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NUMERICAL EXPERIMENTS TO DETERMINE MM5/WRF-CMAQ SENSITIVITY TO VARIOUS PBL AND LAND SURFACE SCHEMES: APPLICATION TO SUMMER 2009 HIGH-OZONE EPISODE IN NORTH-EASTERN SPAIN

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Abstract: The sensitivity of WRF/CMAQ modelling to the various planetary boundary layer (PBL) schemes and land surface models (LSM) is assessed and quantified by comparing model outputs against MM5 outputs and observations. Data comes from 35 and 51 meteorological and air-quality monitoring networks within the North-eastern Spain. The meteorological variables evaluated included surface 1.5-m temperature, 10-m wind speed and direction and 2-m mixing ratio, while the CMAQ species evaluation focuses on ozone concentrations. Results show several differences across the meteorological simulations which affect CMAQ performance.

Key words: Model sensitivity; Planetary boundary layer; Air quality simulations

1. INTRODUCTION

In recent decades, the 5th generation Mesoscale Model (MM5) (Grell *et al.*, 1994) has been one of the most popular models used to provide the meteorological data required for photochemical models such as CMAQ (Byung and Ching, 1999). For the periods May-October 2008 and 2009, the air-quality system composed of MM5, CMAQ and the emission model MNEQA (Numerical Emission Model for Air Quality) (Ortega *et al.*, 2009) has been applied to the North-eastern part of Spain (Catalonia) to forecast ozone concentrations. Their performance has been evaluated demonstrating the ability of the modelling system to forecast ozone concentrations with sufficient accuracy as the statistics fell within the EPA and European recommended performance goals. However, releases of new versions of MM5 by the community have ceased since the Weather Research and Forecasting model (WRF) (Skamarock *et al.*, 2008) has taken its place. Both models have a modular design which allows users to choose several options for the physics involved. However, WRF presents accurate numerical and high-quality mass conservation characteristics, as well as accurate parameterizations to represent physical processes. Several physical schemes are available in WRF for boundary layer turbulence and surface processes which play an important role in the simulation of lower atmospheric winds, temperature and mixing layer depth. These characteristics in turn affect the dispersion simulations. In this way, for air-quality assessments, it is important to ensure accurate meteorological inputs from the weather model to obtain precise estimations from the air-quality models, since meteorological errors in the meteorological fields are passed on to the air-quality model (Gilliam *et al.*, 2006). The present study explores the sensitivity of air-quality estimations predicted using the CMAQ model to various planetary boundary layer (PBL) and land surface (LS) schemes in the WRF model. This is achieved by comparing model outputs, which correspond to different turbulence physics, against observations from a meteorological and air-quality monitoring network within the inner model domain.

2. MODELLING APPROACH

2.1 Modelling components

Meteorological numerical simulations were performed using the WRF-ARW version 3.1.1 and the PSU/NCAR mesoscale model, MM5, version 3.7. Both models were 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 gently 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 updated every six hours with information obtained from the European Centre for Medium-Range Weather Forecasting (ECMWF) model with a 1.5ºx1.5º resolution.

