

# **BOLCHEM, an integrated system for atmospheric dynamics and composition**

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## **Abstract**

The on-line modelling system BOLCHEM consists of a meteorological limited area hydrostatic model (BOLAM) coupled with different gas chemistry models (SAPRC90 and CB-IV chemical mechanisms), an aerosol model (M7, work in progress) and a Lagrangian dispersion model for computation of forward and backward trajectories. The model is under development but recent applications have shown its reliability for air quality studies. Future developments will focus on data assimilation of atmospheric composition and on feedback effects of composition on radiation and dynamics.

## **1 Introduction**

Chemical composition at regional scale is the subject of increasing interest for both air quality and climatological issues. Several models exist but no on-line Italian model was available some years ago. Different expertise are present at ISAC-CNR on several aspect involved in air-quality modelling: atmospheric chemistry, meteorology, microphysics and turbulence, and these were gathered to develop BOLCHEM. The model is part of the European community project GEMS,

sub-project Regional Air Quality models (RAQ) and has been used to study different aspects of air quality related problems.

## 2 Model description

The BOLCHEM model (BOLam + CHEMistry) is the result of an on-line coupling between the mesoscale meteorological model BOLAM (BOlogna Limited Area Model, <http://www.isac.cnr.it/~dinamica/bolam/index.html>) (Buzzi et al., 1994, Buzzi et al., 2003) and modules for transport and transformation of chemical species. BOLAM dynamics is based on hydrostatic primitive equations, with wind components, potential temperature, specific humidity, surface pressure, as dependent variables. The vertical coordinate system is hybrid-terrain-following, with variables distributed on a non-uniformly spaced staggered Lorenz grid. The horizontal discretisation uses geographical coordinates on an Arakawa C-grid. The time scheme is split-explicit, forward-backward for gravity modes. A 3-d WAF (Weighted Average Flux) advection scheme coupled with semi-Lagrangian advection of hydrometeors is implemented. A fourth order horizontal diffusion of the prognostic variables (except for Ps), a second order divergence diffusion and damping of the external gravity mode are included. The lateral boundary conditions are imposed using a relaxation scheme that minimises wave energy reflection. The initial and lateral boundary conditions are supplied from the ECMWF (European Centre for Medium-range Weather Forecasts) analyses available at  $0.5^\circ \times 0.5^\circ$  resolution. Hybrid model level data are directly interpolated on the BOLAM grid.

Transport (advection and diffusion) of tracers (both passive and reactive) is performed on-line at each meteorological time-step using WAF scheme for advection and a "true" (second order) diffusion, with diffusion coefficient carefully estimated from experiments (Tampieri and Maurizi, "submitted"). Vertical diffusion is performed using one-dimensional diffusion equation with a diffusion coefficient estimated by means of an E-l turbulence closure scheme. Dry deposition is computed through resistance-analogy scheme and is provided as boundary condition to the vertical diffusion equation. Furthermore, vertical redistribution of tracers due to moist convection is parameterised consistently with the Kain-Frisch scheme used in the meteorological part for moist convection. Transport of chemical species is performed in mass units while gas chemistry is computed in ppm.

Physical/chemical processes are treated separately for gas phase, aerosol classes and generic tracers (e.g. radioactive species, Saharan dust, ...). Gas phase is treated using the SAPRC90 or CB4 chemical mechanisms. Aerosol is modelled using M7 module from ECHAM5 (coupling still in progress) and generic species are defined by the user case by case providing

chemical/physical properties and equations. More technical details can be found in the COST 728/732 model inventory:

[http://www.mi.uni-hamburg.de/List\\_classification\\_and\\_detail\\_view\\_of\\_model\\_entr.567.0.html?&user\\_cost728\\_pi2\[showUId\]=80](http://www.mi.uni-hamburg.de/List_classification_and_detail_view_of_model_entr.567.0.html?&user_cost728_pi2[showUId]=80)

### **3 Model applications**

The model has been used for a variety of situations in order to test the reliability of the choices made. It also currently runs at ECMWF in the frame of GEMS Project for the ensemble near-real-time experiment. Some of the main results are briefly reported in the following sections.

#### **3.1 Evaluation of model performances for**

##### **3.2 ozone**

The performances of BOLCHEM on the ability to predict O<sub>3</sub> concentration over Italy were evaluated. The comparison between computed and measured concentrations for some periods of 1999 shown that the model is able to predict the diurnal cycle of O<sub>3</sub>, in particular in summer. The agreement between modeled and measured quantities is good during the day while at night there is some problem connected to O<sub>3</sub> destruction. However, US-EPA's criteria are met so that model results can reliably used for air quality predictions. Some time series of O<sub>3</sub> computed with CBIV and SAPRC90 mechanisms are compared to measurements in Figure 1.

