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Modeling SOA formation from alkanes and alkenes in chamber experiments: effect of gas/wall partitioning of organic vapors.

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Oxidation products of Intermediate Volatility Organic Compounds (IVOC) are expected to be the major precursors of secondary organic aerosols (SOA). Laboratory experiments were conducted this last decade in the Riverside APRC chamber to study IVOC oxidative mechanisms and SOA formation processes for a large set of linear, branched and cyclic aliphatic hydrocarbons (Ziemann, 2011). This dataset are used here to assess the explicit oxidation model GECKO-A (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere) (Aumont et al., 2005). The simulated SOA yields agree with the general trends observed in the chamber experiments. They are (i) increasing with the increasing carbon number; (ii) decreasing with increasing methyl branch number; and (iii) increasing for cyclic compounds compared to their corresponding linear analogues. However, simulated SOA yields are systematically overestimated regardless of the precursors, suggesting missing processes in the model. In this study, we assess whether gas-to-wall partitioning of organic vapors can explain these model/observation mismatches (Matsunaga and Ziemann, 2010). First results show that GECKO-A outputs better match the observations when wall uptake of organic vapors is taken into account. Effects of gas/wall partitioning on SOA yields and composition will be presented. Preliminary results suggest that wall uptake is a major process influencing SOA production in the Teflon chambers.

References

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