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SIMULATIONS WITH MM5-CMAQ AND WRF/CHEM MODELS OF A HIGH ELEVATED PM10 AND PM2.5 EPISODE IN GERMANY DURING WINTER, 2003

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1. INTRODUCTION

Simulations of elevated PM10 and PM2.5 concentrations have been always underestimated by modern three dimensional air quality modelling tools. This fact has focused much more attention between researchers during last years. Three dimensional air quality models have been developed during the last 15-20 years and substantial progress has occurred in this research area. These models are composed by a meteorological driver and a chemical and transport module. Examples of meteorological drivers are: MM5 (PSU.NCAR, USA), (Grell et al., 1994), RSM (NOAA, USA), ECMWF (Redding, U.K.), HIRLAM (Finnish Meteorological Institute, Finland), WRF (Janjic et al., 2001) and examples of dispersion and chemical transport modules are EURAD (University of Cologne, Germany), (Stockwell et. Al. 1977), EUROS (RIVM, The Netherlands), (Lagner J. et al. 1998), EMEP Eulerian (DNMI, Oslo, Norway), MATCH (SMHI, Norrkoping, Sweden), (Derwent R. and Jenkin M., 1991), REM3 (Free University of Berlin, Germany), (Walcek, C. 2000), CHIMERE (ISPL, Paris, France), (Schmidt H. et al., 2001), NILU-CTM (NILU, Kjeller, Norway), (Gardner et al. 1997), LOTOS (TNO, Apeldoorm, The Netherlands), (Roemer M. et al. 1996), DEM (NERI, Roskilde, Denmark), (Gery et al. 1989), OPANA model (San Jose R. et al. 1994, 1996, 1997) based on MEMO and MM5 mesoscale meteorological models and with the chemistry on-line solved by (Jacobson M.Z. and Turco R.P., 1994), STOCHEM (UK Met. Office, Bracknell, U.K.), (Collins et al., 1997) and CMAQ (Community Multiscale Air Quality modelling system) (Byun et al., 1998), developed by EPA (USA). In USA, CAMx Environ Inc., STEM-III (University of Iowa) and CMAQ model are the most up-to-date air quality dispersion chemical models. In this application we have used the CMAQ model (EPA, U.S.) which is one of the most complete models and includes aerosol, cloud and aerosol chemistry.

In this contribution we present results from two simulations by two different models. The first air quality modelling systems is MM5-CMAQ which is a matured modelling systems based on the MM5 mesoscale non-hydrostatic meteorological model and the dispersion and chemical transport module, CMAQ. The second tool is the WRF/CHEM (Janjic et al., 2001) air quality modelling system, which 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 so that the interactions between many meteorological and climate variables and the chemistry if at hand and can be investigated. WRF/CHEM is developed by NOAA/NCAR (US) (Janjic et al., 2001). The advantage of on-line models is based on the capability to analyze all variables simultaneously and to account for all interactions (or at least, as much as possible) with a full modular approach.

2. PM10 AND PM2.5 EPISODE

Your submitted manuscript must be in PDF format. During the period January, 15, 2003 to April, 5, 2003, in central Europe (mainly northern part of Germany), we observe three high peaks on PM10 and PM2.5 values in several monitoring stations located in the area of North-East of Germany. The daily averages of PM10 concentrations were close to 80 μgm^{-3} and higher than 70 μgm^{-3} for PM2.5 concentrations. These values are about 4-5 times higher than those registered as “normal” values. The first

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peak on PM10 and PM2.5 concentrations was developed after Feb. 1 until Feb. 15. During this period of time, Central Europe was under the influence of a high-pressure system coming from Russia through Poland and Southern Scandinavia. In Northern part of Germany, we found south-easterly winds and stable conditions with low winds. These meteorological conditions brought daily PM10 concentrations at about 40 μgm^{-3}. The second peak was characterized by a sharp gradient on PM10 concentrations after Feb. 15 and until March, 7. This episode reached daily PM10 concentrations up to 70 μgm^{-3}. The meteorological conditions on March, 2 (peak values) was characterized by a wind rotation composed by South-westerly winds from Poland over the North of Germany and North-westerly and Western winds in the Central part of Germany. Finally a third peak with values of about 65 μgm^{-3} on March, 27 starts on March, 20 ending on April, 5. 2003 was having a similar structure and causes than the second one. The observational data used to compare with the modelling results is referred in San José et al. (2008).

