

## H14-79

### PERFORMANCE EVALUATION OF WRF-MNEQA-CMAQ AND WRF-MNEQA-CHEM AIR QUALITY MODELLING SYSTEMS IN NORTH-EASTERN SPAIN

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**Abstract:** Using data from a case study performed during summer 2009 in the north-east of Spain, the WRF/Chem and WRF-CMAQ models were statistically evaluated and compared, focusing on ozone concentrations. It is shown that the WRF-CMAQ model provides a better forecast of O<sub>3</sub> than WRF/Chem, although both models underestimate ozone concentrations. The major under-prediction of the WRF/Chem could be due to the direct effects of particulate matter on net short-wave radiation and semi-direct effects on air temperature and NO<sub>2</sub> photolysis rate.

**Key words:** Mesoscale models; Air quality simulations

#### 1. INTRODUCTION

The three-dimensional air quality models developed over the last 15-20 years consisted of a meteorological driver, an emissions module and a chemical transport model with the chemistry off-line solved. However, in the last few years, new generations of air quality models have been developed with the chemistry on-line solved with the meteorology because the simulation and prediction of air quality involves both meteorological factor and chemical processes. In the real atmosphere chemical and physical processes are coupled, as several factors such as wind speed and direction, turbulence, radiation, clouds, and precipitation interact with chemical processes such as deposition, and transformations. The chemistry can affect the meteorology, for example, through its effect on the radiation budget, as well as the interaction of aerosols with cloud condensation nuclei. Likewise, clouds and precipitation strongly influence chemical transformation and removal processes, and localized changes in the wind or turbulence fields continuously affect the chemical transport (Grell et al., 2005).

In this contribution we present results from one case study using two different air quality modelling systems. The first system is an off-line matured modelling system based on the Weather Research and Forecasting (WRF) (Skamarock et al., 2005), using the mass coordinate version of the model, called Advanced Research Weather (ARW), coupled to the Community Model for Air Quality (CMAQ) (Byun and Ching, 1999). WRF is a mesoscale non-hydrostatic meteorological model, and the dispersion and chemical transport model CMAQ is one of the most up-to-date air quality dispersion chemical models. The second system is an on-line (one code, one system) tool to simulate air concentrations based on the WRF meteorological driver. In WRF/Chem the chemistry transport and transformations are embedded into WRF as part of the code (Grell et al., 2005), so the interactions between many meteorological variables and the chemistry properties can be explored and analyzed. The same emission model, MNEQA (Numerical Emission Model for Air Quality) (Ortega et al., 2009), was used in both models to test the performance of both modelling systems in forecasting high ozone concentrations that occurred during a case study corresponding to summer 2009 in north-eastern Spain (Catalonia). Comparison of WRF/CMAQ with observations as well as with WRF/Chem for the former pollutant provides the basis of our model evaluation.

#### 2. MODELLING APPROACH

Meteorological numerical simulations were performed using the WRF-ARW version 3.1.1. The model was configured with three nested domains that have grids of 27, 9 and 3 km (Fig. 1), with a two-way interface with the smallest grid. The innermost domain, D1, covers 69x45 grid cells; D2, 70x70 cells; and D3, the inner domain corresponding to Catalonia (NE Spain) covers 94x94 grid cells. The vertical grid is common to all the domains, with 31 vertical levels and a resolution of 15 m close to the surface, decreasing gradually with height, thus enabling low-level flow details to be captured; the top of the domain was at 100 hPa. Initial and boundary conditions were taken from the European Centre for Medium Range Weather Forecasts (ECMWF) with a 1.5°X1.5° resolution every 6 hours, and so boundary conditions could be updated at this time interval.

