Development and preliminary results of a limited area Atmosphere-Chemistry model: BOLCHEM.

Massimo D'Isidoro[1,3], Sandro Fuzzi[1], Alberto Maurizi[1], Mihaela Mircea[1], Fabio Monforti[2], Francesco Tampieri[1], Maria Gabriella Villani[1,4] and Gabriele Zanini[2].

[1]Inst. of Atmospheric Science and Climate (ISAC-CNR), Via Gobetti 101, 40129 Bologna, Italy.
[2]ENEA PROT-INN Section, Via Martiri Monte Sole 4, 40129 Bologna, Italy.
[3] Dipartimento di fisica, Università di Ferrara,Via Paradiso 12, 44100 Bologna, Italy.
[4] Campus Scientifico Sogesta, University of Urbino, 61029 Urbino, Italy.

Corresponding author address: m.disidoro@isac.cnr.it

Summary

The model BOLCHEM has been developed at ISAC-CNR for regional air quality forecast. In this paper we present the first results achieved simulating a high ozone episode over Italy. The model forecasts obtained using two different chemical mechanisms (SAPRC-90 and CB-IV) are compared with ground-based measurements performed in different parts of Italy. The model reproduce well the main features of the ozone episode, in particular the ozone concentration maxima, but there are differences due to the chemical mechanism used and also due to the representation of other physical processes such as dry deposition, boundary layer representation, etc.

1. Introduction.

There are several factors that contribute in determining the air quality forecast such as: emissions, chemistry, microphysics and meteorology. The relevant progresses obtained in the last decades in numerical weather prediction together with the exponential increase of computer power are now exploited to improve the regional air quality forecasts. In particular, over regions with complex topography, the results of an air quality model strongly depend upon the mesoscale features of the meteorology fields that, in turn, depend on the orography description and the parameterizations of sub-grid processes. Italy, especially the Po valley, has such morphology that requires an on-line coupling between the meteorological and chemical fields.

2. Model description.

The model BOLCHEM (BOLam + CHEMistry) stand for an on-line coupling of the mesoscale meteorological model BOLAM (Bologna Limited Area Model) (Buzzi et al., 1994, Buzzi et al., 2003) with a gas phase chemistry processor. The model can run with the two gas-phase chemical mechanisms SAPRC-90 (131 reactions with 35 chemical species; see Carter, 1990) and
CB-IV (85 reactions and 30 chemical species; see Gery et al., 1994). The gas species included in the two chemical mechanisms are showed in Table 1.
BOLAM dynamics is based on hydrostatic primitive equations, with wind components u and v, potential temperature θ, specific humidity q, surface pressure p_s, as dependent variables. The vertical coordinate system is terrain-following (σ), with variables distributed on a non-uniformly spaced staggered Lorenz grid. The horizontal discretization 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 p_s), 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° X 0.5° resolution. Hybrid model level data are directly interpolated on the BOLAM grid.
The meteorological module supplies to the chemical mechanism various prognostic and diagnostic fields such as temperature, specific humidity, wind components u and v and the geopotential height to BOLCHEM at every multiple of its time-step. An interface code allows some operations such as the computation of the photochemical reactions coefficients, the horizontal and vertical advection of the chemical species to be done by means of a semi-Lagrangian scheme and the calculation of the

$$V_d = \frac{1}{R_a + R_b + R_c}$$

vertical diffusion coefficients to be done using the mixing length theory. Moreover, the dry deposition velocities and surface emissions are taken into account in estimating the vertical fluxes of the concentrations. The dry deposition scheme follows a resistance analogy approach (Wesley, 1989) with the deposition velocity (V_d) function of three resistance terms:
where R_a is the aerodynamic resistance and is computed using the friction velocity U_* and the Businger stability functions at the surface layer; R_b, is computed in a different way over land and sea and is considering a quasi-laminar boundary layer resistance depending upon U_* and the molecular diffusivities of the single gases. R_c is the surface resistance and is considered constant, varying only with the species. Finally, the chemical reactions following the chemical mechanism (SAPRC-90 or CB-IV) are solved and then the meteorological processor for the successive time-step is called.

