Improved modelling experiment for elevated PM_{10} and $PM_{2.5}$ concentrations in Europe with MM5-CMAQ and WRF/CHEM

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Abstract

The application of the MM5-CMAQ model (PSU/NCAR/EPA, US) to simulate the high concentrations in PM_{10} and $PM_{2.5}$ during a winter episode (2003) in Central Europe has been performed. The selected period is January, 15 – April, 6, 2003. Values of daily mean concentrations of up to 75 μgm^{-3} are found on average from several monitoring stations in Northern Germany. Additionally, the WRF/CHEM (NOAA, US) model has been applied. In this contribution we have performed additional simulations to improve the results obtained in our contribution (San José et al. (2008)). We have run again both models but with changes in emission inventory and turbulence scheme for MM5-CMAQ. In the case of WRF/CHEM many more changes have been performed: Lin et al. (1983) microphysics scheme has been substituted by WSM 5-class single moment microphysics scheme (Hong et al. 2004); Goddard radiation scheme has been substituted by Dudhia radiation scheme and FTUV photolysis model has been substituted by J-FAST photolysis model. The results improve substantially the PM_{10} and $PM_{2.5}$ patterns in both models. The correlation coefficient for PM_{10} for 80 days simulation period and for daily averages has been increased up to 0.851 and in the case of $PM_{2.5}$, it has been increased up to 0.674.

Keywords: emissions, PM_{10} and $PM_{2.5}$, air quality models, air particles.

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$PM_{2.5}$ 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 the northern part of Germany, we found south-easterly winds and stable conditions with low winds. These meteorological conditions brought daily PM_{10} concentrations at about 40 μgm^{-3}. The second peak was characterized by a sharp gradient on PM_{10} concentrations after Feb. 15 and until March, 7. This episode reached daily PM_{10} concentrations up to 70 μgm^{-3}. The meteorological conditions on March, 2 (peak values) were characterized by a wind rotation composed of 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 started 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. [25].

3 Emission data

In both models, we have applied the TNO emissions [17] 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 [18]. This database gives the PM_{10} and $PM_{2.5}$ 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 $PM_{2.5}$ fraction of the particle emissions was split into an unspecified fraction, elemental carbon (EC) and primary organic carbon (OC). The EC fraction of the $PM_{2.5}$ emissions for the different SNAP sectors was taken from [19]. For the OC fraction, the method proposed by [20] 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 [25] 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 [24] 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 [23] for the biogenic emissions. The MOSAIC sectional approach is used with 4 modes for particle modeling.

5 Changes in model configurations

In the case of MM5-CMAQ the changes in the model simulations compared with the report of [25] affect only the emissions (as explained above) on 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 the case of WRF/CHEM, the changes affect the microphysics scheme, substituting the [26] scheme by the WSM (WRF single moment) 5-class microphysics scheme [27]. 5 represents the number of water species predicted by the scheme. The Goddard/NASA radiation scheme is substituted by the Dudhia radiation scheme [28]. The FTUV photolysis rate [29] model is substituted by the FAST-J scheme [30].

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6 Model results

The comparison between daily average values (averaged over all monitoring stations) of PM_{10} 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/Observed mean (Root Mean Squared Error); percentage within +/- 50% and number of data sets. Figure 1 shows the comparison between PM_{10} 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 $PM_{2.5}$. 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.

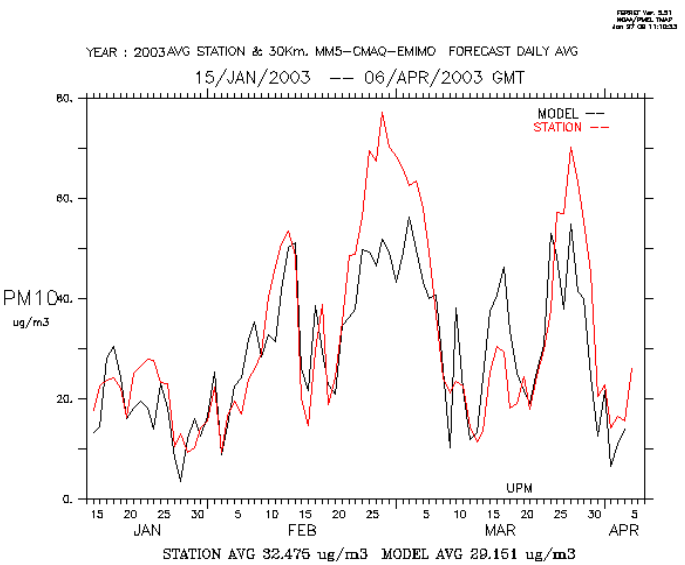

Figure 1: Comparison between daily averaged observed PM_{10} concentrations and model results produced by MM5-CMAQ. The model gets closer to the maximum peak compared with the previous simulation in [25].

