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Evaluating the sensitivity to HOM production rate and vapor pressure in α-pinene ozonolysis using the open-access box model PyCHAM

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Secondary organic aerosols (SOA) cause a significant impact on human health and global climate change. Recent studies indicate that highly oxygenated molecules (HOMs) are important components for the formation and the growth of SOA (Ehn et al., 2012). HOMs can be converted to extremely low volatile organic compounds (ELVOCs), which can irreversibly condense upon particle surfaces with very high efficiency. Field measurements in boreal forest regions have proved that α-pinene comprises a significant fraction of HOM precursors (Ehn et al., 2014), thus making a significant contribution to SOA formation and growth.

The model simulation of SOA mass yield requires quantified understanding of both the chemical mechanisms and the microphysical properties of the relevant chemical species. However, high uncertainty of the mechanism and the vapor pressure of HOM species has made it challenging to reproduce experiment data using box models (Roldin et al., 2014). Additionally, the estimation of vapor pressures of HOM species is challenging: both group contribution methods and quantum chemistry methods are developed from volatility measurements of compounds with relatively high vapor pressure, such that the uncertainty range around the estimates for lower volatility compounds is unquantified (Kurten et al., 2016). Therefore, here we present a model fitting approach to limit the uncertainty of the production rate and the vapor pressure of HOM species generated from α-pinene ozonolysis by applying the newly developed box model PyCHAM (CHemistry with Aerosol Microphysics).

This box model, written in Python, is capable of simulating the gas-phase chemistry and microphysics taking place in an aerosol chamber experiment, with high flexibility and explicitness. It is designed to work with the Master Chemical Mechanism (MCM) and any other schemes following the same protocol (Jenkin, Saunders, & Pilling, 1997).

In this study, an α-pinene ozonolysis scheme is built by combining the inorganic scheme in the MCM and relevant up-to-date research targeting the HOM production mechanism together. Then, a range of vapor pressures and production yields of HOM species are tested, and their agreement with measurements from the Manchester Aerosol Chamber (MAC) is evaluated. Furthermore, the best combinations of the parameters are tested against the Aerosol Interaction and Dynamics in the Atmosphere (AIDA) (Saathoff et al., 2009) chamber data to investigate their applicability. Preliminary sensitivity tests indicate that it is possible to constrain the range of vapor pressures and production yields of HOM species to get satisfying agreement against the chamber experiments, thus lowering their uncertainty for HOM species.

Reference

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