complex sea-land-sea breeze systems. Figure 2 shows area investigated. Numbers indicate the location of meteorological stations from the Italian Military Meteorological

Service, while general informations are summarised in Table 1. Points indicate the emission sources.

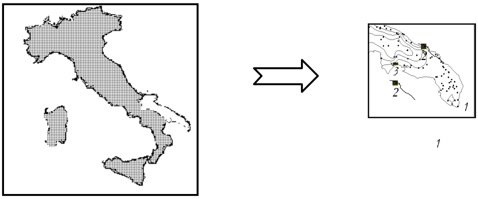

Fig. 2. Area investigated

N.	name	lat.	long.	h (m)
1	S. Maria di Leuca	39° 49'	18° 21'	112
2	Brindisi	40° 39'	17° 57'	10
3	Marina di Ginosa	40° 25'	16° 58'	5

Tab. 1. Location of the meteorological stations and height relative to sea level

4. EMISSION DATA

The emission data for the model's inputs are estimated by means of three different approaches:

1. the national emissions inventory (named CORINAIR) for area sources;
2. the industrial emissions inventory, for industrial sources;
3. a direct estimation, for the road transport, agriculture and biogenic emissions.

Developed in the context the European Community program (1985) concerning in the harmonisation and organization of informations on environment conditions, the CORINAIR (COordination INformation AIR) inventory (Bocola and Cirillo, 1989) represents an important database containing that part of project related to the atmospheric emissions.

For our purpose, the emission data, related to the modelling domain in the selected period, have been obtained by applying a top-down methodology to the Italian inventory data: actually only the 1990 emission inventory are available, but even if it's necessary a certain caution in using them, they represent a valid reference in the regional emissions' description. The inventory includes CH_4, NH_3, NO_x, N_2O, CO, CO_2, VOC (Volatile Organic Compound) and SO_x emissions, given in ton/year, on provincial territorial unit and subdivided by activity sectors: among these, only CO, NO_x, SO_x and VOC have been used, because the only ones to participate in the chemical mechanism implemented in the model.

To estimate the industrial emissions it has been used a database related to all industrial sources in Apulia region, based on each companies' autocertifications.

The estimation of road transport has been obtained from an analysis of mobility and circulation characteristics on every road network arch.

The same approach has been applied for the calculation of biogenic emissions, consisting mainly in VOC emissions: they have been directly estimated on the basis of Apulia area vegetation data and calculated by using appropriate algorhythms.

4.1 The disaggregation procedure

In order to provide the appropriate detail in time and space, needed for the photochemical modelling, the yearly District inventory has been therefore disaggregated through the following steps:

- *spatial disaggregation*, to obtain, starting from the district level and the municipality emissions; it has been then 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;
- *time modulation*, in which the model can provide emission fields for any assigned time interval on a daily or hourly basis; it has been performed by using as much as possible local information about the time behaviour of the activities responsible for the emissions, and so considering for each of them monthly, hourly and working day/holidays factors.

At the end of this procedure, it has been done the speciation of organic compounds: the total amount of VOC emitted by different activity sectors has been splitted into individual organic compounds according to proper speciation profiles and the lumped into the emission classes needed by photochemical transport model.

Figure 3 shows the temporal disaggregation procedure scheme and figure 4 shows an example of spatial disaggregation of NOx emission.