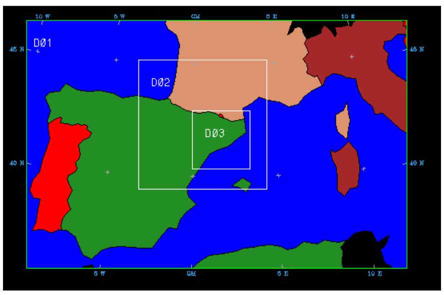

Figure 1. Model domains for MM5, WRF, MNEQA and CMAQ

The photochemical model used in this study to simulate pollutant dispersion is the U.S. Environmental Protection Agency (EPA) model-3/CMAQ model (Byung and Ching, 1999). This model, supported by the U.S. EPA, undergoes continuous development. The CMAQ v4.6 simulations use the CB-05 chemical mechanism and associated EBI solver (Yarwood *et al.*, 2005), including the gas-phase reactions involving N_2O_5 and H_2O, 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. It includes emissions from both natural sources (particles from dust or hydrocarbons emitted by vegetation) 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 basis of the disaggregation method is the soil uses CLC2000 (*Corine Land Class 2000*) with 250 m resolution, coupled with different statistical functions, including socio-economic variables.
In order to explore the sensitivity to the PBL and LS schemes of the WRF model, six sets of experiments were performed. The first compared solutions using the MM5 standard configuration (Table 1), while experiments 2 to 6 compared solutions using different PBL and LS schemes but the same parameterizations for cumulus, microphysics and radiation (Table 2). Although it was intended to isolate the PBL scheme as the sole cause of the model sensitivity, as each of the five PBL schemes required a specific LS model (LSM), model sensitivity was due to the PBL and its associated LSM. Henceforth, this combination will be represented only by the PBL scheme.

Table 1. Physical options for experiment number 1.

PHYSICAL OPTIONS	**MM5**	**WRF-1**
Cumulus parameterizations	Grell	Grell 3D
PBL Scheme	MRF	YSU
Microphysic Scheme	Schultz	Lin
Radiation Scheme	RRTM lw & Cloud-radiation sw	RRTM lw & RRTMG sw
Surface scheme	Noah LSM	Noah LSM

Table 2. Physical options for experiments 2 to 5

WRF	**PBL SCHEME**	**LS SCHEME**
WRF-2	Mellor-Yamada-Janjic (MYJ)	Eta similarity
WRF-3	Asymmetrical Convective Model version 2 (ACM2)	Pleim Xiu surface layer
WRF-4	Quasi-Normal Scale Elimination (QNSE)	QNSE surface layer
WRF-5	Mellor-Yamada Nakanishi and Niino Level 2.5 (MYNN 2.5)	MYNN surface layer

The outputs from the MM5 and WRF options were processed using MCIP version 3.4 into the format required by the MNEQA and CMAQ models.

2.2 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 different 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 located 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 brings them from the coast to the rural territory inland.
Meteorological modelling results were evaluated from a set of 31 surface meteorological stations belonging to the Catalonia Meteorological Service that are distributed throughout Catalonia. The evaluation included wind velocity and wind direction measured at 10 m above ground level (a.g.l.), air temperature at 1.5 m a.g.l. and air humidity measured at 2 m a.g.l. The air-quality evaluation, which focussed on ozone concentrations, was performed using hourly measurements of ozone concentration reported by 51 air-quality surface stations named XVPCA (Xarxa de Vigilància I Previsió de la Contaminació Atmosfèrica) belonging to the regional Catalan Environmental Agency that covers with an accurate territorial distribution the size of the area.
Two single-day episodes, 27 and 28 July 2009 were selected for the simulation to represent summer weather conditions characterized by an anticyclonic situation with small pressure gradients favouring the development of mesoscale circulations such as the sea breeze. This thermally induced circulation plays an important role as it transports pollutants to areas well away from their source, resulting in poor air quality and increases in potential health problems.

3. RESULTS AND DISCUSSION

3.1 WRF sensitivity to PBL and LS
The sensitivity of the WRF-CMAQ modelling to various PBL and LSM schemes used in the summer period was assessed following the procedure recommended in the *Guidance on the use of models for the European Air Quality Directive* (Denby, 2009) and in the *EPA Draft Guidance on meteorological model evaluation* (EPA, 2009). The basic statistical measures were mean bias (MB), the mean absolute gross error (MAGE), the root-mean-square error (RMSE) and the index of agreement (IOA). Table 3 presents both sets of statistics: those corresponding to MM5 simulation with the configuration indicated in Table 1, and those corresponding to different WRF configurations (Table 2). The statistics were computed hourly and averaged over the 31 surface weather stations.

Table 3. Statistics corresponding to MM5 and WRF model performance evaluation.

