Model Simulations of the Ozone Concentrations over Europe during the Summer 2003 Heat Wave

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1 Summary

An intercomparison between meteorological drivers and chemical mechanisms is performed on some days of the Heat Wave event of 2002. The models used are BOLCHEM and CHIMERE, and their results are compared with ground-based concentrations. Both the models reproduce the pollution event. However, different chemical mechanisms and parameterisations produce larger differences on the chemical concentrations than variations due to meteorological fields.

2 Introduction

The investigation of air quality and forecasting of atmospheric pollution events require modelling of the spatial distribution and time evolution of the atmospheric minor components in various meteorological conditions. The atmospheric concentration of gases and aerosols result from the combined effects of emissions, transformations (chemical mechanisms), transport and removal.

Following other works in the literature restricted to simple cases (e.g. Jimenez et al. 2003 [5]), the present study shows the effect of the uncertainties in representing the meteorology and the air chemistry on pollutant concentrations at the regional scale.

Ozone concentrations were simulated with two models BOLCHEM (D'Isidoro et al. 2005, [4]) and CHIMERE (Vautard et al. 2001, [7]) for some days of the Heat Wave Event of the Summer 2003 over Europe, from 30 July to 3 August. These five days are representative of the beginning of a particularly intense episode of photochemical pollution over Northern Europe.

The work presents the effect of different meteorological drivers and chemical mechanisms on the resulting chemical concentrations computed with BOLCHEM and CHIMERE. Models results were evaluated against ground-based observations.

The simulations were performed using the same emissions, and initial and boundary conditions for the chemical species. Table 1 briefly summarises the main characteristics of the models used: chemical mechanisms, meteorological drivers, chemical concentration fields and emissions. The comparison aims at investigating the O_3 concentrations reproduced with:

- CHIMERE driven by different meteorological fields, which are modelled by meteorological models MM5 and BOLAM;
- CHIMERE and BOLCHEM, characterised by two different chemical mechanisms (MELCHIOR2 in CHIMERE, and SAPRC90 in BOLCHEM), but driven by the same meteorological fields (BOLAM).

3 Results

3.1 Horizontal O_3 Concentration Maps

The O_3 concentrations resulting for the cases described in section 2 are plotted in Figure 1. The O_3 concentration fields correspond to 3 August 2003 at 1500 UTC, for the layer closest to the surface. The O_3 fields produced by CHIMERE-MM5 and CHIMERE- BOLAM, shown in Figure 1, exhibit similar patterns, with maximum and minimum values located at about the same areas (e.g. Paris, the Ruhr basin, the coastal region from Marseilles to Genoa) and they are consistent in value. However, at some sites, CHIMERE-MM5 and CHIMERE-BOLAM predict different O_3 concentrations, due to the meteorological fields applied (e.g. BOLAM temperature at 2m height is generally higher during the night and lower during the day than MM5 one, as it can also be seeing in Figure 2). The meteorological fields differ because models contain different representations of local dynamical effects and orography.

By looking at the concentrations produced by BOLCHEM and CHIMERE, both driven meteorologically by BOLAM, it appears that BOLCHEM generally predicts higher maxima and lower minima in the ozone field than CHIMERE. Furthermore, the latter also produces smoother spatial distributions. The overall patterns are similar, though differences in O_3 values and locations are more pronounced than between CHIMERE-MM5 and CHIMERE-BOLAM.

Since CHIMERE and BOLCHEM use the same meteorological fields, variations in the O_3 values are likely due to the different chemical mechanisms and parameterisations adopted (e.g. dry-deposition mechanism has a different formulation in BOLCHEM and CHIMERE, and this explains different O_3 patterns such as those seen over sea).

3.2 Model Results and Ground-Based Measurements at Selected Sites

Models results were also compared with ground-based observations. The data used were taken from the European Air Quality DataBase (AirBase) at six locations: Paris, Frankfurt, Marseilles, Milan, Bologna, Rome. Sites were selected by considering the regions for maxima and minima in the O_3 concentrations or where distributions completely differ (see black dots in the O_3 maps, Figure 1, which give an idea of some the areas described). For each site all the stations within a radius of about 0.5 degree (about the models resolution) were selected, and data were grouped into two main classes: urban (URBAN), and other (OTHER).

Figure 2 shows O_3 timeseries and the difference in models temperature at 2 m height ($T_{BO} - T_{MM5}$) for the chosen locations. As a general view, after the first two-three days of simulation (characteristic spin-up period), the models reproduce the pollution episode both in O_3 trends and values.

Compared to MM5, BOLAM temperature at 2m height is generally higher during the night and lower during the day, and differences can reach values even of ≈ 5 K. Anyhow, the O_3 concentrations produced by CHIMERE-MM5 and CHIMERE-BOLAM differ less than those obtained from CHIMERE and BOLCHEM driven by BOLAM.