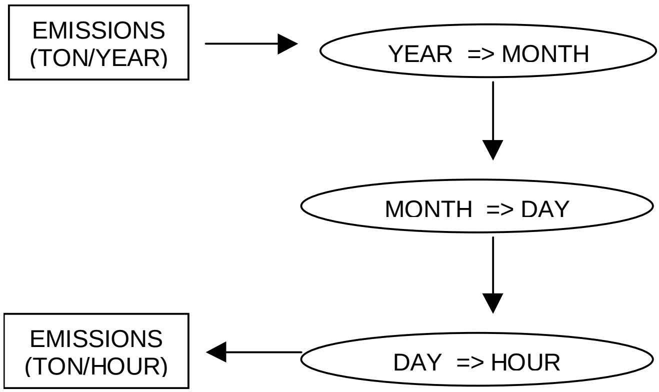

Fig. 3: temporal disaggregation scheme

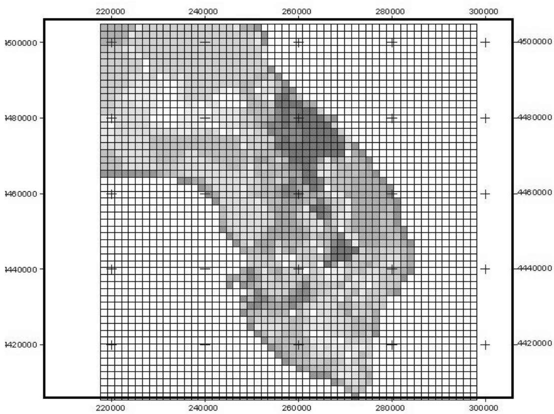

Fig. 4. example of spatial disaggregation

5. METEOROLOGICAL FIELDS

On the basis of the analysis of the weather maps (DWD- Deutscher WetterDienst) relative to the year 1998, one typical summer meteorological situation was selected, from 24 to 27 July 1998. This summer scenario is characterised by a synoptic situation almost constant for all period.

The RAMS model was initialised and driven using the data from the European Centre for Medium-Range Forecast, updating fields every six hours. Three nested grids were selected: the first grid had a mesh of 26x36 points (22.5 km grid spacing); the second grid had a mesh of 47x47 points (7.5 km grid spacing) and the third grid had a mesh of 54x54 points (1.875 grid spacing) .

Twenty one terrain following vertical levels were used in all grids of RAMS, whereas in CALMET were used ten vertical levels.

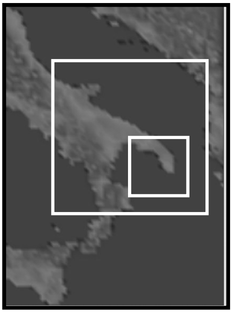

Fig. 5. Simulation grids

5.1 Comparisons between model results and measurements

The wind predictions model are compared with wind data recorded every three hours at six meteorological stations from the Italian Military Meteorological Service.

Preliminary analysis indicates that the meteorological system can simulate the general mean wind field over the area in a realistic way (Figure 6). Some discrepancies are present in the individual stations, particularly evident for station 1 situated in a very critical point. These could due both to uncertainties in the measurements and to the insufficient model resolution of the local effects. It has been noted that measurements are taken at a discrete location while calculated values are representative for a grid cell of 7500x7500m.

Two statistical quantities were compute from the all model results: the normalised mean square error, *nmse*, (characterising the amount of the deviation between predictions and observations), and the fractional bias, *fb*, (showing the tendency and the sign of the deviation):

$$nmse = \overline{(C_o - C_p)^2} / \overline{C_o}\,\overline{C_p}$$

$$fb = \left(\overline{C_o} - \overline{C_p}\right) / \left(0.5\left(\overline{C_o} + \overline{C_p}\right)\right)$$

where subscripts *o* and *p* refer to observed and predicted quantities, and an overbar indicates an ensemble average.

Statistical indexes concerning the comparison are summarised in Table 2.

Wind speed (m/s)		Wind direction	
nmse	**fb**	**nmse**	**fb**
0,29	-0,06	0,09	0,31

Tab. 2: Statistical indexes

6. DISPERSION SIMULATIONS

To simulate the ground concentration level of non-reactive pollutants, it has been used the Lagrangian puff model CALPUFF, while to simulate the ground concentration level of reactive pollutants it has been used the photochemical grid model CALGRID.

The simulations started at 00:00 of 24 July 1998 and lasted for 4 days ending at 19:00 of 27 July.

Figure 7 shows the ground level concentration fields obtained with CALPUFF model at different times. It is evident that pollution level of SO2 is quite high and concentrated in the area downwind the largest emissions, due to the wind direction persistence.

