EVALUATION OF WRF-CHEM SIMULATIONS WITH THE UNIFIED POST PROCESSOR (UPP) AND MODEL EVALUATION TOOLS (MET).

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1. INTRODUCTION

The studies of Air Quality as well as strategies for mitigation of pollution are based largely on numerical models. Therefore it is essential to have tools that systematically evaluate the model performance, including comparison of numerical simulation results against observational data. The Weather Research Forecast (WRF) model is a numerical model widely used for Air Quality studies (Tuccela et al 2012, Tiea et al., 2007), developed at National Oceanic Atmospheric administration (NOAA) (Grell et al., 2005) and later updated (Fast et al., 2006) incorporating chemical transformations and complex gas-phase chemistry, photolysis and aerosols, referred as WRF-chem. Roughly speaking the WRF-chem input must include meteorology, simulation domain, and emissions according with the corresponding chemical module in order to perform simulations. Subsequently, there are several computational packages for viewing and managing the WRF-chem model outputs, ncl (NCAR, 2012), GrADS (GRADS, 2011), netCDF. Also in this respect, the Unified Post Processor, UPP (DTC, 2012) code ingests WRF output files (wrfout_d01_"date") in netCDF format, and interpolates output from model's native grids (netCDF) in another format (GRIB) according to the World Meteorological Organization (WMO) standards, similarly observational data must be processed to conduct further analysis with the recently released Model Evaluation Tool, MET (Gotway et al., 2011). The MET package is able to do performance evaluation in simulations, promotes consistency of results between the users, choice of model configuration, identifying and correcting model flaws, forecast improvement, improved decision making, identify forecast weakness, strengths, differences with observation data (e.g., monitoring stations where the model has the best performance). Fig. 1 shows the overall structure of simulations with WRF-chem and post-processing of data.

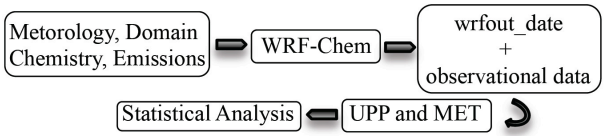

Fig. 1. The WRF-Chem model ingests Meteorology, Chemistry, and Emission data. The WRF output in addition with the observational data is post processed by UPP and MET packages. Finally statistical analysis is done.

The original configuration of UPP can read several fields (eg, U, V, T, Albedo), see chapter 7, table2 (Baldwin et al., 2012). However, as far as we have seen, the chemical species oriented to the study of air quality are not included by default in these fields. Therefore, changes should be made in UPP (and so on in MET) to add new fields to encourage the statistical analysis of air quality modeling.

In this document a detailed description of modifications made in both UPP and MET releases packages is given, this changes must be done in order to incorporate relevant chemical species: nitrogen oxide (NO), nitrogen dioxide (NO2), sulphur dioxide (SO2), carbon oxide (CO), Particle Matter (PM10 and PM2.5), ozone (O3) and meteorological parameters into the verification process. These modifications has been tested in UPPV1.0 and METv3.0.1 releases, under linux86-64 cluster with the corresponding Fortran, C and C++ Portland Group (pgi-9.0) compilers.

Likewise, here we consider an specific episode of high weekend ozone concentration to illustrate the verification process, were MET is used to evaluate agreement between simulated species concentrations and monitoring stations data of the Automatic Atmospheric Monitoring

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System (SIMAT) in Mexico City (http://www.calidadaire.df.gob.mx/).

Finally, the use of UPP and MET considering our modifications allows us to perform a systematic statistical analysis, and then amend the National Emissions Inventory (2004) to adjust as best as possible the simulations against data from SIMAT monitoring stations. This is done by means of the proposed hourly emission coefficients for key species in the ozone production. This work is organized in the following way. Section 2 is devoted to underline the modifications in MET and UPP packages. Section 3 contains a brief description of the model setup including the National Emissions Inventory (NEI) and the Automatic Monitoring Network. Finally, results and remarks are given in section 4.

2. UPP AND MET MODIFICATIONS

In order to include new chemical species in the post-processing procedure is necessary modify and add new lines in UPP and MET packages. The following UPP files suffer modifications: *DEALLOCATE.f, INITPOST.f, MDLFLD.f, MPI_FIRST.f, RQSTLD.f, VRBLS3D_mod.f and wrf_cntrl.parm*. A general guide of changes is shown in Fig. 2, but the specific line codes for each file are available from the authors of this manuscript.

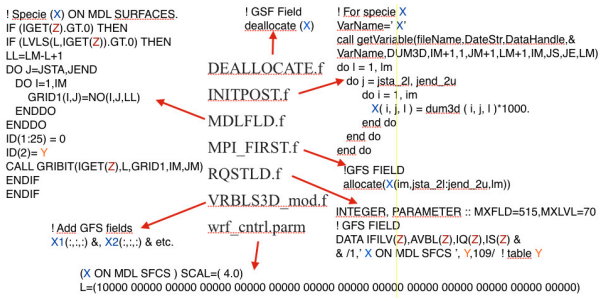

Fig. 2. Main modifications made over several subroutines in UPP code.

