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

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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 improved to better communicate the changes in the code and remove apparent contradictions. 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.

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 need 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.

Specific Comments:

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

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

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.

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.
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.

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.

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

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

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

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.

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

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.

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.

Page 5, line 15: What is “more consistent” mean? Why isn’t it completely consistent?

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.

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

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.

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

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?

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.

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

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?

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

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.

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.

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.

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.

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.

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?

Page 11, line 36: The authors mention “WRF cloud parameterization” but they should specifically state in their model setup 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.

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.

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?

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

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.

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?

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

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?

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.

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

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.

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