Geoscientific Model Development Discussions

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Comment on gmd-2021-295

Anonymous Referee #1

Referee comment on "Simulation of organics in the atmosphere: evaluation of EMACv2.54 with the Mainz Organic Mechanism (MOM) coupled to the ORACLE (v1.0) submodel" by Andrea Pozzer et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-295-RC1, 2021

This manuscript updates the treatment of oxidation products of VOCs in a general circulation model EMAC, by integrating a comprehensive VOC oxidation chemistry model Mainz Organic Mechanism (MOM) and calculating the gas/particle partitioning of the oxidation products with the ORACLE model. The treatment of organic oxidation products here is different from many previous studies in that the identitities of the oxidation products are explicitly tracked, whereas many previous studies lump the oxidation products by volatility with the VBS framework. This allows direct comparison between modeled and measured atmospheric concentrations of species of interest (e.g., CH3OH, HCOOH etc). The model predictions are then evaluated against atmospheric measurements from a wide range of sources (ground stations, aircraft, satellite and assimilated model results) for a number of important atmospheric species, including, most importantly, PM2.5, organic aerosol, and aerosol optical depth (AOD). The model generally caputres PM2.5, AOD and ground organic aerosol, but significantly underestimates organic aerosol for the free troposphere. Nevertheless, this study still represents an important step towards a complete VOC oxidation mechanism in atmospheric models to simulate organic aerosol loading, compositition, and other properties (e.g., optical or hygroscopicity). This reviewer recommends publication. Some comments for the manuscript are:

1. line 16: use "secondary organic aerosols" instead of just "aerosols", because it is already said that the aerosols discussed here are from VOCs.

2. line 37: Can the authors elaborate in the manuscript why explicit chemical identities would be useful in atmospheric simulations here?

3. For the OA treatment (starting from line 103), has the MOM + ORACLE approach been tested against chamber SOA experiments of, for example, alpha-pinene, to see if the model correctly captures SOA mass production in the experiments? This reviewer trusts

that the two submodels have been well tested in previous studies but just wonders if this can be done for closure.

4. For section 4.2.2, the authors do not seem to offer a potential explanation for the underestimation. Can this be added to the text?

5. In the outlook section, the authors discuss potential improvements to the model. Since SOA lifecycle in the atmosphere can also be affected by aerosol phase state, heterogeneous reaction with oxidant, etc., which are still highly uncertain, could the authors include these processes in the discussion as well, and talk about how they can be captured in the MOM+ORACLE framework?