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Interactive comment on "The Community Multiscale Air Quality (CMAQ) Model Versions 5.3 and 5.3.1: System Updates and Evaluation" *by* K.AppelWyat Appel et al.

Anonymous Referee #2

Received and published: 5 January 2021

Overview:

The paper (i) documents the model changes introduced in CMAQ versions 5.3 (and 5.3.1) compared to the previous version 5.2 and (ii) presents the evaluation of mean daily 8-hr average (MDA8) surface ozone, average PM2.5 and PM2.5 speciation over the USA. Hemispheric and regional model configuration of 5.2 and various variants of 5.3 are included in the evaluation.

General comments:

Peer-reviewed publication on model updates should be of interest to the scientific community, also beyond the specific user community of that model. These papers are

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expected to differ from other types of documentation such as user-guides and comprehensive documentation because they should follow a certain scientific narrative.

The presented paper is generally a welcome and well-written overview of the CMAQ updates of version 5.3. However, the balance between a readable scientific paper and a user-guide presenting all possible configuration options was too often shifted to the latter, which made it sometimes difficult to understand the main points of the paper.

I strongly recommend making a more selective and clearer choice of the discussed 5.3 and 5.3.1 configuration options. A single 5.3. default configuration (it could also be 3.5.1) should be more clearly identified and compared against the default version 5.2. The subvariants of 5.3 and 5.3.1 can then be used to discuss further issues or to better substantiate the findings of the paper. Table 1 is central to the paper and should be introduced much earlier and it should be a more verbose.

Further, it should be better distinguished between 5.2 to 5.3 updates that change scientific result and technical updates of the modelling infrastructure such as MCIP or DESID, whose impact is not evaluated. I recommend shortening the description of these technical modifications, if their impact is not assessed in the paper.

The presented model run versions do often vary in more than one aspect, which makes pin-pointing the reasons for the differences in the model performance difficult. It is common practise that developments of comprehensive modelling systems are often implemented in “packages” containing various modification but a more detailed discussion on the dominating reasons for differences in the modelled concentrations and fluxes would be helpful. For example, a novelty aspect of STAGE compared to M3Dry seems to be the multi-tile approach. However, the dry deposition simulations seem to differ also in other aspects and a clear message on the importance of the tiled approach is not provided.

A discussion of the representativeness of the observations is required for scientifically sound evaluation paper. For AQ application it is common practise to distinguish differ-

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ent air quality regimes such as “urban”, “rural” and “street”. While representativeness is mentioned it is not acted upon as no stratification of the observations is applied in the many time series plots.

The evaluation of the model runs is limited to MDA8 ozone and seasonal averaged and speciated PM2.5. While these quantities might be the most important for air quality legislation purposes, the scientific validity of the paper could be greatly improved by also presenting the impact of the model changes on the diurnal cycle and simulated maximum values. Also including NOx and SO2 evaluation results in the main paper would be very welcome to understand the discussed changes in MDA8 ozone and PM2.5. If the model upgrade to 5.3 did not noticeably modify the aforementioned variables, it should be pointed out more clearly.

Overall, version 5.3. seems to be only a small improvement in ozone over 5.2 with the strong caveat of the increased ozone spring time bias and the general degradation in California throughout the year. It would be interesting to discuss the reasons in more detail and to explain why 5.3. is considered to be an improvement.

It is an interesting result that the pollutants boundary conditions simulated by the hemispheric configuration are one of the most influential aspects for the regional model differences. It would therefore also be useful to evaluate the hemispheric configuration with the AQS (or other) observations and not only show model differences between these simulations. Likewise, the performance of the regional and hemispheric runs should be assessed and compared.

Specific comments:

L 25ff The text seems to jump between version 5.3. and 5.3.1 and it is not clear to which you refer (see my general comment on a clearer 5.3 version choice)

L 27 Please quantify better the bias changes (x % or y ppb)

L 32 as above for PM.

L 43 Please mention if the tiling approach contributed to these differences.

L 93-99 I recommend referring already here to table 1 or insert a new overview table of the various model modification, which you will discuss in that section. Also make much clearer, which of the following updates are used only in the hemispheric and the regional configuration. It took a while to realise that the halogenic chemistry updates are not part of the regional model configuration, which is the focus of this paper.

L 115-129 It is not quite clear, if this refers to the 5.2 to 5.3 update or to a previous update.

L 124 How far inland there is a noticeable difference?

L 144 Is this loss rate only applied at the lowest model level or throughout the atmosphere?

L 163 The difference between AERO7 and AERO7i is not clear and if this is relevant to the paper. According to my understanding of Table 1 only AERO7 is used (?). Why do you mention 7i here?

L 176 “half organic” or “half of secondary organic” aerosol ?

L 200 Please explain “biogenic mapping”

L 194 -203 I find this a bit confusing. Please only discuss configuration options you are going to assess in the paper.

L 211 Please provide reference or explanation, why the coarse mode dry deposition velocities were considered to be too high in 5.2

L 216 Please explain “in areas of high sigma”. Is the modification in 5.3 a numerical bugfix or does it imply a modification of the algorithm?

L 225 ff Again, it is not always clear which aspects of the aqueous and heterogenous chemistry are modified between 5.2. and 5.3 and if you test any in the paper.

L249-257 The reported changes in SO4 and O3 are substantial. It is not clear if they are derived from the represented simulation. If anything, they should be included in the results section 4.

L 270 FF: The main update of M3Dry seems to be the much more detailed input of NH3 information from fertilisation. It is not clear, if this is a 5.2 vs. 5.3 difference.

L 300 FF: Does STAGE use the M3Dry approach including its input data and differs it only w.r.t the sub-grid (tile) approach.

