Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2018-316-RC3, 2019

Geoscientific Model Development Discussions

Interactive comment on "Chemistry and deposition in the Model of Atmospheric composition at Global and Regional scales using Inversion Techniques for Trace gas Emissions (MAGRITTEv1.0). Part A. Chemical mechanism" *by* Jean-François Müller et al.

Anonymous Referee #3

Received and published: 3 February 2019

This paper compiles a new set of isoprene oxidation mechanism for a global model, based on recent laboratory and theoretical developments. The authors did a thorough job on explaining chemical reactions on major pathways. I find Section 2 is particularly useful for future model development. However, I feel that Section 3 could be improved by including more discussion. I have a few comments:

1. The authors use SEAC4RS dataset for their model evaluation, and compare their

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results to Fisher et al. (2016) extensively for RONO2 budgets and speciation. It should be pointed out that this paper uses a RONO2 yield of 13%-14% from isoprene RO2+NO reaction, in contrast to 9% assumed in Fisher et al. (2016). Such difference would presumably lead to significant differences between these two models. I believe some caveats should be provided in the text to make reader aware of these differences.

2. Similar to Fisher et al. (2016), the authors find a model underestimate of RONO2, as shown in their Figure 5. A recent study by Li et al. (2018), suggests that a large part of discrepancy could be due to terpene nitrates and nighttime isoprene nitrates. In particular, the authors assume a 100% recycling of NOx from APINONO2 + OH. This choice may have a large impact on total RONO2. For nighttime chemistry, the authors have ignored the formation of dinitrate (N31 for Table 2), which could also contribute to RONO2, according to Li et al. (2018). Some discussion on the uncertainties of terpene nitrates and nighttime isoprene nitrates, should be included in the text.

3. The reader is also wondering how this model performs on HNO3 and PAN, which are major NOy reservoirs. Examining these species may help to justify the 60% reduction of U.S. NOx emission inventories in their model.

4. It seems that Section 3.4, Global budget of formic and acetic acid, is disconnected from the rest of the paper. It appears that the authors want to recalculate the global budget of these two acids, without any comparison to field observations. It is unclear how this new mechanism has improved current knowledge on formic and acetic acid. Some model sensitivity tests and comparison to observations would be useful.

5. While reading Section 3.4, the authors suggest CH3CO3+HO2 is the major source of CH3COOH. This seems like another good reason to examine PAN in their model.

6. Given the extensive research on isoprene oxidation over Southeast US, the authors should include two review papers on this topic in their introduction, Carlton et al. (2018) and Mao et al. (2018).

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