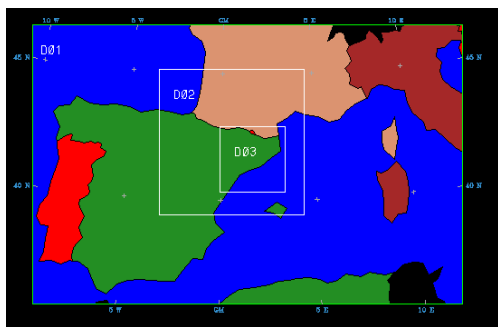


Figure 1. Model domains for WRF-Chem, MNEQA and CMAQ.

The major physics options used in WRF/Chem include the Goddard shortwave radiation scheme, the Rapid Radiative Transfer Model (RRTM) longwave radiation scheme (Mlawer et al., 1997), the Fast-J photolysis rate scheme (Wild et al., 2000), the Yonsei University (YSU) PBL scheme (Hong et al., 2006), the (NOAH) land-surface module (Chen and Dudhia, 2001; Ek et al., 2003), the modified Purdue Lin microphysics module of Lin et al. (1983) and Chen and Sun (2002), and the Grell-Devenyi cumulus parameterization (Grell and Devenyi, 2002). The gas-phase chemistry is based on the Carbon-Bond Mechanism version Z (CBM-Z, Zaveri and Peters, 1999). The aerosol module is the Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) (Zaveri et al., 2008).

The particle size distribution is simulated in MOSAIC for eight size bins between 0.0390625 and 10 mm with six bins for PM<sub>2.5</sub> and two bins for PM<sub>10-2.5</sub>. The bulk aqueous-phase chemistry of Fahey and Pandis (2001) is used. The direct effect of aerosols on shortwave radiation is simulated based on Mie theory following the approach of Fast et al. (2006). The indirect effect of aerosols on cloud formation is accounted for through the effects of clouds on shortwave radiation. More detailed

chemistry, aerosol, and cloud treatments can be found in Fast et al. (2006), Gustafson et al. (2007), and Chapman et al. (2009).

The photochemical model, CMAQ, is the U.S. Environmental Protection Agency (EPA) model-3/CMAQ, which undergoes continuous development. The CMAQ v4.6 use the CB-05 chemical mechanism and the associated EBI solver (Yarwood et al., 2005), including the gas-phase reactions involving N<sub>2</sub>O<sub>5</sub> and H<sub>2</sub>O, and it removes obsolete mechanism combinations (e.g. gas+aerosols w/o). In addition to these changes, version 4.6 includes modifications in the aerosol module (AERO4).

MNEQA is an emissions model developed by our group (Ortega et al., 2009). It includes emissions from both natural sources (particles from dust or hydrocarbons emitted by vegetation based on the description of Guenther et al., (1993)) and anthropogenic sources (mainly traffic and industry). As nested domains are commonly applied to air quality modelling systems because the constituent meteorological, emission and photochemistry models must deal with grid variability and various domain ranges, the MNEQA methodology differs from one domain to another. For smaller domains such as D3, MNEQA uses a bottom-up methodology to calculate pollutant emissions. This involves working out each type of source in a particular way using local information. For larger domains (D1 and D2), MNEQA uses a top-down methodology, which incorporates pollutant emissions from the European annual inventory EMEP/CORINAIR into the model. The disaggregation method in MNEQA model is based on the soil uses CLC2000 (*Corine Land Class 2000*) with 250 m resolution, coupled with different statistical functions, including socio-economic variables.

Further information about the physical configuration of WRF-CMAQ and WRF-Chem is provided in Table 1. The model is executed with 24h as spin-up.

