Unveiling the Chemical Pathways of Secondary Organic Aerosol Formation in Hangzhou using Explainable Machine Learning

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Abstract

Secondary organic aerosol (SOA) is a significant component of fine particulate matter, exerting important environmental and climate effects. This study employing explainable machine learning (SHAP), investigated the pollution characteristics, sources, and formation mechanisms of SOA in Hangzhou City, Zhejiang Province during summer and autumn in 2023. The average concentration of organic aerosols (OA) in Hangzhou was 9.31 μg/m^3, accounting for 49% of $PM_{2.5}$, with SOA concentration reaching 5.36 μg/m^3. The H:C and O:C ratios of OA, indicative of the degree of oxidation, were 1.62 and 0.46, respectively, with oxidation processes predominantly occurring in the afternoon and early morning. Six distinct OA sources were identified: hydrocarbon-like organic aerosols (HOA, 19%), cooking-related organic aerosols (COA, 12%), nitrogen-containing organic aerosols (NOA, 12%), oxidized primary organic aerosols (OPOA, 26%), less-oxidized oxygenated organic aerosols (LO-OOA, 9%), and more-oxidized oxygenated organic aerosols (MO-OOA, 22%). Explainable machine learning revealed that meteorological conditions and precursors significantly influenced SOA formation, with meteorological conditions contributing 30-44% to SOA variation. Notably, the inhibitory effect of meteorological conditions on SOA dispersion increased with pollution severity. Different formation pathways of SOA were revealed by combining various precursors, aerosol liquid water, and machine learning methods. By combining precursors, aerosol liquid water, and machine learning methods, different SOA formation pathways were elucidated. Specifically, OPOA was derived from NOA and COA through photochemical pathways; LO-OOA formed via the photochemical reaction of MACR and subsequent condensation onto particles; and MO-OOA resulted from both photochemical oxidation and aqueous phase reaction, potentially involving transit metal ions (Fe^{2+}).

Early Career Scientist

NO, I am not an early career scientist.

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