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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A new model mechanism for atmospheric oxidation of isoprene: global effects on oxidants, nitrogen oxides, organic products, and secondary organic aerosol" *by* Kelvin H. Bates and Daniel J. Jacob

Anonymous Referee #2

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Overview:

This paper presents an updated isoprene oxidation mechanism (RCIM) that is suitable for global modelling studies and has consequences for the burdens of several important trace species in the atmosphere; namely NOx, ozone, HOx, as well as the secondary organic aerosol (SOA). Given isoprene's importance in the troposphere, and the large amount of activity spent over the last decade elucidating its oxidation mechanism, this is clearly important work.

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Discussion paper

The paper starts with a brief description of the important changes to the mechanism relative to other mechanisms such as the MCM v3.3.1. These include new products from H-shift intramolecular reactions, new parameterisations for the nitrate yield from NO + RO2 reactions, explicit treatment of the tetra-functionalised compounds and more detailed NO3 chemistry. The effects of the new mechanism relative to other isoprene oxidation mechanisms are investigated using two box model studies and incorporation of the reduced mechanism into the GEOS-Chem global model.

While overall it is felt that this is a good paper representing a valuable addition to the literature, the reviewer has some concerns that should be addressed before the paper is published.

General comments:

In section 2.2, the three methods of analysing the RCIM are discussed. The first is a fixed radical box model where the concentrations of NO, HO2 are kept constant and the only oxidant present is OH. The second is a diurnal steady state box model which has varying radical concentrations and temperature, as well as varying emissions of isoprene and NO to simulate a tropical boundary layer. Finally, RCIM is incorporated into the global model GEOS-Chem. This is initialised for 18 months before being run for 1 year. The diurnal steady model is well explained with the daytime average value from the 8th day serving as the output. The GEOS-Chem run is also adequately explained. However, it is felt that more explanation about the analysis of the fixed radical box modelling is necessary. It is understood that the model is run until complete conversion to CO2 but it is not explained how the concentration for a particular species is calculated; is it the maximum value achieved by a species, the average concentration over a period of time or another metric?

It appears the main aim of the paper is to compare the effect of the new isoprene mechanism with older mechanisms. Therefore, it is felt that Figure 7, which compares global model results of the new isoprene mechanism with a no-isoprene scenario, is

much less relevant than Figure S17 in the SI which compares global model results between the new mechanism and the standard GEOS-Chem vn11.02 mechanism. The general effect of isoprene on NOx, O3 and OH is well known in the field. Fig S17 should replace current Figure 7 and the discussion in section 4 should focus more on the differences in global model output between vn11.02 and RCIM rather than RCIM vs. no isoprene. Furthermore, the no-isoprene scenarios plots in Figure 5 should be removed for clarity and more attention paid to the differences between the various mechanisms' outputs.

Continuing on this issue, with respect to the global model comparison section, it would be beneficial to see how the model output using RCIM and vn11.02 compare to observational data. In particular the significant predicted changes to OH, NOx, CO and HCHO over the Amazon and the CO change over much of the southern hemisphere should be compared to observational data if one is to have confidence in the use of RCIM.

The SOA yield is predicted to be significantly higher than previous models. The contribution to SOA from various species is explained. However, little detail is provided regarding the estimates of SOA production from each species aside from IEPOX. Specifically, the estimates of SOA from HMML, non-IEPOX non-IDHPE species, nitrates, glyoxal and the tetrafunctionalised species are not explained. The decision to treat the tetrafunctionalised species as LVOCs within the GEOS-Chem framework also warrants further discussion as the species span a wide range of volatilities.

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