Table 5. WRF-CMAQ and WRF-Chem model configuration

Physical and chemical options	Off – line modelling system	On – line modelling system
Cumulus	Grell 3D (Grell and Debenyi, 2002)	Grell 3D
PBL Scheme	Yonsei University (Hong et al., 2006)	Yonsei University
Cloud Microphysics	Lin (Chen and Sun, 2002)	Lin
Radiation Scheme	RRTM lw (Mlawer et al., 1997) & Goddard sw (Chou, M.-D. and Suarez, M.J., 2001)	RRTM lw & Goddard sw
Surface Layer Scheme	MM5 similarity (Skamarock et al., 2005)	MM5 similarity
Land Surface Scheme	Noah LSM (Chen and Dudhia, 2001)	Noah LSM
Anthropogenic Emissions	MNEQAv4.0 (Ortega et al., 2009)	MNEQAv4.0
Biogenic Emissions	Guenther parameterizations, (Guenther et al., 1994) in MNEQAv4.0 (Ortega et al., 2009)	Guenther option in WRF\Chem (Grell et al., 2005)
Dust Emissions	Dust emissions in MNEQAv4.0 as parameterizations described in Marticorena and Bergametti (1995) and Vautard et al. (2005).	MOSAIC dust emissions option in WRF \ Chem (Zaveri et al., 2008)
Sea-salt emissions	Sea-salt emissions in CMAQ calculated as a function of wind speed and relative humidity	MOSAIC sea-salt emissions option in WRF \ Chem
Gas-phase mechanism	CB05 (Yarwood et al., 2005)	CBMZ (Fast et al., 2006)
Aerosol module	AERO4 (Shankar et al., 2005)	MOSAIC8 (Zaveri et al., 2008)
Photolysis scheme	Photolysis rates from JPROC and PHOT modules in CMAQ model (Byun and Ching, 1999)	Fast-J photolysis (Wild et al., 2000)
Nesting	2-way (WRF) and 1-way (CMAQ)	2-way

### 3. AREA CHARACTERISTICS, DATA USED AND EPISODE SELECTION.

The area of study was Catalonia in North-east Spain, bounded by the Pyrenees to the North and by the Mediterranean Sea to the South and East. Catalonia is a Mediterranean area with complex topography; from a topographic point of view, it can be divided into three areas. One area runs more or less parallel to the coastline and includes the coastal plain, the coastal mountain range and the pre-coastal depression. The second area is a central depression; and the third area includes the Pyrenean foothills and the Pyrenees Mountains proper. The main industrial areas and most of the population are distributed along the coast. In summer, there are high ozone concentration episodes inland, sometimes in rural areas, due to the advection of pollutants by the sea breeze, which carries them from the coast to the rural territory inland.

The air quality evaluation, which focused on ozone concentrations, was performed using hourly measurements of ozone concentration reported by 40 air quality surface stations named XVPCA (*Xarxa de Vigilància i Previsió de la Contaminació Atmosfèrica*) belonging to the regional Catalan Environmental Agency, which covers the entire area with an accurate territorial distribution.

A case study from summer 2009 was selected for the simulation, as it represents typical summer weather conditions. These are characterized by anticyclonic situations, with slight pressure gradients favouring the development of mesoscale circulations such as the sea breeze. This thermally induced circulation transports pollutants to areas well away from their source, resulting in poor air quality and an increase in potential health problems.

#### 4. MODELS EVALUATION

The WRF model with the same configuration presented in this study was evaluated during two periods in summer 2009 (Arasa et al., 2011) using available observational data following the evaluation protocol recommended by EPA (2005) and Denby (2010). Results showed that the YSU scheme with Noah LSM as land surface scheme produces the best results, mainly for wind speed, humidity and temperature, therefore this justifies the use of this configuration. We analyzed the performance of both models focusing on hourly, maximum 1-h and 8-h average ozone concentrations. Results of the evaluation are presented in Table 2. They show that the performance for WRF/Chem (On-line) is worse than WRF-CMAQ (off-line), although both models underestimate ozone concentrations.

Table 2. Summary statistics corresponding to air quality stations associated with air quality simulations of ozone concentration for the case studied with  $30\mu\text{g m}^{-3}$  as a cut-off value.

