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Geoscientific Model Development Discussions

Interactive comment on "Photochemical grid model implementation of VOC, NO_x, and O_3 source apportionment" *by* R. H. F. Kwok et al.

Anonymous Referee #1

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Summary: The authors have implemented and applied ozone "source apportionment" in the Community Multi-scale Air Quality model (CMAQ). Implementation is a significant effort that provides important capabilities to CMAQ that are relevant to scientific exploration and regulatory application. Application and evaluation showed results that would be expected from implementation in similar models.

The paper would be improved by addressing three things. 1) The weaknesses inherent sensitivity metric application, particularly with respect to biogenic VOCs. 2) Discussion different ozone endpoint for results. 3) Minor comments.

1 Sensitivity Metrics:

The source apportionment technique relies on the PH2O2/PHNO3 indicator that has

been extensively used for Carbon Bond IV. The PH2O2/PHNO3 ratio, often referred to as the Sillman ratio, is a simplification of a more complex relationship (Sillman, 1995, A5 (PH2O2+PROOH)/PHNO3). The Carbon Bond IV mechanism lacks an organic peroxide (ROOH), which requires the simplification of based on the ratio of PROOH/PH2O2 in a 1995 Lack Michigan simulation. Though Dennis and Tonnesen showed it's robustness, I am not aware of a published comparison to the robustness of (PH2O2+PROOH)/PHNO3.

The poor performance of biogenic zero out could be related to ROOH production. The speciation of VOCs are important in determining the PH2O2/PROOH ratio in the presence/absence of NOx. The PH2O2/PROOH dependence could suggest that biogenic VOC sensitivity would be mischaracterized by PH2O2/PHNO3. Though the explanation of non-linearity is suggestive, it is not definitive. In fact, the first order sensitivity shows better performance for BIOG for both the slope and correlation.

At least some discussion of the metric is warranted, as well as more discussion of the fundamental issues with applying a binary metric.

2 Ozone Endpoint:

The authors show only daytime-average for most results and all-hour averages for ISAM/DDM. I suspect that the choice to average was based on the autocorrelation of hourly results, but this is not discussed. Averaging, however, removes variability. An alternative metric that would be more relevant, would be maximum daily 1-hour average or maximum daily 8-hour average. The 8-hour average would still have some reduction in variability, but would be more relevant to the regulatory application that is likely to use this tool. Thus, the brute-force evaluation of 1- or 8-hour average would be more interesting.

In addition, why do some results use all-hour and others daytime only?

3 Minor comments:

Page 5802, line 23-24 - add some more detail than just a hanging line.

Page 5803, line 5 - is J = J*something?

Page 5803, line 11 - The effect on accuracy will likely depend on the time of day, as sensitivity typically shifts with time. During the PH2O2/PHNO3 transition, this could be important if the synchronization time step is not controlled. Some discussion is warranted.

Page 5803, 5804 - consider harmonizing subscripts in equation 7 with 8 and 9.

Page 5812, line 2-5 - reword.

Page 5812, line 11 - consider splitting this paragraph to help distinguish between what I believe are very distinct points.

Interactive comment on Geosci. Model Dev. Discuss., 7, 5791, 2014.