3. EMISSION DATA

In both models, we have applied the TNO emissions (Visscherdijk, A. and H. Denier van der Gon, 2005) as area and point sources with a geographical resolution of 0.125º latitude by 0.25º longitude and covering all Europe. The emission totals by SNAP activity sectors and countries agree with the baseline scenario for the Clean Air for Europe (CAFE) program (Amann et al., 2005). This database gives the PM10 and PM2.5 emission for the primary particle emissions. We also took from CAFE the PM splitting sub-groups, height distribution and the breakdown of the annual emissions into hourly emissions. The PM2.5 fraction of the particle emissions was split into an unspecified fraction, elemental carbon (EC) and primary organic carbon (OC). The EC fraction of the PM2.5 emissions for the different SNAP sectors was taken from (Schaap, M. Et al., 2004). For the OC fraction, the method proposed by Beekmann et al. 2007, is applied as follows: an average OC/EC emission ratio of two was used for all sectors, i.e. the OC fraction were set as twice the EC fractions, except if the sum of the two fractions exceed the unity. In this case ($f_{EC} > 0.33$), f_{OC} was set as: $f_{OC} = 1 - f_{EC}$. With this prepared input, the WRF/CHEM and CMAQ took the information as it is. The hourly emissions are derived using sector-dependent, monthly, daily and hourly emission factors as used in the EURODELTA (http://aqm.jrc.it/eurodelta/) exercise. The differences with (San Jose et al., 2008) simulations for MM5-CMAQ are established as follows: Albania, Croatia, Bosnia and Serbia use the Bulgaria daily factors; Turkey uses the Hungary daily factors; Belarus, Moldavia, Ukraine and Russia use the Romania daily factors; Germany use the Federal Republic of Germany daily factors; Czech Republic uses the Slovakia monthly factors. The VOC to TOC factor is 1.14. In case of WRF/CHEM the changes are the same than for MM5-CMAQ but the VOC to TOC factor in the VOC splitting scheme is changed to 3.2.

4. MM5-CMAQ AND WRF/CHEM: ARCHITECTURES AND CONFIGURATIONS

MM5 was set up with two domains: a mother domain with 60 x 60 grid cells with 90 km spatial resolution and 23 vertical layers and 61x61 grid cells with 30 km spatial resolution with 23 vertical layers. The central point is set at 50.0 N and 10.0 E. The model is run with Lambert Conformal Conical projection. The CMAQ domain is slightly smaller following the CMAQ architecture rules. We use reanalysis T62 (209 km) datasets as 6-hour boundary conditions for MM5 with 28 vertical sigma levels and nudging with meteorological observations for the mother domain. We run MM5 with two-way nesting capability. We use the Kain-Fritsch 2 cumulus parameterization scheme, the MRF PBL scheme, Schultz microphysics scheme and Noah land-surface model. In CMAQ we use clean boundary profiles for initial conditions, Yamartino advection scheme, ACM2 for vertical diffusion, EBI solver and the aqueous/cloud chemistry with CB05 chemical scheme. Since our mother domain includes significant areas outside of Europe (North of Africa), we have used EDGAR emission inventory with EMIMO 2.0 emission model approach to fill those grid cells with hourly emission data. The VOC emissions are treated by SPECIATE Version 4.0 (EPA, USA) and for the lumping of the chemical species, we have used the (Carter, W. P. L., 2007) procedure, for 16 different groups. We use our BIOEMI scheme for biogenic emission modeling. The classical, Atkin, Accumulation and Coarse modes are used (MADE/SORGAM modal approach). In WRF/CHEM simulation we have used only one domain with 30 km spatial resolution similar to the MM5. We have used the Lin et al. (1983) scheme for the microphysics,

Yamartino scheme for the boundary layer parameterization and (Guenther et al., 1995) for the biogenic emissions. The MOSAIC sectional approach is used with 4 modes for particle modeling.

In case of MM5-CMAQ the changes in the model simulations compared with the report of (San Jose et al., 2008) affect only to the emissions (as explained above) an the Kz (eddy diffusivity coefficient). The option to use the so-called KZMIN as detailed in CMAQ code is applied. If KZMIN is activated the Kz coefficient is calculated by:

$$Kz = KzL + (KzU - KzL) * UFRAC \quad (1)$$

Where Kz is the eddy diffusivity in m^2s^{-1}. KZL is 0.5 (lowest) and KzU is 2.0 (highest). The UFRAC represents the percentage (rage 0-1) of urban landuse in the grid cell.

In case of WRF/CHEM, the changes affect to the microphysics scheme, substituting the (Lin, Y.-L. et al., 1983) scheme by the WSM (WRF single moment) 5-class microphysics scheme (Hong, S-.Y. et al.,2004). 5 represents the number of water species predicted by the scheme. The Goddard/NASA radiation scheme is substituted by the Dudhia radiation scheme (Dudhia J., 1993). The FTUV photolysis rate (Tie, X. X. et al., 2003) model is substituted by the FAST-J scheme (Wild, O. et al. 2000).