3. The case study.

In this study, we focused on an ozone episode that occurred over Italy during the first week of July 1999, when a west moving wave coming from northern Africa crossed the Italian peninsula with temperatures reaching values up to 20°C at 850 hPa level, creating ideal meteorological conditions for the developing of photochemical pollution at lower atmospheric levels, especially over the highly industrialized and urbanized region of Po valley.
The BOLCHEM was run in horizontal with 20 km resolution grid and with 28 sigma vertical levels. The lower level was approximately at 20m above the surface. Figure 1 shows the model domain and orography. The period studied starts on 1st July 1999, 00 UTC and ends 7th July 1999, 00 UTC. The meteorological fields are supplied by ECMWF and lateral boundary conditions are updated every 6 hours. The weather fields were re-initialized every 48 hours with the analyses in order to avoid an excessive error growth in the meteorological forecast. The chemical fields are driven by hourly surface emissions and 3 hourly lateral boundary conditions after the initialisation. Emissions, initial and boundary conditions were obtained from the 1999 base case run of the MINNI model (Zanini et al., 2004). Point source emissions are not taken into account in this experiment.

4. Results.

Figure 2 shows the synoptic situation: the 850 hPa level temperature field simulated by the model on 2nd July , at 15 UTC, when the heat wave mainly influenced central and northern Italy.
The predicted ozone concentrations using the two chemical schemes (SAPRC-90 and CB-IV) on 2nd July at 15 UTC in the lowest level of the model are shown in Figure 3.. The ozone fields show a very similar spatial distribution.. There are differences in the maximum concentrations: SAPRC-90 showing in general higher values than CB-IV. The model behaviour was also evaluated by comparing the modelled and measured time series between 2nd and 7th July at four locations shown in Figure 2. Figure 4 shows the time series of ozone concentration at three rural and one sub-urban (Torino Lingotto) stations. It can be seen that the diurnal cycle is generally well reproduced by the two chemical mechanisms and the concentrations computed with the two schemes are similar. However, SAPRC-90 gives higher values than CB-IV, as already seen in Figure 3, and this indicates that the simulations using SAPRC-90 scheme can exceed the alarm threshold for ozone concentration in some cases while that using CB-IV does not.
The large departures of computed ozone concentrations from measurements observed in some locations can be due to different factors such as the model resolution: 20 km grid size could be not optimal for a comparison with single station measurements, in particular for urban and sub-urban locations. Another cause of the departures between observed and simulated ozone concentrations can be the parameterizations of the physical processes included in BOLCHEM. Higher resolution simulations, with a better representation of orography and mesoscale features could yield to an improvement of the air quality forecast, provided that a realistic description of the surface emissions is available.

5. Discussion and future development.

The atmosphere-chemistry model BOLCHEM, developed at ISAC-CNR for regional air quality studies, was used to simulate a case of elevate ozone concentration over Italy on July 1999. The purpose of this study was to evaluate the model ability in reproducing photochemical pollution, focusing on ozone concentration. Two simulations were accomplished using SAPRC-90 and CB-IV gas phase mechanisms for the week 1-7 July 1999. The results of the simulations were evaluated and compared with ground-based measurements performed over Italy. The relative good agreement between the maximum ozone concentrations predicted by BOLCHEM and the measurements point out that the model is an useful tool for air quality forecast for ozone episodes. The future development of BOLCHEM will focus on the implementation of a wet removal scheme for gases and an aerosol module as well as on improvements of dry deposition scheme and computation of the photochemical reactions coefficients..

References.

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GAS CHEMISTRY MECHANISMS						
SAPRC-90				CB-IV		
131 reactions 35 species (10 fast, 25 slow)				85 reactions 30 species (11 fast, 19 slow)		
HNO3	RNO3	ARO1	MEK	PNA	CO	C2O3
HONO	MGLY	ARO2	CRES	HONO	FORM	XO2
HNO4	AFG2	O3	RCHO	HNO3	ALD2	CRO
CO	SO2	NO	ALK2	PAN	MGLY	CRES
HO2H	ETHE	NO2	C2CO3	H2O2	OPEN	HO2
OOH	OLE1	NO3		MEOH	ETOH	ROR
PAN	OLE2	N2O5		PAR	O3	ISOP
PPN	OLE3	HO2		ETH	NO	NTR
HCHO	OLE4	RO2		OLE	NO2	N2O5
CCHO	ALK1	CCO3		TOL	NO3	XYL

Table 1: Gas species included in the SAPRC-90 and CB-IV chemical mechanisms in BOLCHEM.

