Geoscientific
Model Development
Discussions

Interactive comment on **"Overview and evaluation of the Community Multiscale Air Quality (CMAQ) model version 5.1"** *by* **K. Wyat Appel et al.**

Anonymous Referee #1

Received and published: 7 October 2016

This paper describes recent updates to CMAQ, a chemical transport model used for regulatory and research purposes. The topic of the paper is certainly suitable to GMD and will likely be useful to users of CMAQ. However, the manuscript needs to be im- proved to better communicate the changes in the code and remove apparent contra- dictions. In particular, I found the discussion for some on the updates to be too general and did not include sufficient citations justifying those updates.

Major Comments:

1) In general, I found the discussion for some on the updates to be too general and did not include sufficient citations justifying those updates as indicated by some of my specific comments below. In addition, the end of Section 1 and Section 2 need to be reordered to have common steps to improve the clarity of the text. I also have concerns

regarding how the two versions of CMAQ are compared given other differences in WRF and the emissions. I understand that there are often complicating factors that make a more fair comparison possible. Some discussion is included to state why those differences in the configuration arise, but those points could have been made more clearly.

Response: Hopefully we've addressed most of this concern by addressing the specific comments below. In general however, we tried to include enough detail so that the reader understood what basic changes were made and why. If the reader wishes to get more detailed specifics of the changes made, they are referred to the technical documentation for the model release.

2) Section 5.2: I like evaluating the models using profiles from the DISCOVER-AQ data, since observations at the surface only provide a small slice of the atmosphere. However, Section 5.2 seems rather brief and overly simplistic. Extensive measurements were collected during the campaign I presume, yet only one profile is shown. It does illustrate the differences between models, but only for one case. The authors needs to either delete the section, provide a more extensive evaluation, or justify why only one profile is needed. One way to summarize the aircraft data is to showing percentiles of both model and observations as a function of height. In addition, why not use the NASA lidar data to illustrate differences in PM? The authors describe changes in aerosol optical properties but do not evaluate this part even though data is available to evaluate the optical properties.

Response: Since the objective of this section is to evaluate the change in model performance for NOY, AN and PNs, the section has been retitled to reflect its purpose and not suggest to the reader that this section will be a comprehensive evaluation against aircraft measurements. Several statistical metrics of NOY performance have also now been included in the section to help expand the analysis provided and highlight the greatly improved performance of NOY in CMAQv5.1. While it would be nice to be able to show additional profiles from other days and include measurements from other networks, the point of the section was to simply inform the reader of the large improvement in NOY performance and an example of the change in ANs and PNs mixing ratios that can be expected in the new model. Future evaluations of CMAQ will focus specifically on the DISCOVER-AQ time period and utilize the measurements made to a much greater extent.

Specific Comments:

Page 1, line 27: Does "thereby reducing the PM2.5 bias" refer to the previous bias? Please be specific.

Response: Added a statement indicating underestimation of PM2.5 by CMAQ in the summer to clarify what bias is being reduced.

Page 1, lines 28-29: The text in these to lines seem to contradict one another in terms of the PM2.5 bias.

Response: Clarified that this refers to the consideration of the effect from all the changes made to the model and not just a single update as previous referred to.

Page 1, lines 31-32: Line 31 says v5.1 has a higher O3 bias, but in next line says error is better. I can understand that the correlation could be better in v5.1 even though the bias is worse, but the authors are not clear what they mean here.

Response: Corrected text to read that only the correlation improved and not the error.

Page 1, line 36: What does "significantly" really mean? This is not specific. Page 2, lines 20-24: Consider making this text a bulleted list.

Response: Removed the word significantly since it is subjective. Opted to avoid introducing bulleted text into the manuscript.

Page 2, lines 18-29: I was trying to relate the changes described in this paragraph, with Section 2. But upon first reading the paper, it was not clear to me that these two parts were necessarily referring to the same changes. The text could be improved if lines 18-29 were written to be parallel to Section 2, or visa versa.

Response: Reordered this paragraph to make it consistent with the order in which the model updates were presented in section 2.

Page 3, lines 18-24: Please include a reference justifying the revised stomatal conductance. As written, it seems the modification is simply a tuning parameter that improves some quantities in the predictions. There could be easily other changes in the model that could improve the quantities that were mentioned.

Response: A reference was added regarding the origin of the stomatal conductance values.

Page 3, line 25: Mention values of the heat capacity used in the old and new versions.

Response: These values were added to the text.

Page 3, line 32: So what is the Pr now? The authors say they changed it, but are not specific about this parameter.