Statistic	Hourly (Off-line)	Hourly (On-line)	1-h Maximum (Off-line)	1-h Maximum (On-line)	8-h Maximum (Off-line)	8-h Maximum (On-line)
MB ( $\mu\text{g m}^{-3}$ )	-10.57	-18.73	-10.77	-21.59	-11.23	-17.82
MAGE ( $\mu\text{g m}^{-3}$ )	20.34	22.28	14.98	23.25	14.55	19.73
MNBE (%)	-9.14	-22.59	-8.22	-18.05	-10.07	-16.07
MNGE (%)	30.68	30.59	13.17	20.16	14.88	19.72
RMSE ( $\mu\text{g m}^{-3}$ )	24.13	27.20	19.90	28.82	17.87	24.56
IOA	0.818	0.782	0.866	0.732	0.916	0.858

Spatial distribution of some discrete statistics as mean bias (MB) and root mean square error (RMSE) from the hourly ozone concentrations forecasted by WRF-CMAQ and WRF/Chem models are presented in Figure 2.

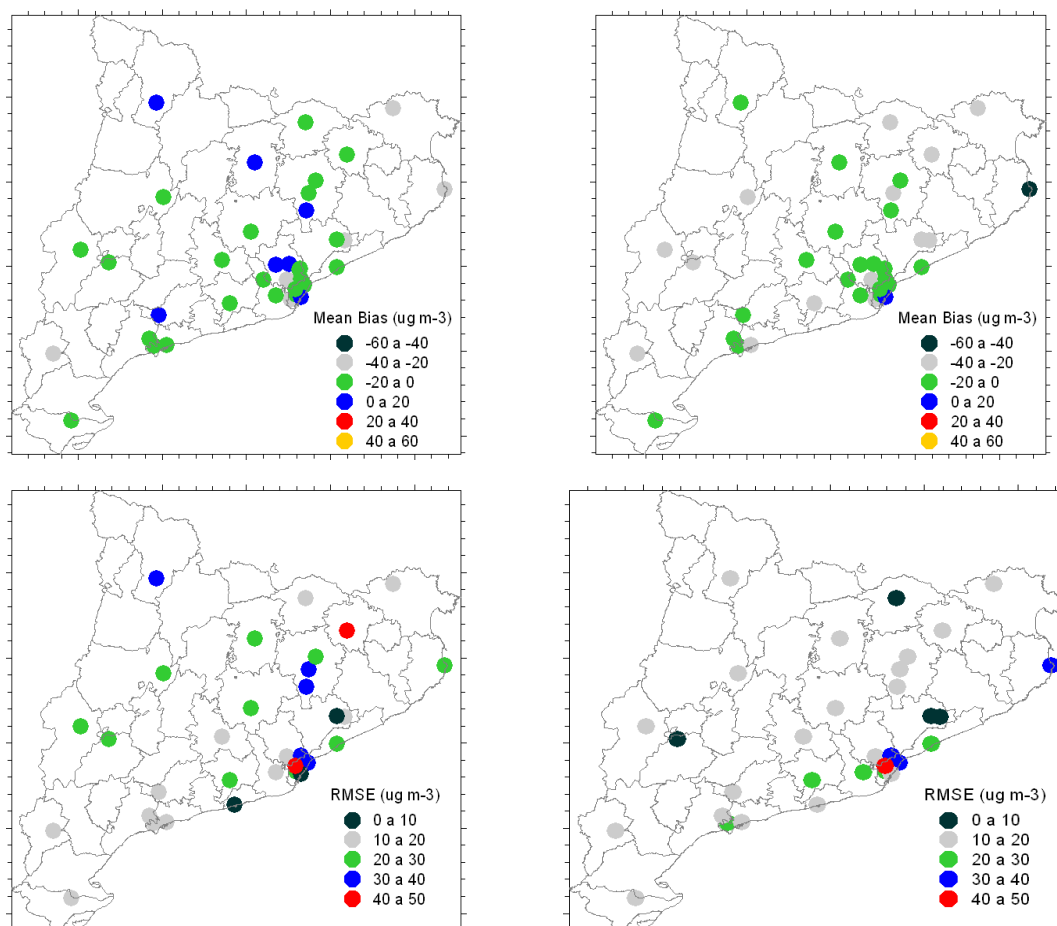


Figure 2. MB and RMSE for WRF-CMAQ (left panels) and WRF/Chem (right panels) models comparing hourly ozone concentrations with the air quality stations network for the case studied.