Meteorological variable	Statistic	MM5 WRF	WRF-1 YSU	WRF-MYJ	WRF-3 ACM2	WRF-4 QNSE	WRF-5 MYNN2.5
Wind velocity	RMSE (ms$^{-1)}$	1.73	1.60	1.86	1.61	1.84	1.53
	MB (ms^{-1})	0.60	0.53	0.94	0.59	0.97	0.51
	IOA	0.64	0.70	0.66	0.67	0.66	0.73
Wind direction	MAGE(º)	56.43	58.28	57.55	61.58	60.03	57.08
	MB (º)	4.21	5.50	1.03	7.25	3.35	9.52
Temperature	MAGE (K)	2.10	1.88	1.75	1.68	1.83	1.69
	MB (K)	-1.83	-0.77	-0.95	-0.94	-1.13	-0.78
	IOA	0.89	0.90	0.91	0.93	0.91	0.93
Specific humidity	MAGE(g kg^{-1})	1.78	1.58	1.79	1.74	1.74	1.67
	MB (g kg^{-1})	1.24	0.60	0.50	0.84	0.48	0.77
	IOA	0.41	0.46	0.29	0.35	0.31	0.38

For the 10-m wind velocity, the MB value was always positive. This indicates an overestimation of the wind velocity; YSU and MYNN 2.5 schemes yielded the best values of MB, RMSE and IOA, while QNSE yielded the largest MB value. For wind direction, YSU yielded the best BIAS while MYNN 2.5 yielded the largest. The poor statistics found for this variable could be attributed to the complex topography of the simulated area. For air temperature, all 6 simulations resulted in slightly negative biases; the lowest value was for the YSU scheme and the largest one for MRF in the MM5 model. MAGE values were similar: the largest value also corresponded to the MRF scheme in the MM5 model. Finally, for specific humidity, the best MB was for the QNSE scheme, while the MRF scheme in MM5 had the largest value. All simulations resulted in very poor IOA. Although no single scheme or option yielded the best results for all variables, it seems that for temperature and wind velocity the best results corresponded to the YSU and 2.5 schemes. Our results agree with those of Borge *et al.*, (2008) for the Iberian Peninsula.

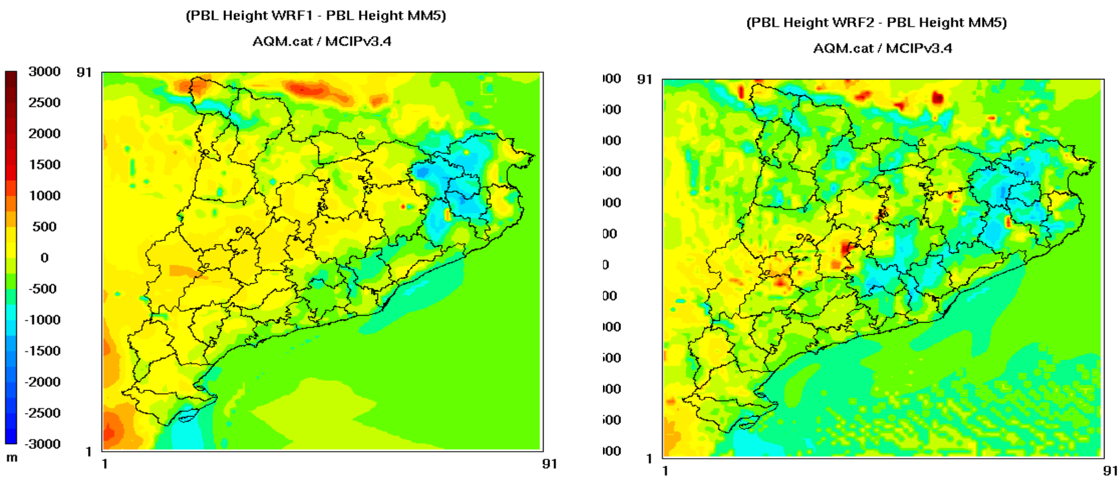

Figure 2. PBL height differences between YSU and MRF (left) and MYJ and MRF (right) on 28 July 2009 at 1400 UTC