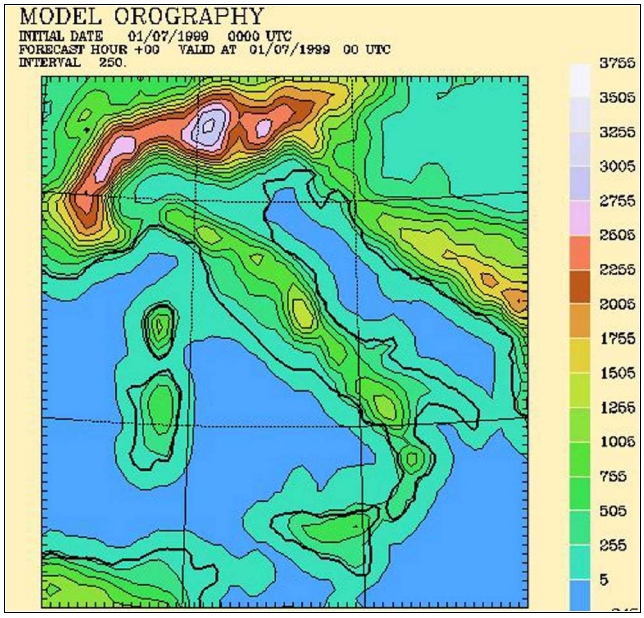

Figure 1: Model domain and orography.

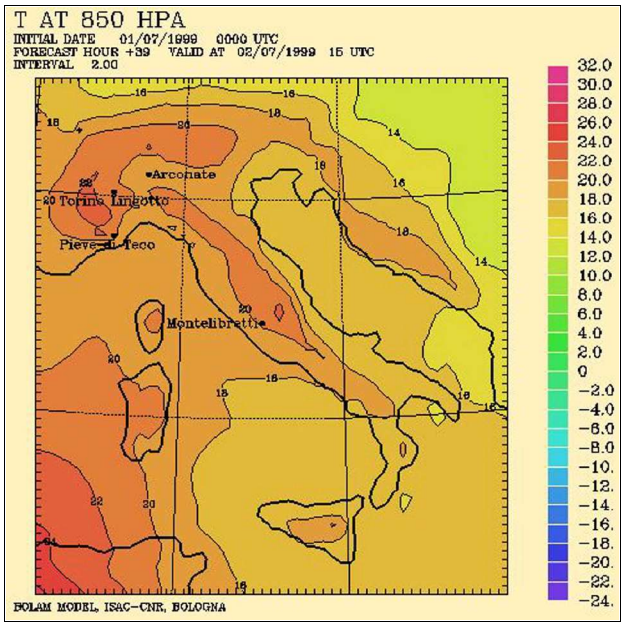

Figure 2: BOLCHEM simulated 850 hPa level temperature field at 2nd July, 15 UTC. Ground based stations locations are shown.

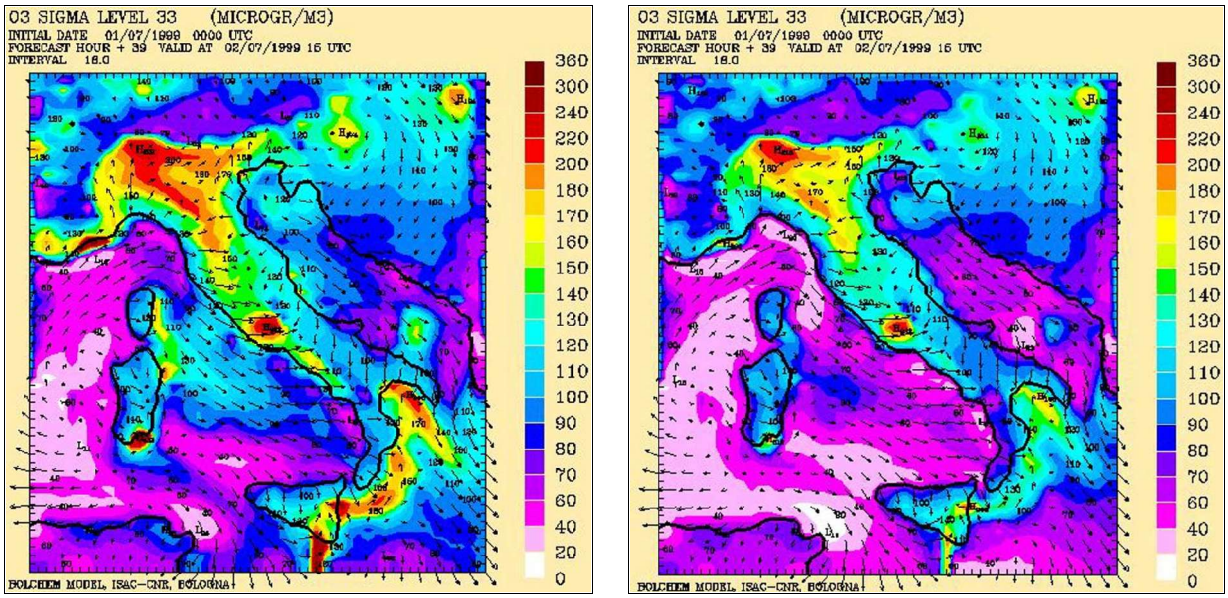

Figure 3: Predicted 20m ozone concentration fields ($\mu g/m^3$) at 2nd July, 15 UTC for SAPRC-90 (left) and CB-IV (right).

