Geoscientific
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Interactive comment on "Evaluation of dust and trace metal estimates from the Community Multiscale Air Quality (CMAQ) model version 5.0" *by* K. W. Appel et al.

K. W. Appel et al.

appel.wyat@epa.gov

The authors would first like to thank the reviewer for the extremely thorough review of the article. We greatly appreciate his/her time and effort to provide the well thought-out comments and suggestions. We've done our best to answer these questions and update the manuscript accordingly.

1. Abstract. Overall the abstract summaries the main ideas of the paper, but in some part is a little bit subjective at qualifying the model behavior using words like "did well" or "good". I think it could be more forceful if authors quantify model performance using statistics. Here some examples: P1860, line 12-14: could you replace the sentence

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"The CMAQ modeling system generally did well [: : :] the western United States;" by something more quantitative, e.g. indicating the annual mean bias or correlation coefiňĄcient in order to compare with eastern coast. The same thing should be considered in the summary section, e.g. P1881, lines 11-13.

Response: We've included some of the quantitative statistical values from the main text in the the abstract to give the reader some sense of the model performance. However, there are far too many quantitative measures in the main text to include in the abstract.

2. Chemical boundary conditions. P1867, line 10-19: the way as the boundary condition is treat is not very clear explained in the manuscript. On the one hand, GEOSChem dust concentrations are speciated into CMAQ trace metals and lumped species using a composite of four desert soil proïňĄles from SPECIATE. My questions at this issue are: did you create a mean proïňĄle from the four ones? Which proïňĄles are they? Which is the percentage of composition of each species? On the other hand, it is not clear the chronological order that the authors applied to treat GEOS-Chem to feed CMAQ for PM boundary conditions. I guess that ïňĄrst, they grouped aerosols by size matching bins and corresponding CMAQ modes; and second, they speciated aerosols from the PM2.5 fraction (which came from mainly from the ïňĄrst GEOS-Chem bin) as AFEJ, AALJ, ASIJ, ATIJ, ACAJ, AMGJ, AKJ, and AMNJ, using the composite of four desert soil proïňĄles. From the text is not clear, please clariïňĄed how you performed that.

Response: The section discussing the chemical boundary conditions has been expanded to include a greater discussion of how the BCs were created. In addition, a new table will be added that shows how the mapping between the GEOS-Chem and CMAQ species was done. This should clarify the process in which the BCs were created.

3. Soil variable deïňĄnition and comparison with observations. Soil from CMAQ is postprocessed using the Equation 1. However, this equation is not very well supported in the manuscript. Furthermore, the link the authors use as reference does not work.

From Equation 1, one can guess that your only evaluate soil in fraction PM2.5. In this sense, which is the size of PM in the measurements? Do the authors think that the size between model and measurement is a source of uncertainty in the present evaluation?

Response: We tested the link, and it still appears to work. I'm not sure why the author was unsuccessful with the link. The soil equation was used in liue of examining all the soil species individually, as such a task becomes tedious and overwhelming to the reader. We have added a sentence in the text explaining why we use the soil equation. Yes, we are only examining the fine fraction of soil. While there may be some uncertainty introduced by comparing PM2.5 measurements to I and J mode sums from CMAQ, it should very small in most cases and not affect the conclusions of the evaluation significantly.

4. Reasons for CMAQv5.0 soil overestimation. The results show that overall CMAQv5.0 overestimates observed soil, where bias is bigger in CSN stations than in IMPROVE stations. Authors attribute part of such overestimation to underestimation of nighttime mixing in the urban area and uncertainties in spatial and temporal distribution of dust related emission sources in the emission inventory. This conclusion is present in the abstract and in the conclusion. However, along the paper there is not enough evidences about that. In this sense, have the authors quantiïňĄed the model day-time and night-time cycles of PBL, wind direction and velocity? This evaluation could give an objective idea in what extend meteorology is affecting to under-/overestimation of concentration.

Response: We've added a reference that deals with the inadequacies of the WRF model to represent mixing in the urban environments. The deficiencies in WRF in this area are well researched, and number of groups are currently working to improve the representation of mixing in the urban environment in WRF.

5. Effect on sulfate chemistry. P1875, line 23: author suggest that one reason that SO_4^{2-} decrease between both CMAQ version is related to the fact that Fe(III) and

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Mn(II) concentrations in the CMAQv5.0 are often lower that the prescribed Fe and Mn used in previous version. In this sense, my question is: how lower are these Fe(III) and Mn(II)? On the other hand, at P1875, line 25-28 the paragraph appears confusing. From this sentence is not clear if the new rate constant is pH dependent or not. Please clarify this issue.