L 321 Please provide a reference or explanation for “bulk accommodation coefficient”

L 351-378 Please consider removing descriptive parts, which are more a user guide than information important for the conclusions of the peer-reviewed paper.

L 422 Here or elsewhere it be good to give more information about the kind of the impact of the different options for LAI and VF input into WRF on meteorological model results relevant for CMAQ such 2mT, PBL height or soil moisture.

L 441 Please provide more detail on the EPA wildland fire emissions for the regional runs. Has FINN been used?

L480 Table 1 needs to be introduced much earlier in the paper because it is the “life-line” for the reader to understand the different tested model variants. Also, I strongly recommend to be more descriptive in the table (e.g if halogenic chemistry was used) and not only provide abbreviations.

L495 Using WBD, or not, needs further discussion. Why was WBD considered acceptable for the hemispheric runs and not for the regional runs ? What were the negative implications of not using WBD in areas affected by dust ?

L 510 Please clarify if you stratified the data in AQ regimes such as urban, rural and street ? An evaluation of an AQ model at 12 km resolution may not be representative for locally highly polluted areas. A discussion of the representativeness of the obser-

vations is required for scientifically sound paper.

L 543 Please clarify, if the statistical measures are calculated for each station by meaning over time or also for specific times meaning over space.

L 578 I think showing the mean values (as in Fig S2 and S6) and not the biases (Fig1 and 3) would be a better choice for the paper. Please comment on the reason for the spring time underestimation in both 5.3 and 5.2

L587 The differences in ozone are attributed to changes in dry deposition. It seems that differences in meteorology (WRF38 vs WRF 411) also impact the mean ozone values. WRF411 ozone is about 1ppb higher than WRF38. Please provide more detail what the reasons are for this increase in ozone.

L 593 As the degradation in spring is striking, please provide more information why this is the case.

L 600 As the degradation in California is striking, please provide more information why this is the case.

L 611 The large summer underestimation is a common feature in 5.3 and 5.2 (see Fig S6). Please comment, why this could be the case.

L 615 Please provide more details on the impact of OH and Ozone in winter on OC. What are the main pathways? Why does the opposite ozone difference (i.e. higher O3 on 5.2) during the rest of the year do not lead to higher PM2.5 in 5.2 ?

L 616 Please specify in more detail what modelled species NCOM entails.

L 636 I find this explanation (different RWC emission in Canada) confusing because I had assumed the emissions are the same for both 5.2 and the considered 5.3 run. Please comment and point out this fundamental difference earlier. I assume that PCSOA on RWC is not applied in the presented case.

L 657 Please provide more information what species are included in the OTHR group

of the model results.

L 670 Please comment why BELD5 has been used despite that it is not publicly available and seem to degrade the PM results in summer, when the model is already biased low.

L 675-600 Please also provide (a) an evaluation of the HCMA runs with observations and (b) compare the performance of the regional and hemispheric runs (see general comment). Please mention the ozone sonde evaluation in the supplement, which shows larger negative biases with 5.3 in the troposphere.

L 712: Please clarify, if the difference between WRF411 and WRF38 runs also includes the differences in vegetation parameters (MODIS based) for dry deposition and biogenic emission modelling, or not.

L730-742 Please make clearer if this paragraph is meant to be the explanation for the differences mentioned in the paragraph before. It would also be helpful to stress more (if it is the case) that the differences in ozone are mainly driven by the vegetation data updates not by other WRF changes.

L 740 Is the reduced O3 wet scavenging something quantified by model diagnostics or is it more a guess. One would not expect a large impact of wet deposition, especially when aerosols seemed to be not effected (see next paragraph).

L 759 Please summarise here the main differences. An important difference of STAGE seems the tile-approach but it seems to make no differences at all as it is not mentioned in the section. Please remark more clearly if that aspect has an (positive) impact.

L 778 Please discuss the reasons for the differences in ozone based on the differences between M3Dry and STAGE.

L 796 The NH3 evaluation is a very interesting aspect of the paper. I strongly recommend to also show in Fig 12 a run of the noBIDI configuration to demonstrate the impact of the bi-directional approach. Fig 12 is very busy and I suggest considering

separate plots for the different error measures.

L 805: It would be interesting to know why the differences are so large at a few particular stations shown in Fig 13. whereas the differences are much smaller for the majority of the stations. Is this the tile -approach or other issues related to vegetation cover?

L 813-850 Figures 14 and 15 provide a very welcome overview of the model performance. I would strongly recommend to prepare the graphs not only for 5.3 but also for 5.2. In that case the reader would get the possibility to compare the performance of the two configurations, which is after all the main topic of the paper.

L 881 Please mention the specific differences between STAGE and M3Dry that cause the described differences in the results.

Table 1: Please make it more self-contained, i.e. readable without need to refer to the paper for each acronym. Please add information if the run is evaluated with observations. Please consider to chose a 5.3 runs as the default 5.3 version.

Figure 1/3: Please mention which lines are on top of each other. It is not clear where the blue line is. In my opinion, there is no need to repeat the color-code information of the legend. Refer to table 1 for the different options.

Figure 2/4: Please mention briefly why the specific 5.3 version is chosen (5.3 default ?) Refer to table 1 for details.

Fig 5: Spell out unfamiliar acronyms such as OTHR and NCOM.

Fig 6/7: Say this are surface values

Fig 8-11: consider saying more clearly in the caption what aspect is different (i.e. meteorology or deposition model)

Fig 12: Consider adding a model run without bi-directional-flux approach. Do not show to many statistical parameters in one plot. Please clarify if the correlation is spatial or temporal.

Fig 14/15: Please include and juxtapose the graphs for a 5.2 and 5.3 CMAQ simulation.

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