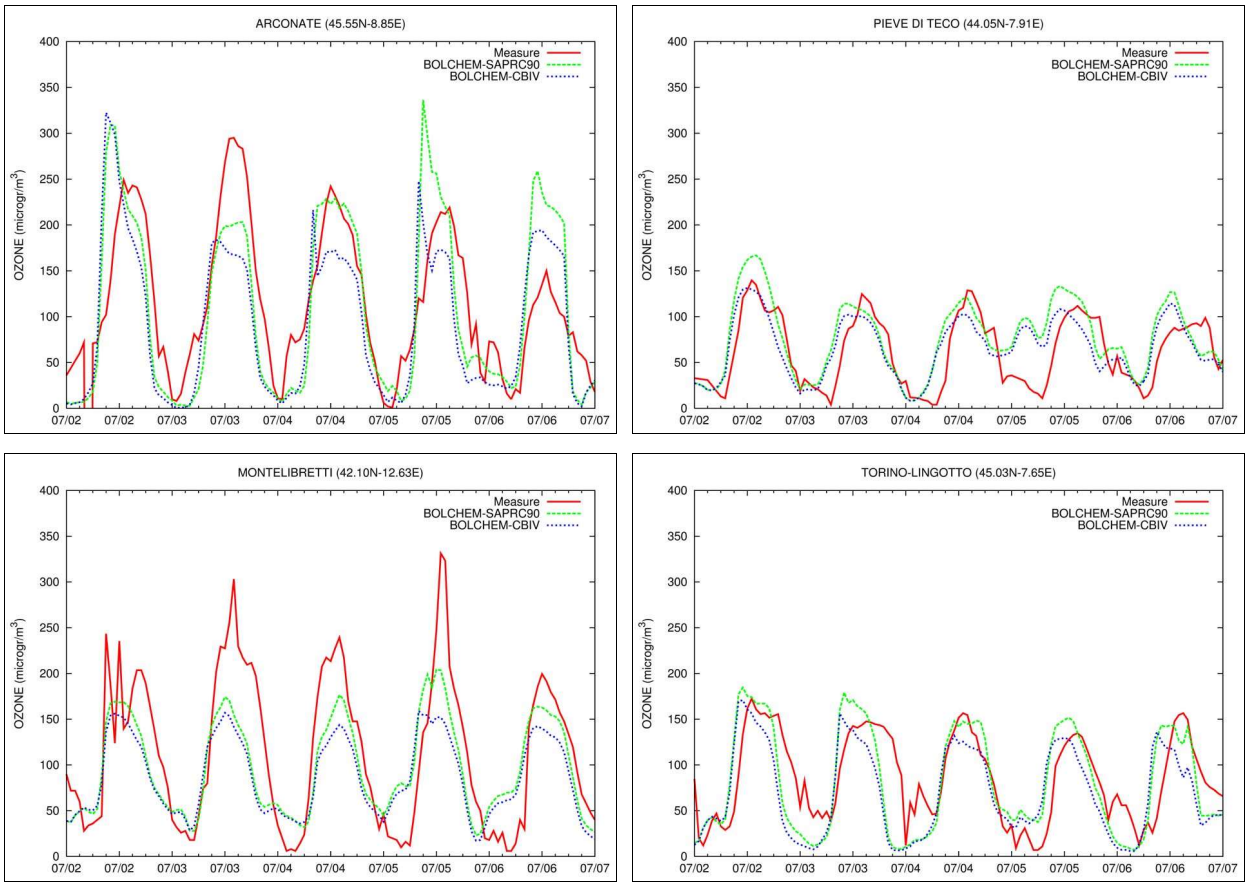

Figure 4: Time series. BOLCHEM computed (SAPRC90, green curves; CBIV, blue curves) and observed concentrations (red curves) over four selected Italian locations. Units in $\mu g/m^3$.