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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.

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Reply to Anonymous Referee #3

We thank the referee for their comments and respond to the points raised below.

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

This is correct. This difference in RONO2 yield between the two studies is now mentioned in the discussion of the NOx loss through RONO2 formation (Sect. 4.2) and again in the evaluation of total RONO2 against SEAC^{4}RS measurements (Sect. 4.3).

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.

Thank you for these valid points. We include now a more complete discussion of the possible causes of RONO2 underestimation in the model: "There are several possible explanations for the discrepancy, including the neglected reactions of NO_3 with unsaturated oxidation products from isoprene and other BVOCs, the neglected formation of unsaturated dinitrates from the reaction of dinitroxyperoxy radicals (NISOPO2) with NO (Li et al., 2018), a possible overestimate of the tertiary nitrate hydrolysis sink (for dinitrates from ISOP+OH), and a misrepresentation of alkyl and hydroxyalkyl nitrates from other precursors than isoprene. The monoterpene nitrates are very crudely represented in the model. In particular, the assumption of 100% NOx recycling in their reaction with OH could lead to a significant overestimation of RONO2 loss. "

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.

We now include PAN in the model comparison with SEAC^{4}RS (Fig. 9). A moderate model overestimation is found, similar to previous studies (Travis et al. 2016, Li et al. 2018). The model also overestimates HNO_3 measurements from SEAC^{4}RS, but reproduces well the average NO_3^- wet deposition measurements over the U.S. (data obtained from R. Larson, NADP Database Manager, Wisconsin State Laboratory of Hygiene). A detailed discussion and justification of the NOx emission reduction (similar to a previous model study, Travis et al. 2016) is clearly beyond the scope of our study.

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.

As reported in the text, there is wide consensus that models underestimate formic and acetic acid abundances by large factors. This has been shown through numerous model comparisons with aircraft, ground-based and in situ measurements. Our study does not claim to reconcile models with observations. Since our newly-derived global sources of those acids are similar as (or even lower than) in previous modelling studies, it is clear that the large model underestimations remain, and extensive comparisons with atmospheric observations are not needed to make that point. We added the following sentence to Section 4.4: “Despite the newly-proposed large production of formic and acetic through hydroperoxycarbonyl photolysis, our derived total sources of those acids remains similar as (or even lower than) in previous modelling studies

(Paulot et al., 2011; Stavrakou et al., 2012; Millet et al., 2015; Khan et al., 2018), and are therefore insufficient to explain their high observed abundances."

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.

PAN is now included in the model comparison against SEAC^{4}RS observations.

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).

Done.

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