Figure 8 shows the ground level concentration of O3, NOx and VOC obtained with CALGRID model at different times. In the morning there are high concentrations of NOx and VOC; these two species react and, during warmer hours due to solar radiation, create O3. The O3 level concentrations diminish in the night hours.

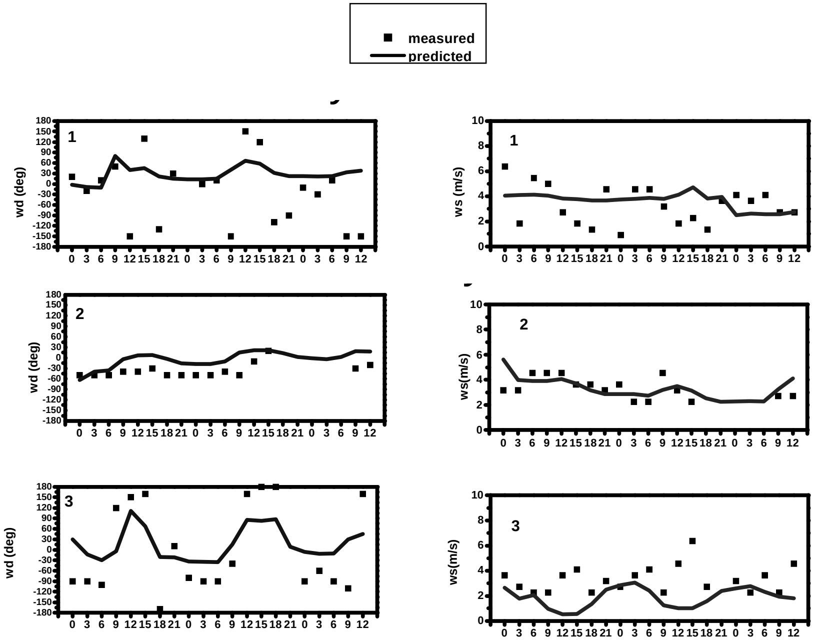

Fig. 6. Comparison among predicted and measured wind data

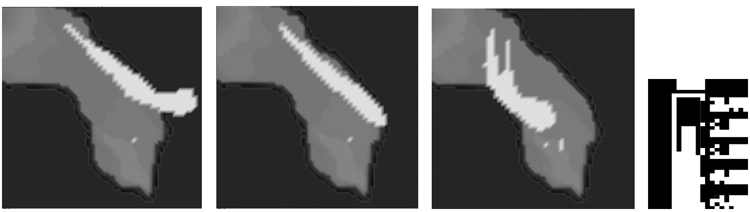

Fig. 7. CALPUFF simulation (μg/m^3)

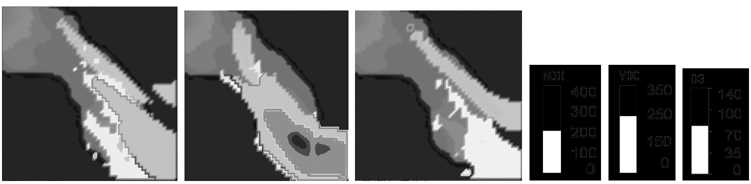

Fig. 8. CALGRID simulation (μg/m^3)

7. CONCLUSIONS

The RAMS-CALMET modelling system has been implemented to investigate the capability of such a system to represent and reproduce mesoscale circulations, while the CALPUFF and CALGRID models have been used to simulate the transport and dispersion of air pollutants. Simulations were performed over the Salento peninsula in a typical summer scenario.

Comparison between RAMS predictions and measured wind fields shows that the model can simulate the mean wind field over a complex terrain in a realistic way. The discrepancies in some stations could be due to the insufficient spatial representation of topography that does not allow the resolution of the local terrain effect.

The global system can be considered a useful tool to investigate the impact produced by pollutant sources in complex terrain and to support decisions in planning air quality monitoring network.

Acknowledgements.

The present work was partially supported by the CNR-Project CNRG00ED51

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