Response: The Pr is (and was) a function of the eddy diffusivity values of momentum and heat. Previous, these values were the same and there Pr was always equal to unity. That is no longer the case.

Page 3, line 32-36: Similarly, what are the new stability functions and are there some published results to describe them?

Response: The stability functions are described in Pleim et al. 2016 which is provided as a reference in this section.

Page 4 line 7, This line is confusing. I am missing some details since the phrase "little difference between the initial MOL estimate and the final re-calculated value" is basically saying the code will do nothing. Then what is the point of the code? To me the test associated with MOL assumes the reader is already somewhat familiar with this subject, but I do not understand the logic here.

Response: This statement was removed from the text as it was unnecessary and requires a greater understanding of the use of the MOL value in CMAQ and WRF that described in the text.

Page 4, lines 9-16: The text on gravitational settling seems out of place in this section.

Response: This description has been moved to the end of Section 2.5.

Page 4, line 26: There are many studies, not just the two cited, that indicate IVOCs are missing in the emission inventory. Suggest changing text to include "e.g." or "for example" or something similar.

Response: Changed the text to indicated the provided references are examples.

Section 2.2: In general, I found the text in this section to be confusing in terms of what is actually new in v5.1 compared to older versions. The level of detail is rather minimal.

Response: The goal of this section is to provide an overall understanding of what was updated and why. It is not intended to document in detail every change made to the aerosol code in CMAQ. Text was added to the beginning of the section that points the reader to the CMAQv5.1 technical documentation which includes in detail all the changes made to the model.

Page 5, line 15: What is "more consistent" mean? Why isn't it completely consistent?

Response: We have revised the paragraph to better define what is and is not consistent with the meteorological model. The updates in photolysis calculations in CMAQ v5.1 related to clouds were intended to ensure internal consistency between cloud mixing, aqueous chemistry and photolysis. The reason cloud treatment in CMAQ is not currently "completely consistent" with WRF is the way that sub-

grid convective clouds are handled. The sub-grid convective cloud scheme in CMAQ, which is responsible for convective transport of chemical species, aqueous chemistry, and wet scavenging, is a simple bulk scheme based on the convective cloud model in the Regional Acid Deposition Model (RADM; Chang et al., 1987) but with convective transport based on the Asymmetric Convective Model (Pleim and Chang, 1992). Since the CMAQ cloud scheme uses the convective precipitation rate to diagnose sub-grid mass fluxes, the location and timing of precipitating convective clouds are consistent with WRF. A new convective cloud scheme for CMAQ based on the Kain-Fritsch scheme in WRF is currently being tested to improve consistency across chemical and meteorological components of the system.

Page 5, lines 20-21: What does "run time options" mean? I assume the authors mean the user has the ability to choose these options. "run time options" sounds like unnecessary jargon.

Response: We removed the term and added text on how a user may use either of the two options.

Page 5, lines 24-25: This sentence does not describe how "cloud fraction, sub-grid cloud fraction, resolved cloud water content" are actually used.

Response: These parameters are simply provided in the text as examples of new diagnostic values that are available as output in the new version of the model in case a user wishes to examine them. They are not new variables used in the CMAQ model. We also added text to the paragraph briefly describing the calculation method for photolysis rates and how the clouds contribute to the calculation.

Page 5, line 27: The satellite data can be used to evaluate clouds, but it cannot be used to directly evaluate photolysis calculations. The authors need to be more specific here. I think the authors mean that the clouds indirectly determine where photolysis rates may be high or low, but the satellite does not provide any quantitative estimate of photolysis.

Response: We agree and revised the paragraph to state this point. Note that this paragraph was also moved to section 4.3 since the focus is on model evaluation. The revised sentences now state:

"Additional diagnostic evaluation of photolysis/cloud model treatment in CMAQ was conducted based on the model predicted cloud albedo at the top of the atmosphere. The predicted cloud albedo from WRF3.7, CMAQv5.0.2 and CMAQv5.1 were evaluated against cloud albedo from NASA's Geostationary Operational Environmental Satellite Imager product (GOES; http://satdas.nsstc.nasa.gov/). This evaluation was used to qualitatively determine if one CMAQ version better considers how clouds affect calculated photolysis rates."

Page 5, line 34: Do you mean photolysis rates at the surface? Please be specific. Surface values will differ from those aloft.