##### **3.3 Ozone sensitivity to precursor emission reduction**

An important aspect for emission reduction policies, is the study of the regional sensitivity to precursor emission reduction. For this purpose indicator species are computed to asses reduction in NO<sub>x</sub> and VOC over the whole Italy and on subdomains centered on specific spots: the Milan and Rome areas and some of the major industrial areas. Different periods were selected and runs with both chemical schemes were performed over Italy comparing indicator species computed for different reduction scenarios. For all the periods investigated, it is found that Italy, including the big islands Sicily and Sardinia, is mostly dominated by NO<sub>x</sub> chemical regimes, independently of the photochemical mechanism used. However, the effect of the reduction of NO<sub>x</sub> predicted with the CB-IV mechanism is lower than that

predicted with SAPRC90 mechanism. In addition, the urban areas around cities as Milan, Rome, Naples or industrialised areas around harbours as Genoa, Messina, Venice are always in a marked VOC sensitive regime. It can be also noted that the differences in the spatial distribution of the chemical regimes due to the photochemical mechanism used and due to the meteorological conditions are comparable. Example of maps of sensitivity of ozone to reduction of VOC and NO<sub>x</sub> are reported in Figure 2.

### **3.4 Saharan dust transport**

Saharan dust is a major component of the aerosol load over Italy due to the vicinity to the African continent. The direct forcing of dust aerosol may be comparable to or even exceed the forcing of anthropogenic aerosols. To correctly treat this aspect, a proper modelling of surces is needed. A sensitivity experiment was carried out to test the sensitivity of the emission model (Tegen eta al, 2002) to the friction velocity treshold during a strong Saharan dust outbreak that occurred from 15 to 19 July 2003, transporting the dust particle almost over the whole Italy (Figure 3). The comparison of model results with the observations (surface concentrations from EMEP stations and aerosol optical depth (AOD) from AERONET stations) allowed to select the better treshold.

### **3.5 Lagrangian transport and Etna eruption**

A Lagrangian transport model is implemented in BOLCHEM (BOLTRAJ variant) that can be used in conjunction with the Eulerian part. This is useful as an analysis tool for a better interpretation of Eulerian simulations through the computation of the probability matrices of pollutant origin. It is also useful to study specif events of concentrated sources when the resolution of the Eulerian grid would be too small to represent dispersion at short time. The first application was the Mt. Etna eruption on Autumn 2002 (Villani et al., 2006). The joint analysis of Lagrangian trajectories, satallite data, meteorology and lidar measurements allowed to estimate the tropospheric dispersion coefficient and to clarify some features observed by lidar located at Potenza. Lidar measurements recorded a strong signal with clear sulphate signature, along with weaker layers above. Satellite images gave no clear evidence but trajectory analysis revealed the nature of the complex picture: part of the trajectories passing over Potenza took a long tour through the sahara region, possibly carrying some silicate and passing over Potenza at the same time (and at different heights) of those coming directly from Mt. Etna (Figure 4).

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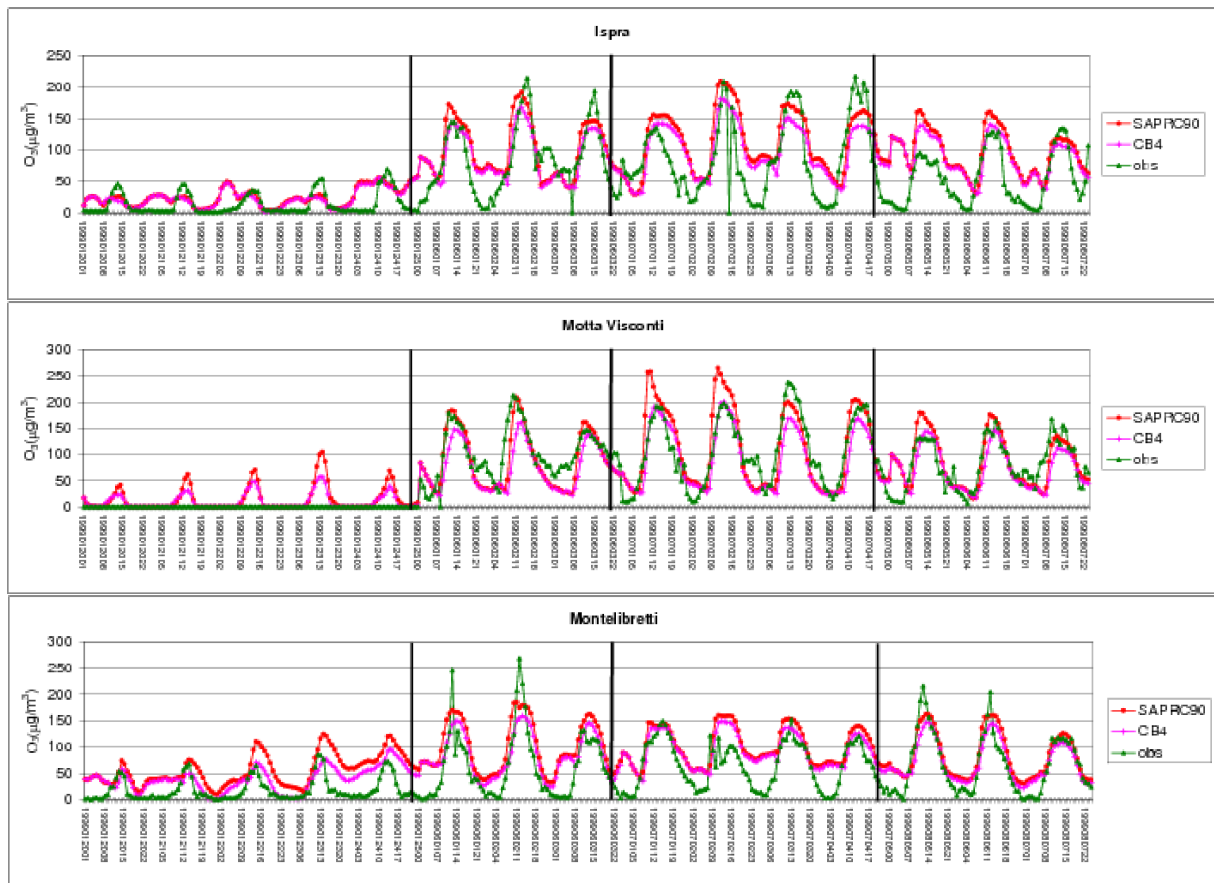
through the Program Italy-USA Cooperation on Science and Technology of