5. MODEL RESULTS

The comparison between daily average values (averaged over all monitoring stations) of PM10 concentrations and modeled values has been performed with several statistical tools such as: Calculated mean/Observed mean; Calculated STD/Observed STD; bias; squared correlation coefficient (R2); RMSE/Obsrved mean (Root Mean Squared Error); percentage within +/- 50% and number of data sets. Figure 1 shows the comparison between PM10 observed averaged daily values and the modeled values by MM5-CMAQ. The results show that for MM5-CMAQ, the new configuration related to emission data and eddy diffusivity improves the correlation coefficient from 0.828 to 0.851 but the pattern show a substantial improvement with the central peak much closer to the observed data. Figure 2 shows the comparison between observed and modeled average daily data for the episode with the new configuration for the WRF/CHEM model. The results show a much better correlation coefficient going from 0.782 to 0.852 with the new configuration. Figures 3 and 4 show similar results for PM2.5. In case of MM5-CMAQ the improvement is from 0.608 to 0.674 and for WRF/CHEM the change is from 0.760 to 0.759. These results show that the new configuration is substantially better than the previous one. New experiments are needed to determine the impact of emissions and the eddy diffusivity respectively.

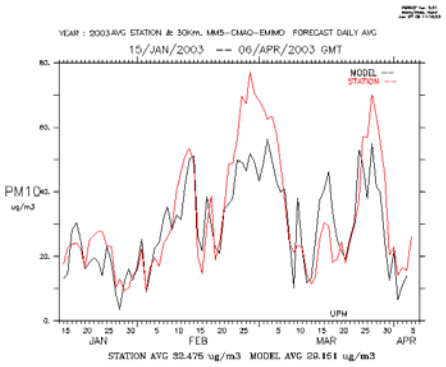

Figure 1. Comparison between daily averaged observed PM10 concentrations and model results produced by MM5-CMAQ. The model gets closer to the maximum peak compared with the previous simulation in (San Jose et al., 2008).

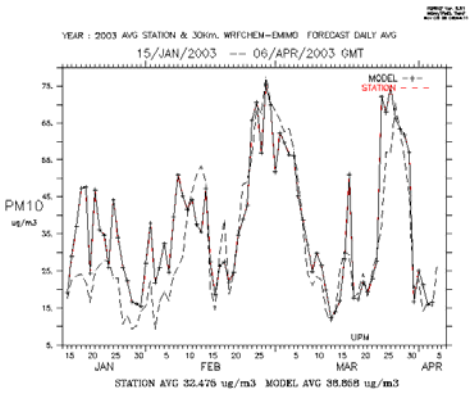

Figure 2. Comparison between daily averaged observed PM10 concentrations and model results produced by WRF/CHEM. The model captures even better than in the previous simulation (San Jose et al., 2008) the magnitude of the PM10 peaks.

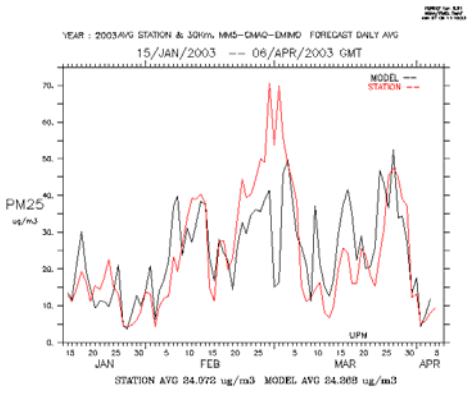

Figure 3. Comparison between daily averaged observed PM2.5 concentrations and model results produced by MM5-CMAQ. The model gets closer to the simulation performed in San Jose et al. (2008).

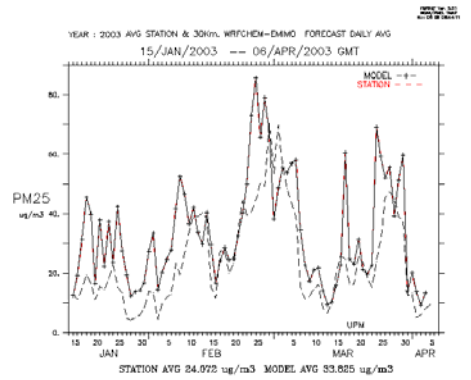

Figure 4. Comparison between daily averaged observed PM2.5 concentrations and model results produced by WRF/CHEM. The model overestimates a little bit the observed data but the correlation coefficient gets a light improvement (up to 0.759).

6. CONCLUSIONS

We have implemented and re-run two different models (MM5-CMAQ and WRF-CHEM) for the same episode over Northern part of Germany during the winter period of 2003 (Jan. 15-Apr. 5, 2003). The comparison between these simulations and those performed in San Jose et al., 2008, produce the following results: we have improved substantially the correlation coefficients for the daily averages when comparing observed and modelled data for both models. The WRF/CHEM continue to show better results than MM5-CMAQ but the peaks for PM10 and PM2.5 for MM5-CMAQ are getting closer to the observed peaks. The patterns for MM5-CMAQ have improved substantially compared with the results obtained in San Jose et al., 2008. New experiments are necessary to determine the impact of eddy diffusivity and emission inventory on the new results.

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