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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 #2

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The present manuscript details the condensation of the isoprene oxidation mechanism which has been subject of revived and intense research, both experimental and theoretical, in the last decade. The authors integrated all the major advancements and originally contributed to large portion of them. Their critical understanding of the relevant chemical processes, far from being all achieved, adds to the value of manuscript. Impact of recent experimental and theoretical advancements of the global budgets of organic acids is very interesting. The model is fairly well described and the evaluation

seems appropriate for use in global models. However, a box model comparison between MAGRITTEv1.0 and MCMv3.3.1, the mechanism presented by Wennberg et al. 2018 or even their detailed mechanism would add useful information about the model performance. I wish the authors could provide such data and information.

I have two major concerns.

1) Bulk isomerization rates

Please explain more the counter-intuitive concept by which the bulk isomerization rate of the lumped (beta- and delta-) species ISOPBO2 and ISOPDO2 should linearly increase with the traditional RO2 sink rate (kp). Why is it not or it has to be different than what Crounse et al. (2011) reported? Even if correct, neglecting the RO2 sink due to permutation reactions should yield non-negligible errors/deviations from the analytical solution. Please explain why the neglect and in case provide an estimate of the deviation caused by it.

2) Reproducibility of results

The chemical mechanism of MAGRITTEv1.0 is not exactly what can be downloaded at the link given. A few sample differences are listed below.

The reaction of CH3OH with OH is standard in the manuscript but in MAGRITTE.eqn file one finds two reactions with one including the water vapor catalysis by Jara-Toro et al. 2017.

The rate constant for the reaction

CH3O2 + HO2 = 0.9 CH3OOH + 0.1 HCHO

is 4.1E-13*exp(750/TEMP) and 3.8E-13*exp(780/TEMP), respectively.

Concerning the 1,6-H-shift of ISOPDO2 in the .eqn file one finds

ISOPDO2 = 0.25 HO2 + 0.25 HPALD2 + 0.75 OH + 0.75 CO + 0.75 DIHPCHO :

4.253E8*exp(-7254/TEMP) ;

ISOPDO2 + NO = NO + 0.25 HO2 + 0.25 HPALD2 + 0.75 OH + 0.75 CO + 0.75 DIHPCHO : 6.29E-19*exp(4012/TEMP) ;

ISOPDO2 + HO2 = HO2 + 0.25 HO2 + 0.25 HPALD2 + 0.75 OH + 0.75 CO + 0.75 DIHPCHO : 4.90E-20*exp(4962/TEMP) ;

The last two reactions constants are not the ones reported in Table 2.

PYRA (pyruvic acid) is listed in Table 1. However, it is neither in Table 2 nor in the .eqn file.

Overall, it might be that the authors uploaded another version of MAGRITTE. Please upload a v1.0 that is faithful to the Tables in the manuscripts. The files should bear the information about the exact model version.

Moreover, no file with the actual functions used for many rate constants is given. This is also the case for the cross-sections and quantum yields used for computing the photolysis frequencies. Please also provide this information.

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