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HO_x and NO_x reformation during isoprene oxidation – implications for atmospheric chemistry using a regional-scale chemical transport model

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Recent laboratory and theoretical studies have provided new insight into the oxidation of isoprene – including more detailed understanding of the formation and fate of isoprene nitrates, formation of epoxides under low-NO_x conditions, and reformation of HO_x via isomerization reactions. We have incorporated these updated chemical mechanisms into the CMAQ regional atmospheric chemical transport model and simulate the time period of the INTEX-A field campaign.

When compared with ambient measurements, we find this updated chemistry provides a more accurate simulation of isoprene oxidation products: methacrolein, methyl vinyl ketone, and alkyl nitrates. In addition, including limited HO_x radical regeneration in the oxidation of isoprene improves simulated OH concentrations, especially when isoprene concentrations are high. Over the southeastern United States, a region of high isoprene emissions, simulations including this chemistry show a 2-4 ppb increase in ozone and 30% increase in secondary organic aerosol. As NO_x emissions decrease, this chemistry is likely to grow in importance over this region.