Response: The figure shows what the cloud parameterization between version 5.0.2 and 5.1 implies about the cloud albedo or reflectivity at the top of the atmosphere. Changes in photolysis rate are integrated over the vertical column so the paragraph does not discuss photolysis rates at a specific altitude. Also, the revised text attempts to better explain the analysis and displayed results.

Page 5, lines 37-38: This statement is about the clouds, but c) and d) are about photolysis rates. I understand the photolysis rates reflect the cloud distributions, it is just strange the way the sentence is stated. As I said before, the use of "more consistent" leads me to wonder in what ways the clouds in WRF and CMAQ still differ. What are those ways?

Response: We revised the paragraph in section 2.3 to better explain how WRF and CMAQ differ in the cloud description, specifically the sub-grid or convective clouds (please see response to previous question for more details). The paragraph describing the figure has been moved to section 4.3. The figure is now referred to as Figure X and the statement in question has been reworded to more accurately describe that what is being plotted is based on the cloud parameterization in the CMAQ system, not just within the photolysis module:

"Figure X shows the average cloud albedo or reflectivity at the top of the atmosphere during daytime hours in July 2011 derived from the GOES satellite product (5a), and the cloud parameterizations within: (5b) WRF3.7, (5c) CMAQv5.1_RetroPhot and (5d) CMAQv5.1_Base."

(Note that the "CMAQv5.1_RetroPhot" and "CMAQv5.1_Base" abbreviations have been defined at the beginning of section 4.3.)

Page 6, line 6: How was "most important" determined? More important than what? It seems that the modifications are being added based on recent research activities, but it is not clear why these are more important than other new pathways that may have been reported in the literature. Please explain.

Response: Since the term "most important" is inherently subjective, we opted to remove that statement since it was not important to the discussion regarding the mechanism updates.

Page 6, line 12: N and Fc need to be defined.

Response: The statement referencing these values has been removed since it's not critical at all to discuss these variables and they are described in the citation provided.

Page 7, lines 6-9: This text is really only saying that some updates have been made, but gives no real specifics on what those updates actually are. How will this help users?

Response: The specifics of these updates are providing in the technical documentation available through the CMAS website. A link to the documentation is provided in the beginning of the section. Here we're making the reader aware of the changes and why they were made.

Page 7, line 26: The text mentions overestimates of biogenic VOCs at coastal sites, but this sentence seems to require a reference to know what study pointed that out and how.

Response: The text has been modified to better explain how the overestimation was determined and addressed, and now also includes a reference.

Page 8, Section 3: What is missing from this section is a list of parameterizations used in WRF.

Response: Modified the text to include the specific parameterizations that were employed in the WRF simulations. In addition, now include the WRF namelists in the supplemental material.

Page 8, line 14: I am not sure why the same version of WRF was not used to drive the two versions of CMAQ. I assume it is to have their older treatments in the land-surface and PBL parameterizations; however, there are likely other changes in the model as well that could cause differences. Please comment, and I think it is worthwhile to reiterate at this point why the two versions of WRF are used.

Response: The text was modified to explain why different versions of WRF were used. In short, because the updates made in WRFv3.7 were tied to similar updates made in CMAQv5.1, those two version of the models need to be used together (without modifications to the MCIP code). Similarly, WRFv3.4 is tied to CMAQv5.0.2 without additional modifications to the MCIP preprocessor. Hopefully this is now clear to the reader in the main text.

Page 8, lines 19-39: I am also confused why different emission inventories are used. This will drive differences in the v5.0 and v5.1 simulations that are beyond just the changes to the parameterizations.

Response: A new emissions platform became available after the v5.0.2 simulations were complete. It was felt that in order to obtain the best model results the latest emissions platform should be used and therefore was used for the v5.1 simulations. Sensitivity tests were performed to assess the impact that the changes in the emissions platform had on the model results and the impacts were determined to be small. A figure showing the impact of the emissions platform change on ozone and PM2.5 in January and July has been added to the text to quantify to the reader the impact from the emissions platform

change.

Page 10, lines 27-28: While I cannot disagree with these sentence, I think the explanation is rather simplistic. SOA depends on photochemistry and has been shown to be correlated with O3. So if O3 increases, one could expect increases in SOA and therefore an increase in PM2.5.

Response: Added a statement regarding how the change in oxidant concentration could impact the formation of SOA and therefore PM2.5 concentrations.

Page 10, line 39: The authors note that the total concentration of the new SOA species are small. One could conclude here that why were they included in the first place? It would be useful to reiterate that the PAH species are for health reasons and will need to be evaluated in the future. I am less sure about the ALK species. In section 2, the authors not that only the "most important" changes are made, but it is not clear why this is important.