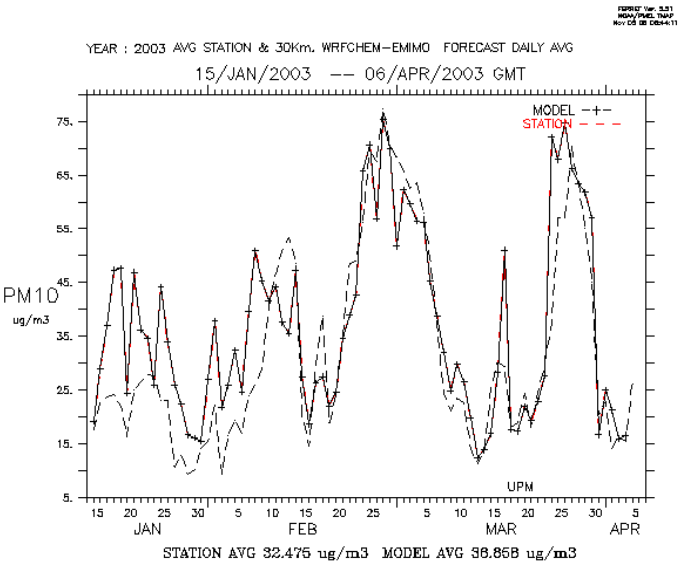

Figure 2: Comparison between daily averaged observed PM_{10} concentrations and model results produced by WRF/CHEM. The model captures even better than in the previous simulation [25] the magnitude of the PM_{10} peaks.

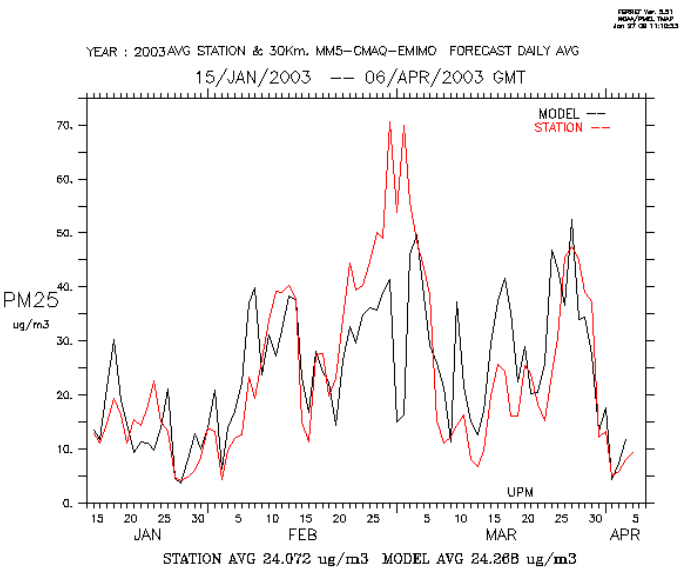

Figure 3: Comparison between daily averaged observed $PM_{2.5}$ concentrations and model results produced by MM5-CMAQ. The model gets closer to the simulation performed in [25].

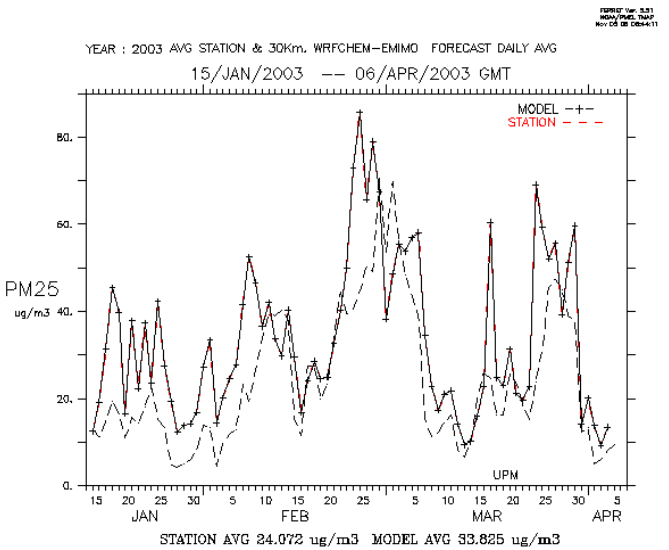

Figure 4: Comparison between daily averaged observed $PM_{2.5}$ concentrations and model results produced by WRF/CHEM. The model overestimates a little bit the observed data but the correlation coefficient gets a light improvement (up to 0.759).

7 Conclusions

We implemented and re-ran two different models (MM5-CMAQ and WRF-CHEM) for the same episode over the northern part of Germany during the winter period of 2003 (Jan. 15-Apr. 5, 2003). The comparison between these simulations and those performed in [25] 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 PM_{10} and $PM_{2.5}$ for MM5-CMAQ are getting closer to the observed peaks. The patterns for MM5-CMAQ have improved substantially compared with the results obtained in [25]. New experiments are necessary to determine the impact of eddy diffusivity and emission inventory on the new results.

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