

Research Highlight

A team of researchers simulated the production and composition of secondary organic aerosols (SOA) in Mexico City pollution outflow plume. They found that the SOA loading several days downwind was more than three times that leaving the city. These results suggest significant radiative impacts of Mexico City SOA in the outlying regions, several hundred kilometers downwind. Researchers used the gas phase photochemical box-model GECKO-A (Generator of Explicit Chemistry and Kinetics of Organics in the Atmosphere) to explicitly simulate oxidation of precursor hydrocarbons (emitted as part of vehicle exhaust in Mexico City) to tens of thousands of chemical compounds over the course of four days. The vapor pressures of these compounds were estimated and used to determine gas-particle partitioning to form SOA. The model successfully reproduced the magnitude and daytime shape for both primary organic aerosols (POA) and SOA within the city, with POA peaking in the early morning and SOA peaking during mid-day. The model also showed that SOA composition became progressively more chemically diverse with time in the outflow plume.

The majority of the model SOA originated from reaction products of the large n-alkanes, used as surrogates for all emitted hydrocarbons of similar volatility. The remaining SOA originated mostly from light aromatics. Simulated organic aerosols' elemental composition reproduced the observed hydrogen-to-carbon and oxygen-to-carbon ratios reasonably well, although the modeled ratios developed more slowly than observations suggest. SOA chemical composition was initially dominated by α -hydroxy ketones and nitrates from the large alkanes, with contributions from peroxy acyl nitrates and, at later times when nitrogen oxides are lower, organic hydroperoxides.

Despite dilution-induced particle evaporation of semi-volatile SOA compounds, the simulated plume-integrated organic aerosols mass continued to increase for several days downwind. This continued SOA production was attributed to further gas-phase oxidation of evaporated organic compounds to produce compounds of lower volatility, which then repartitioned to the particle phase to form even more chemically diverse SOA.

Reference(s)

Lee-Taylor J, S Madronich, B Aumont, M Camredon, A Hodzic, GS Tyndall, E Aperl, and RA Zaveri. 2012. "Explicit modeling of organic chemistry and secondary organic aerosol partitioning for Mexico City and its outflow plume." *Atmospheric Chemistry and Physics*, 11, 13219-13241.

Contributors

Rahul Zaveri, *Pacific Northwest National Laboratory*

Working Group(s)

Aerosol Life Cycle