

Modeling secondary organic aerosol formation from oxidation of α -pinene, β -pinene, and *d*-limonene

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The biogenic species α -pinene, β -pinene, and *d*-limonene are among the most abundant monoterpenes emitted globally. They are also important precursors to secondary organic aerosol (SOA) formation in the atmosphere. This study involves the development of proposed oxidation mechanisms for these three species. Semi- and non-volatile oxidation products with the potential to lead to SOA formation are predicted explicitly. Simulation code that describes the gas-phase oxidation mechanisms including reactions that lead to ozone (O₃) formation is coupled to an equilibrium absorptive partitioning code. The coupled model is used to simulate both gas-phase chemistry and SOA formation associated with oxidation of these three species in chamber experiments involving single as well as multiple oxidants. For the partitioning model, required molecular properties of the oxidation products are taken from the literature or estimated based on structural characteristics. The predicted O₃ and SOA concentrations are typically within $\pm 50\%$ of measured values for most of the experiments except for the experiments with low initial hydrocarbon concentrations and the nitrate radical experiments with α -pinene. The developed model will be used to update a gas-phase chemical mechanism and a SOA formation module used in a three-dimensional air quality model.

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