Response: The previous versions of the model use prescribed constant values of 0.01 ug/m3 for Fe(III) and 0.005 ug/m3 for Mn for SO2 oxidation via metal catalysis oxidation pathway. However, CMAQv5.0 uses predicted Fe and Mn concentrations, then applies solubility and oxidation state, and calculate Fe(III) and Mn(II) for SO2 oxidation following Alexander et al. (2009). It uses a constant solubility of 10% for Fe and 50% for Mn. Ninety percent (90%) of the dissolved Fe is taken in the form of Fe(III) at night and 10% is taken in the form of Fe(III) during the day while all dissolved manganese is taken in the form of Mn(II) (Sarwar et al, 2013). Predicted Fe and Mn concentrations vary; consequently, available Fe(III) and Mn(II) for SO2 oxidation also vary in space and time. We calculate monthly mean Fe(III) and Mn(II) concentrations available for SO2 oxidation and compare with the prescribed constant values used in the previous versions of the model. Higher SO_4^{2-} concentrations are predicted mostly in the eastern US. Thus, we calculate monthly mean values in this region. In January, we find that mean Fe(III) concentrations range 0-0.07 ug/m3 while mean Mn(II)concentrations range 0-0.06 ug/m3 in the eastern US. The domain-wide monthly-mean Fe(III) concentration in the same region is 0.003 ug/m3 which is three times lower than the prescribed constant value used in the previous versions of the model. Similarly, the domain-wide monthly-mean Mn(II) concentration is 0.0008 ug/m3 which is six times lower than the constant prescribed value used in the previous versions of the model.

Previous versions of the model use the rate constant suggested by Walcek and Taylor (1986) while CMAQv50 uses the rate constant suggested by Martin and Good (1991) for metal catalysis oxidation pathway. Alexander et al. (2009) implemented the reaction of Martin and Good (1991) into a global chemical transport model and examined global

implications of the sulfur budget. Sarwar et al. (2013) followed the procedures of Alexander et al. (2009) and implemented it into the CMAQ model. The new rate constant was developed at a pH of 3.0. Similar to Alexander et al. (2009), the new rate constant in CMAQv50 is used for all pH. Note that while the rate constant in previous versions of the model is pH dependent, it contains discontinuity.

6. Impact on soil concentrations from African dust event. CMAQv5.0 underestimates soil concentration in summer under some specific episodes. The authors suggest that these underestimations (the days 13 July, 28 July and 3 August) are related with mineral dust long-range transported from the Sahara desert. However, the performed analysis does not justify the present of this event. Could the author confirm that the soil in these events come from Sahara desert or other part of Africa? At least, could the author confirm that air masses come from this continent? Maybe you can use trajectory analysis, global model or satellite data to support the evidence of a long-range transport of dust from African desert.

Response: Based on the reviewers comment, we obtained some satellite derived aerosol optical depth (AOD) data for late July and early August 2006, which showed relatively high AOD values for that time period. We added a sentence in the text stating such, but did feel it was necessary to add an additional figure showing the satellite AOD values. We feel confident that elevated dust during that time period was largely contributed to by transported dust from Africa.

7. The number of available stations form IMPROVE network is 161 (P1870, line 24). However, the number of stations which appear in Figure 1 is 160. Are there any special reasons for that?

Response: No. It's likely that one of the sites was just missing a significant amount of data for that year.

8. Figure 5 b shows the change in bias between the two CMAQ simulations at IM-PROVE, CSN and CASTNET. Here, CASTNET appear for the first time. You should

introduce the network properly in section 3 as you did for the other networks.

Response: Yes, that was on oversight. We've added a description of the CASTNET data in section 3.

9. Figure 4. I suggest including the number of observed data available to have an idea of the temporal coverage of the measurements.

Response: Done. The number of observations available was added to both the text and figure.

TECHNICAL CORRECTIONS - P1863, line8: the references "Xiu and Pleim, 2007" and "Pleim and Xiu, 2003" are not in the References section.

- P1863, line15: the reference "Otte and Pleim, 2009" is not in the References section.

- P1877, line24: the reference "Fairlie et al. (2006)" is not in the References section.

- P1883, line 28: Davis and Swall (2006) is not referenced along the manuscript.

- P1885, line 14: Otte and Pleim (2010) is not referenced along the manuscript.

- P1885, line 32: Pleim and Xiu (1995) is not referenced along the manuscript.

Response: We fixed those references.

- P1863, line25: the link does not work.

- P1870, line20: the link does not work.

Response: We checked the links and they appear to work.

- P1864, line17: replace "single emissions category" by "single emission category"

- P1864, line25: replace "PM2.4" by "PM2.5"

- P1865, line27: BEIS acronym is previously deïňĄned in Pg 1864, line2.

- P1867, line4: remove capital letter in "Chemical".

- P1874, line14: deïňĄne MI as Michigan, I guess.

- P1890, caption Fig. 1: the sentence "the IMPROVE network sites (blue) and CNS (red)" should be replace by "the IMPROVE network sites (red) and CNS (blue)". - P1892, caption Fig. 3: replace "RMSE" by "root mean squared error (RMSE)" as for the other statistics IA and r.

- P1892, caption Fig. 3: replace "correlation" by "correlation coefiňĄcient".

- P1893, Fig. 4: Figure 4 left panel makes reference to Mn but in the caption you indicate it as K. I guess you should replace "K" by "Mn" in the caption since the plot and the discussion is based on Mn.

- P1893, Fig. 4: Could you indicate in both plots the number of observation for Mn and Ca?.

- P1893, Fig. 4: in the caption replace "MI" by "Michigan".

- P1894, Fig. 5a: the colour chart indicating low positive bias is in green range and low negative bias is also in green range. Could you make this colour chart consistent with the one in Fig. 5b?

Response: All of the above corrections and suggestions were made to the manuscript.

Interactive comment on Geosci. Model Dev. Discuss., 6, 1859, 2013.