

Geosci. Model Dev. Discuss., referee comment RC2  
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## Comment on gmd-2022-240

Anonymous Referee #2

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Referee comment on "AMORE-Isoprene v1.0: a new reduced mechanism for gas-phase isoprene oxidation" by Forwood Wiser et al., Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2022-240-RC2>, 2022

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### General comment

The authors present a work describing the construction of a very reduced isoprene oxidation mechanism by use of an original semi-automatic algorithm also developed by the authors. The manuscript is well written, and the reduction algorithm is explained well. I only have concerns (detailed below) model performance at low NO conditions.

### Major comments

- The mechanism presented has not been developed and tested for real low NO conditions (< 200 ppt) that are not that seldom in high-isoprene environments. In general, unimolecular decompositions are not considered among the "oxidation pathways". However, Bates and Jacob (2019) report ISOPO<sub>2</sub> isomerization to be 22% of the total loss on average. Reaction 2 in Table S.2 look like to be such a unimolecular reaction, but it is not found in the final mechanism. This is likely to be the main reason the authors need to add 0.6 HO<sub>2</sub> to the ISOP + HO<sub>2</sub> reaction in order to improve the comparisons with the Caltech mechanism as shown in Fig. 3. However, the comparison for ambient conditions is presented for HO<sub>2</sub> and HCHO only. The deviations of AMORE are not small but may be accepted given the extreme computational cost saving. What is worrying is the absence of a comparison for predicted OH, especially at low NO. It is by now well known that photolysis of HPALDs and other H-shifts (unimolecular decompositions) are key in determining OH-recycling and OH levels under relevant atmospheric conditions. The authors should show a comparison for OH. I mean, model bias reduction for ozone and formaldehyde simulated by CMAQ are significant (as shown in Sect. 3.3) but I wonder that could be partly for the wrong reasons. For

instance, at low O<sub>3</sub> the model bias worsens. Why is that? Anyway, errors in predicting OH cause errors in magnitude and timing of VOC oxidation and SOA production. A hint could be provided if plots like the ones in Fig. 3 and 4 were done for OH and ISOP. In Fig. 6 the error for "HOx" should be split in the error for OH and HO<sub>2</sub>.

- The pathway importance algorithm is said to be very sensitive to initial conditions (p. 9, l.219). However, the elevated values for mixing ratios of OH and NO<sub>2</sub> does not seem to be give a balanced breadth of atmospheric conditions. Measurements of OH and NO<sub>2</sub> often exceed the respected elevated values in Table 2 (2.5E6 molec/cm<sup>3</sup> and 10 ppt, respectively). I would like to see how the results change by using values like 1E7 molec/cm<sup>3</sup> and 1ppb for OH and NO<sub>2</sub>, respectively.

#### Minor comments

- The authors seem neither to explore nor to be aware that by neglecting most intermediate species (which deposit on surfaces, react in aqueous media and are transported away) any 3D-model would commit an error in the predictions of the priority species. I think this aspect should be discussed or at least mentioned.