Secondary organic aerosol formation through chlorine-initiated VOCs oxidation in East Asia

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The Community Multiscale Air Quality (CMAQ) model v5.0.1 with a modified SAPRC-11 gas-phase mechanism and heterogeneous reactions for reactive chlorine species is further updated in this study to include formation and gas/particle partitioning of semi-volatile products from chlorine-initiated oxidation of aromatic compounds, terpenes and isoprene (CI-SOA) to provide a full assessment of the impact of chlorine chemistry on the formation of secondary organic aerosol (SOA). Reported SOA-yield data on CI-SOA formation from environmental chamber studies are used to derive the mass-yield and volatility data for the two-product equilibrium partitioning model. The updated model is applied to study CI-SOA formation in east Asia in January (winter) and July (summer) of 2013. The results during the winter show that heterogeneous reactions of chloride ion (pCl-) with gas-phase N₂O₅ and O₃ lead to a significant increase in the Cl₂ and CINO₂ and subsequently chlorine (Cl) and hydroxyl radical (OH) concentrations. A large augmentation of SOA mass concentration up to 5-15% due to irreversible uptake of the glyoxal (GLY) and methyl-glyoxal (MGLY) is predicted as a result of the increased OH concentrations. In addition, the CI-SOA from the reactions of CI radical with VOCs adds to additional SOA concentrations up to 0.5-2.5 ug/m³, which accounts for 5-10% of total SOA mass concentration. Overall, an increase of SOA concentrations by ~10-25% is predicted due to chlorine reactions in winter. The impact of chlorine reactions in the summer on SOA is much smaller due to lower concentrations of pCI- and high levels of OH that dominates the oxidation of VOCs during daytime hours.

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