For WRF/Chem model there is hardly any spatial dependence for the mean bias, as all the values range between 0 to  $-20\mu\text{g m}^{-3}$  and between  $-20$  and  $-40\mu\text{g m}^{-3}$ , whilst for WRF-CMAQ the mean bias values range between 0 to  $-20\mu\text{g m}^{-3}$  and 0 to  $20\mu\text{g m}^{-3}$ , indicating that there are some areas where the model overestimates ozone concentrations. Results for RMSE values

indicate a wide range of values from 10 to 50  $\mu\text{g m}^{-3}$ , although for WRF-CMAQ all values lie between 10 and 30  $\mu\text{g m}^{-3}$  and therefore the results are slightly better.

The major under-prediction of the WRF/Chem could be due to the direct effects of particulate matter on net short wave radiation and semi-direct effects on air temperature and  $\text{NO}_2$  photolysis rate. Differences in short-wave flux at the surface forecasted by the two models (WRF/Chem – WRF) are negative in all parts of the area, with values ranging from -2 to -16  $\text{W m}^{-2}$ . The greatest differences are observed near the coast and the mountain areas, mainly in the Pyrenees. This result indicates that the effect of the aerosol concentration provided by WRF/Chem is higher in these areas, probably due to greater dust and sea salt emission, as it depends on the wind velocity, which is higher in these areas. Related to near surface temperature, results are similar to those found previously, as aerosols affect radiation and temperature. First they can reduce incoming solar radiation via backscattering, therefore increasing the surface albedo and decreasing surface/ near surface temperatures. This cooling effect (from 0.1 to 0.5°C) would be more evident where surface shortwave radiation fluxes have been reduced. However, the relative reductions in air surface temperature are less than those in solar radiation, because near-surface temperatures are also affected by other factors such as soil moisture and soil temperature. Aerosol decreases latent heat flux and soil temperatures, which increases soil moisture and water vapour, and thus near surface temperature. Such an increase compensates for some decreases in near surface temperature, leading to less net decreases in near surface temperature (Zhang et al., 2010).

## 5. CONCLUSIONS

This study compares two models: WRF/Chem (on-line) and WRF-CMAQ (off-line), focusing on ground-level ozone ( $\text{O}_3$ ) predictions. Results of the evaluation show that the performance for WRF/Chem is worse than WRF-CMAQ, although both models underestimate ozone concentrations.

The major under-prediction of the WRF/Chem could be due to the direct effects of particulate matter on net short-wave radiation and semi-direct effects on air temperature and  $\text{NO}_2$  photolysis rate. The greatest differences are observed near the coast and the mountain areas, mainly in the Pyrenees, probably due to greater dust and sea salt emission as it depends on the wind velocity, which is higher in these areas. Related to air surface temperature, results are similar, as aerosols affect radiation and temperature. The cooling effect would be more evident where surface shortwave radiation fluxes have been reduced. However the relative reductions in air surface temperature are less than those in solar radiation, because near-surface temperatures are also affected by other factors such as soil moisture and soil temperature. This study is an initial attempt to analyze the complex feedback mechanisms between chemistry and meteorology, and future research is needed in order to achieve conclusive results.

## ACKNOWLEDGMENTS

This research was supported by the Spanish Government through the project CICYT CGL 2009-12797-C03-02. The authors gratefully acknowledge the assistance of technicians at the Catalan Environmental Agency for providing information regarding the emissions inventory and air-quality measurements.

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