The model CHIMERE, after the spin-up period, seem to follow data better than BOLCHEM. However, differences in the modelled O_3 timeseries are comparable with the variance of the observations.

4 Conclusions

This study shows that both CHIMERE and BOLCHEM reproduce the photochemical pollution event, with predicted O_3 concentrations in fair agreement with the ground-based observations.

The O_3 concentration maps and timeseries show that different chemical mechanisms and parameterisations used in models produce differences that are generally larger than the variations due to different meteorological fields applied to the same model.

This intercomparison suggests that further investigations need to be carried out to better quantify the impact of different parameterisations of the dry deposition velocity, initial chemical fields, and the orography representations on the reproduced chemical concentrations fields.

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Characteristics	CHIMERE (V200301G) http://euler.lmd.polytechnique.fr/chimere/	BOLCHEM [4],[2],[1]
Chemical Mechanism	Melchior2 (gas-phase) [6]	SAPRC90 [3]
Number of Reactions	120	131
Number of Species	44	35
Dry Deposition	Weseley 1989 [8]	D'Isidoro et al. 2005 [4]
Photolysis Rates	Tabulated values www.acd.ucar.edu	Tabulated values [3]
Resolution	$0.5^o \times 0.5^o$ deg	$0.5^o \times 0.5^o$ deg
Meteo	MM5/BOLAM ($0.4^o \times 0.4^o$)	BOLAM ($0.5^o \times 0.5^o$)
Chemical IC/BC	MOZART2 ($\approx 2^o \times 2^o$)	MOZART2 ($\approx 2^o \times 2^o$)
Emissions	EMEP ($0.5^o \times 0.5^o$)	EMEP ($0.5^o \times 0.5^o$)

Table 1: Main characteristics of the models, meteorological and chemical inputs, and emissions used for the simulations