Likewise, to run MET, is desired to use unipost.exe to place the data in the format(s) expected by the statistics tools, this executable re-grid observations to match model output. The WRF-Chem considers the ARW core therefore the utility copygb.exe was not used. Point observations may be supplied in PREPBUFR or ASCII format. In our case the SIMAT observational data is supplied in ASCII, for example:

ADPSFC 76225\ 20080101\060000\ 19.455-99.202.\ Y\776.-9999.\ 6.000,

then reformatted by the ascii2nc tool to create an intermediate NetCDF file for point stat evaluation (Point-Stat tool). The output NetCDF file can contain meteorological and chemical variables, the latter are setup in different parameter table versions, see Office Note 388 - Table B in (NCEP, 2012).

3. TEST EPISODE AND MODEL SETUP

To illustrate the scope of the modifications made on UPP and MET, we considered a high weekend ozone episode for the period of April 13 through 14 April 2007 in Mexico City. This episode has been studied previously and corresponds to the so-called “ozone weekend effect” (Stephens et al., 2008, Garcia-Reynoso et al., 2009), this means despite the fact vehicular emissions are reduced during the weekend the ozone concentrations remain the same and even higher than during the weekdays. Atmospheric Science Center, UNAM, compiled the emissions inventory used in this study, based on the official emissions inventory for Mexico City Metropolitan Area (MCMA) in 2004. The emitted VOC's, CO, NOx, were distributed across mobile, area and point sources and transformed into temporally and chemical speciated emissions to include this as input for WRF-chem. Regional Acid Deposition Model, RADM2 (Stockwell et al., 1990) is considered as a chemical module. Emissions were updated to fill in a 3km spatial resolution and simulations were carried out for 40h time period. Also the North American Regional Reanalysis (NARR) data for Meteorological boundary and initial conditions were used (http://www.emc.ncep.noaa.gov/mmb/rreanl). Finally, the observational data required by MET is provided by the MCMA monitoring stations (RAMA).

4. RESULTS

The Point-Stat tool computes several statistics to evaluate the forecast performance in monitoring stations. Fig. 3 provides a comparison of O3 and CO simulated concentrations against observed data from April 13, 2007 at 6:00h to April 14 at 03:00h local time of Mexico City. The simulated O3 concentrations (continuous line with fill squares) in the Cerro de la Estrella (CES) monitoring station slightly fit with the observational data (filled circles) in most of the time domain,

except for the high ozone concentration time interval (from 12-15 hours), where the simulations underestimate the ozone peak (Apr 14 15:00h). During all the time period the CO simulations systematically are underestimated according to the measured CO concentrations at San Agustin (SAG) monitoring station, shown on bottom of Fig. 3. Likewise, CO simulations follow the same measured data pattern, this suggest modifications in the emission inventory, and further work should be done regard this point.

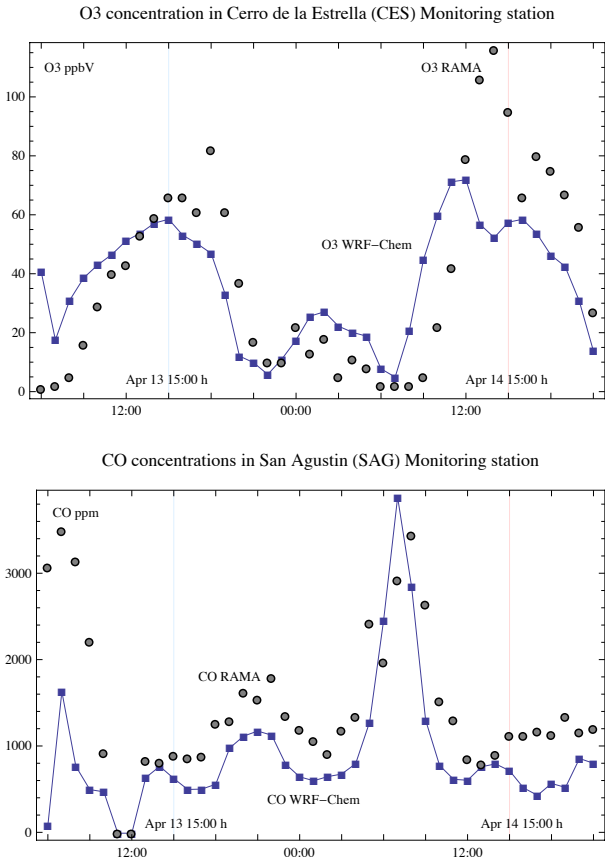

Fig. 3. Ozone and CO concentrations in Cerro de la Estrella and San Agustin monitoring stations are shown above and below respectively, for the period of time from April 13, 2007 at 6:00h to April 14 at 03:00h local time of Mexico City. In both cases the filled circles correspond to the measurements of ozone and carbon oxide concentrations measured in ground-based air quality monitoring network (RAMA) in MCMA and the continuous line (fill square) are the simulations made with WRF-Chem model.