The performance of the model options at forecasting PBL height or mixing layer was validated using the simulation of the MM5 model as a benchmark and compared to the other simulations to asses the differences across modelled PBL heights. Figure 2, as an example, shows a map of the PBL height differences between the YSU, MYJ and MRF schemes on 28 July 2009 at 1400 UTC, a typical summer afternoon when PBL was fully developed. The differences of the mixing depth varied over a broad scale. Generally, the MRF scheme produced higher mixing depths over the coastal mountain range and mountain areas, while over flat areas, MRF yielded lower mixing depths than those yielded by WRF options. Similar behaviour was found for the other WRF options.

3.2 CMAQ sensitivity to PBL and LS

In addition to the MB, MAGE, RMSE and IOA used in MM5 and WRF performance evaluation, other statistics such as mean normalized bias error (MNBE), mean fractional bias (MFB), mean normalized gross error (MNGE), normalized mean error (NME), normalized mean bias (NMB), and unpaired peak accuracy (UPA) were introduced in the CMAQ sensitivity analysis. Summaries of domain-wide CMAQ model performance statistics for daily peak 1-h values and daily peak 8-h ozone concentrations are provided in Tables 4 and 5. As the CMAQ sensitivity analysis focussed on ozone concentration, the WRF4 option corresponding to the QNSE scheme designed for very stable conditions is not included.

Table 4. Summary statistics corresponding to air-quality stations associated with air-quality simulations of maximum 1-h ozone concentration for the period studied.

Specie	Statistic	MM5	WRF-1	WRF-2	WRF-3	WRF-5
O_3	MB (µg m^{-3})	7.31	-0.54	-1.52	4.15	1.02
	MNBE (%)	11.46	4.04	2.41	9.27	3.88
	MFB (%)	5.42	-0.30	-0.84	2.99	0.37
	MAGE (µg m^{-3})	31.34	24.99	20.37	30.88	18.01
	MNGE (%)	30.50	23.42	19.64	29.32	18.39
	NME (%)	27.86	22.21	18.11	27.45	16.01
	NMB (%)	6.50	-0.48	-1.35	3.69	0.91
	RMSE (µg m^{-3})	37.07	31.64	25.57	38.86	25.34
	IOA	0.579	0.610	0.735	0.479	0.792
	UPA (%)	4.48	-7.05	-10.38	-0.93	-4.21

Table 5. Summary statistics corresponding to air-quality stations associated with air-quality simulations of 8-h ozone average concentrations for the period studied.

Specie	Statistic	MM5	WRF-1	WRF-2	WRF-3	WRF-5
O_3	MB (µg m^{-3})	1.35	-2.76	-2.29	-3.36	-1.19
	MNBE (%)	5.71	0.26	-0.24	0.06	-0.11
	MFB (%)	1.01	-2.49	-2.48	-3.40	-2.14
	MAGE (µg m^{-3})	24.33	17.37	13.94	19.71	13.61
	MNGE (%)	26.76	18.60	15.32	20.87	15.16
	NME (%)	24.60	17.57	14.09	19.93	13.76
	NMB (%)	1.36	-2.79	-2.31	-3.40	-1.20
	RMSE (µg m^{-3})	28.05	21.19	18.13	24.28	17.23
	IOA	0.795	0.893	0.925	0.860	0.936
	UPA (%)	-4.14	-5.70	-3.60	-9.50	5.77

For these metrics, the US EPA (2005) developed guidelines indicating that it is inappropriate to establish a rigid criterion for model acceptance or rejection (i.e. no pass/fail test). However, building on past ozone modelling applications (US EPA, 1991) a common value range for bias, error and accuracy has been established. The accepted criteria are MNBE, ±5 to ±15%; MNGE, +30 to +35%; UPA ±15 to ±20%.