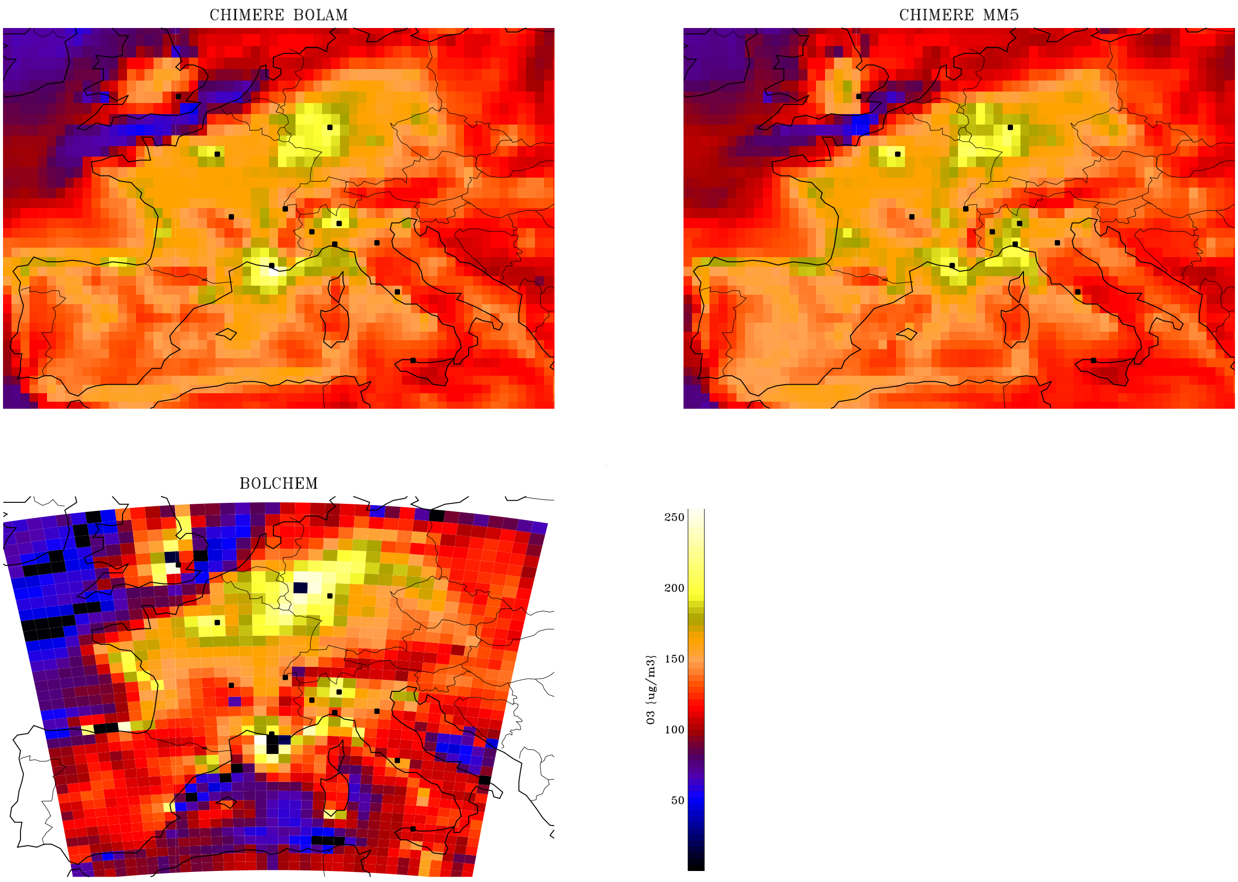

Figure 1: The O_3 distributions in the atmospheric layer closer to the surface for CHIMERE-BOLAM (top left), CHIMERE-MM5 (top right), and BOLCHEM (bottom left).

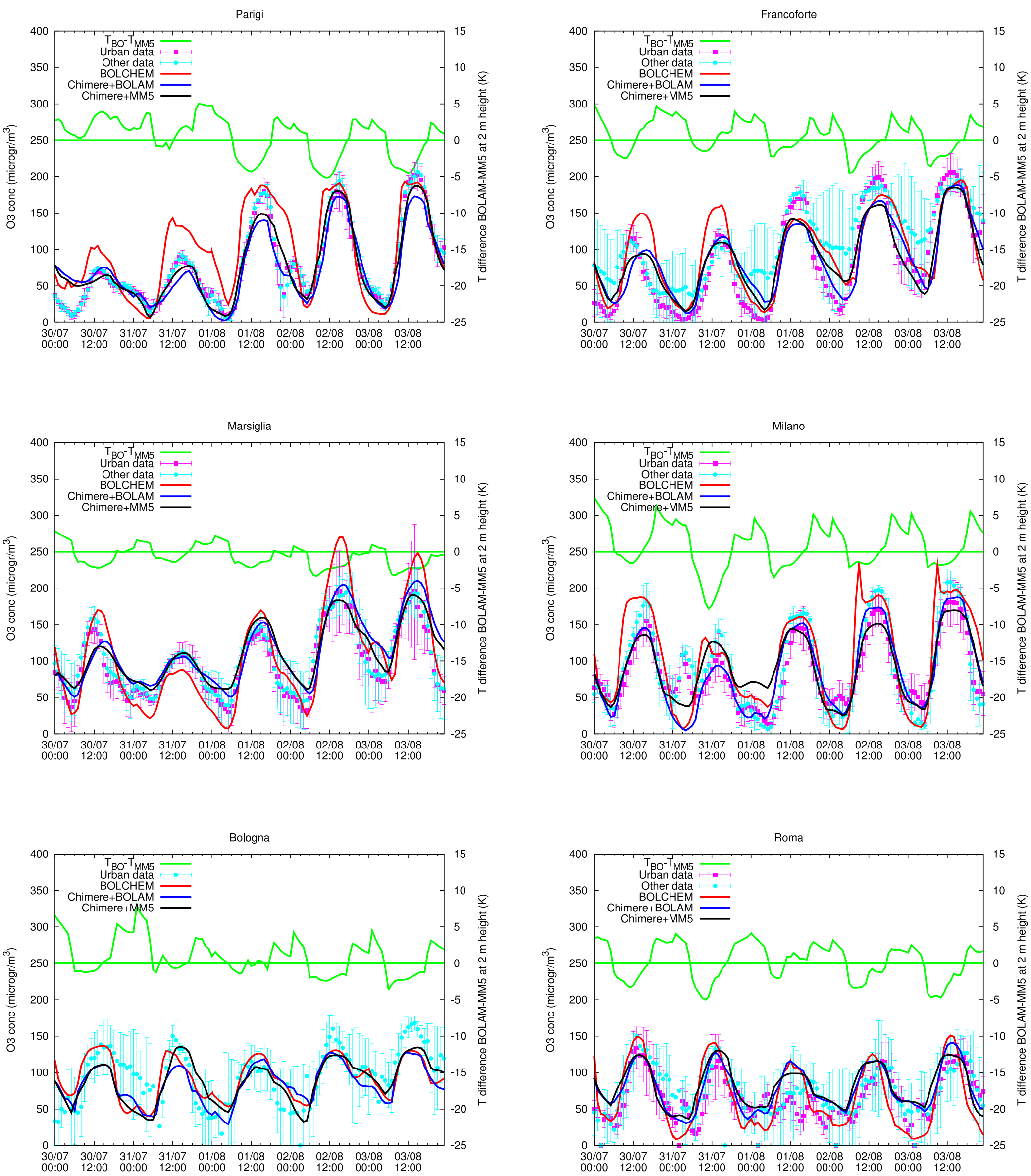

Figure 2: O_3 timeseries and the difference in models temperature at 2 m height ($T_{BO} - T_{MM5}$) plotted for six locations: Paris, Frankfurt, Marseilles, Milan, Bologna, Rome