Response: Statements were added to indicate that while the overall monthly difference in concentration of these species is small, the episodic isolated concentration can be higher. Also indicated the importance of these species in health related studies.

Page 11, lines 1-10: Was the temperature the same between the two versions? Since biogenic emissions are temperature dependent, I am wondering how much difference here is due to meteorological effects versus the changes in chemistry.

Response: The temperature difference between the two simulations is very small due to the use of four-dimensional data assimilation in the WRF simulations and does not affect the biogenic emissions significantly.

Page 11, lines 30-31: Here is a first mention that CMAQ produces more clouds than WRF. The reason for the differences would be useful to describe in Section 2. I still do not understand why CMAQ would have a different representation of clouds, which can only complicate interpretation of the effects of clouds on chemistry. Later in lines 37- 38, they mention differences in sub-cloud treatments. Again this should be stated more upfront in the text. Why is it difficult to have consistent treatment of clouds between the models?

Response: Moved this paragraph to Section 2.3 as it seemed more appropriate there. Greater effort has been made in that section to explain why the clouds in WRF differ from the clouds in CMAQ.

Page 11, line 36: The authors mention "WRF cloud parameterization" but they should specifically state in their model set up which microphysics and cumulus parameterization they used. The way the text is stated, it implies

WRF has only one when in fact there are many options. It is not clear that the underprediction in clouds they have could have been fixed or improved using another choice of microphysics or cumulus parameterization.

Response: The text now includes which WRF parametrizations were used in the simulations. In addition, the WRF namelists used have been added to the supplemental material.

Page 12, line 19: The second phrase of this sentence is redundant with the first phrase and adds no new information; therefore, it should be deleted. For the same reason, the second phrase in the sentence in lines 20-22 should be deleted.

Response: The redundant lines were removed.

Page 12, line 28, the authors mention low (I assume lower) PBL heights. So the difference in O3 are driven by the differences in meteorology and it would be useful to quantify this difference in PBL height. If the difference in PBL is on the order of 10's of meters, how does that compare to the vertical grid spacing of the model to actually make a difference?

Response: This was to note the relatively low PBL heights that typically occur over water versus land and as a result the change in ozone precursors can amplify the change in ozone due over water to low PBL heights. This is not a statement of the actual difference in PBL height between the two WRF simulations.

Figure 5, Perhaps it would be more useful to use percentage changes instead?

Response: As a compromise, added the approximate percent change in O3 and PM2.5 to the text describing Figure 5.

Section 4.4: The differences described in this section seem small, so how does this demonstrate a major update of the code? Does this mean the code changes are important theoretically, but they do not make big difference in the predictions.

Response: Some of the differences are actually quite large for monthly averages. However, the changes made to the atmospheric chemistry are incremental in nature.

Page 12, line 32: I am thrown a bit by the phrase "operational performance". "operational" may mean different things to different communities. Section 4 had a comparison of the models, which is repeated here but now include observations. Maybe just say the performance is evaluated by comparing the models with one another and observations?

Response: Removed the word "operational" as this was a source of unnecessary confusion without the

appropriate context.

Page 13, line 37: Is the change statistically significant?

Response: Statistical significance doesn't apply in this case since we're comparing two model simulations against the exact same set of observations. So, any change is by default statistically significant. However, it would remain in the hands of the reader to determine whether the change is significant to their application.

Page 14, lines 10-11: The authors note an improvement in certain aerosol species, yet emission are different between the simulations. On the next page on line 16, they mention the differences are due to emissions. Why is this then important in terms of the code changes in CMAQ?

Response: I don't actually see where in line 16 it is mentioned that the differences are due to emissions. It is stated that the difference are primarily the result in differences in the concentration of primary emitted species, but that it likely the result of changes in the meteorology (lower or higher PBL heights) and changes in the emissions.

Page 15, line 22: Abbreviations are used for states here, but not elsewhere so there is an inconsistent use. I suggest writing out all state names since international readers will not necessarily know what the state abbreviations are.

Response: Abbreviations are no longer used for the state names.

Page 18, line 32: References to papers in preparation should not be included. Are there other references that can be used?

Response: This paper is actually referenceable as it is online and includes a doi. The text has been changed to no longer indicate the paper as in-preparation.

Page 18, line 33: This section is titled "discussion" but this section contains little new discussion regarding the model results. It reads more like a summary section.

Response: The title of this section has been changed from "Discussion" to "Summary" as it does constitute a summary of the work and not a new discussion.