Also, it is possible that MET compute the grid average of fields, Grid-Stat tool provides verification statistics for a matched forecast and observation grid. Grid averages of observations and simulations are shown in Fig. 4, the grid average of simulated variables (continuous line with fill squares) is compared against the average of all RAMA stations (filled circle) for the same episode. On the top of Fig. 4 the average ozone concentration against RAMA data is shown, maximum measured O3 concentration take place at 15:00h Apr 14 and is pretty close to 140 ppbV, this maximum is bigger than the previous one happening around 15:00h Apr 13 (Ozone weekend effect). Numerical simulations underestimate the second ozone peak with a relative error around 42%. This means that at most monitoring stations the ozone concentration is underestimated by the model.

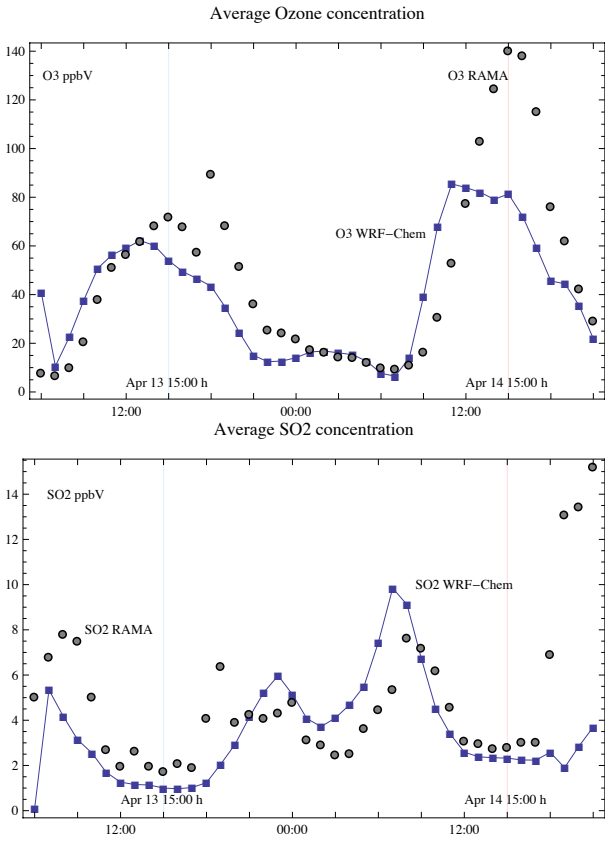

Fig. 4. Simulated and observed averaged fields (O3 and SO2), from April 13, 2007 at 6:00h to April 14 at 03:00h local time of Mexico City. Continuous line represents the average field calculated with WRF-chem model and filled circles the average measured field from the ground-based air quality-monitoring network (RAMA) in MCMA.

At the bottom of figure 4, the grid average SO2 concentration both with model and observations is shown. This chemical specie is well reproduced by the model especially in the first hours of high ozone episode. Additionally in Table 1 examples of several verification measurements for the SO2 are shown. The first parameter on this table

correspond to Accuracy contingency parameter (ACC), in our simulation ACC=0.88328 meaning the fraction of forecast that were correct, ACC ranges from 0 to 1. The other two parameters are the Hanssen-Kuipers Discriminant (HK) and Heidke Skill Score (HSS), they range from -1 to 1 and −1 to 1 respectively. A perfect forecast have HK=1 and HS=1. For a comprehensive description of verification measurements see Appendix C in (Gotway et al., 2011).

ACC	ACC_NCL	ACC_NCU	ACC_BCL
0.88328	0.84326	0.91412	0.84850
HK	HK_NCL	HK_NCU	HK_BCL
0.62474	0.57798	0.67150	0.52034
HSS	HSS_BCL	HSS_BCU	
0.68068	0.58239	0.76499	

Table 1 Statistical analysis results for SO2 evaluation. Accuracy (ACC), Hansen-Kuipers Discriminant (HK) and Heidke Skill Score (HSS) for 662 total observations defined in appendix C of [6].

5. CONCLUDING REMARKS

The modifications made over the UPP and MET files are directed to WRF-chem users and developers interested in Air Quality modeling and forecast. They allow to include O3, CO, NO, PM10 and PM2.5 among other species and parameters, in further statistical analysis. We show that the use of tools as UPP and MET in a systematic way are important to assess the reliability of simulations and now are public available. In some cases the results from the analysis may show differences between measured and modelled values, which may involve further investigation in meteorological parameterizations and emissions inventory characterization. On this regard we are preparing the document to explain the differences in ozone concentrations weekend in Mexico City.

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