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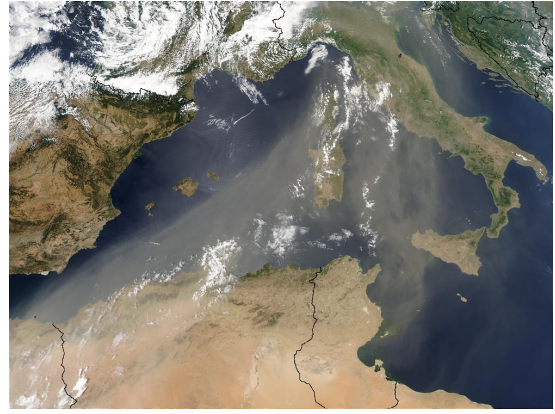
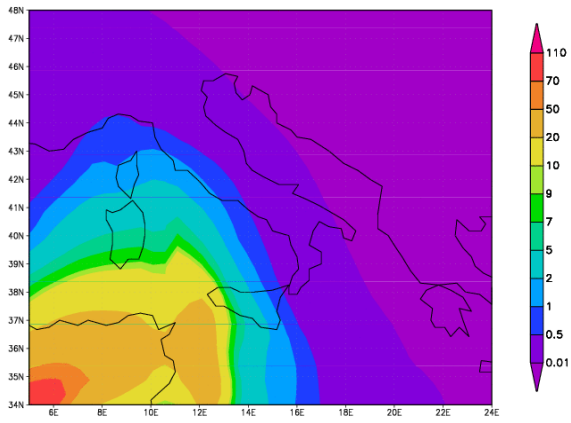
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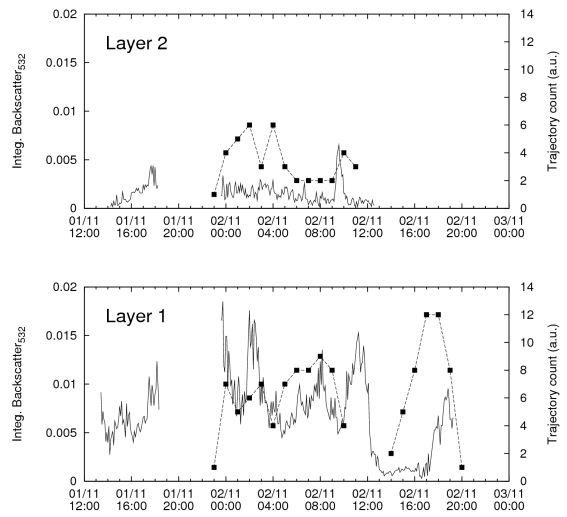
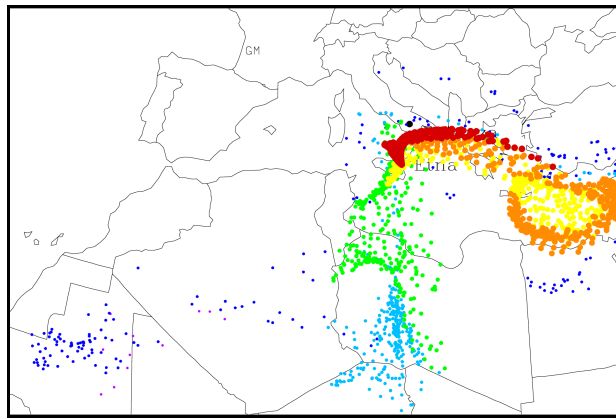
**Figure 1.** Time series for O<sub>3</sub> in three locations in Italy: Ispra, Motta Visconti (MI) and Montelibretti (RM) for four periods: January, June, July and August.







**Figure 3.** Vertically integrated aerosol load simulated with BOLCHEM (left) and seen by MODIS AQUA (right).



**Figure 4. Left panel: position of particles released at Mt. Etna from 26-10-2002 to 01-11-2002. Different colours denote different ages (in days). Right panel: comparison of LIDAR signal measured over Potenza and simulated by BOLCHEM.**