Following these criteria, Tables 4 and 5 show that CMAQ performance is within the EPA recommended performance. The results also show that CMAQ was fairly consistent across MM5 and WRF options. For 1-h maximum concentrations, MM5 tends to overestimate ozone concentrations, while WRF across the different options tends to slightly overestimate (ACM 2 and MYNN 2.5 options) and to underestimate (YSU and MYJ options). For 8-h ozone average concentrations, MM5 statistics show that the model continues to overestimate ozone concentrations, while WRF across all the options tended to underestimate it. The difference between the maximum and minimum performance statistics shows that there was no single PBL scheme in WRF that resulted in extremely good or poor CMAQ model performance, but focussing on MNGE and IOA statistics, WRF-2 and WRF-5 provided the best results. However, to better understand CMAQ sensitivity, simulated CMAQ concentrations were compared with measurements at the local scale. Figure 3, in particular, shows the time series of simulated and observed hourly ozone concentrations for "La Plana de Vic" on 28 July 2009. In this area, during summer time, ozone concentrations sometime exceed the prescribed limit value (180 µgm^{-3}). The results show that all five CMAQ runs corresponding to MM5 and WRF experiments underestimated the maximum ozone and overestimated the night-time minimums. In fact, CMAQ was positively biased during the night. The mid-layer height of the first CMAQ layer was about 15 m a.g.l., whereas the ozone monitoring sensors' heights were on average below 5 m. Given a large vertical gradient of the near-surface O_3 concentration after sunset (Zhang and Rao, 1999; Mao *et al.*, 2006), i.e., O_3 decreasing sharply towards the ground, the simulated O_3 concentrations were much higher than the observations at relatively lower elevations. It should be noted, however, that these results may not completely represent the robust characteristics of the CMAQ performance as the number of O_3 samples above the threshold was very limited during the period.

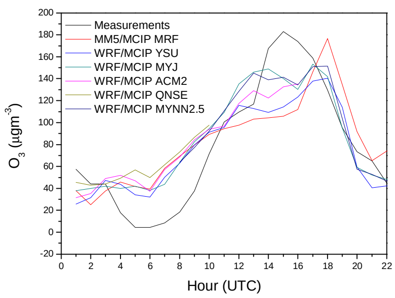

Figure 3. Time series of observed and simulated hourly ozone concentrations at "La Plana de Vic"

4.- CONCLUSIONS

A numerical experiment was conducted over a summer period of 2009 to study air-quality modelling sensitivity to various PBL schemes used in WRF. The YSU, MYJ, ACM2, QNSE and MYNN 2.5 schemes as well as MRF in MM5 were used in the sensitivity experiments. Although it was intended to isolate the PBL scheme as the sole cause of model sensitivity, as each of the five PBL schemes required specific LSM, model sensitivity was due to the PBL and its associated LSM.
The sensitivity of WRF was assessed by comparing surface variables against hourly observations from 31 surface stations within the inner domain. Results from CMAQ were evaluated against hourly measurements averaged from 51 surface monitoring sites. Several basic statistical measures were applied to the sensitivity assessment and evaluation. The results show that although no particular scheme or option yielded the best results for all variables, it seems that for temperature and wind velocity the best results corresponded to the YSU and MYNN 2.5 schemes. For PBL height, there were no measurements to evaluate model simulations, but comparing the MRF scheme in the MM5 model with the WRF options, the first model yielded higher mixing depths over the coastal mountain range and mountain areas, while in flat areas MRF yielded lower mixing depths than the WRF options did.

Assessment and evaluation of CMAQ results indicate that CMAQ is not significantly sensitive to the different PBL options for the domain-wide average for ozone concentrations, however the WRF-2 and WRF-5 options yielded better results than the MM5 model. At a local scale however, differences in ozone concentrations across the CMAQ simulations were considerable. Summary results from this work illustrate that further work simulating a long time period will be necessary in order to infer the relative performance of the models.

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