환경 및 응용기상 분과 [P-085]

Simulation of secondary organic aerosol mass formed via multiphase reactions of hydrocarbons using CAMx-UNIPAR

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The UNIfied Partitioning-Aerosol phase Reaction (UNIPAR) model was integrated into the Comprehensive Air quality Model with extensions (CAMx) to process secondary organic aerosol (SOA) formation by capturing multiphase reactions of hydrocarbons (HCs) in regional scales. Secondary organic aerosol (SOA) mass in the Southern USA during winter-spring 2022 was simulated with CAMx-UNIPAR. UNIPAR streamlines multiphase partitioning of oxygenated products and their heterogeneous reactions by using explicitly predicted products originating from 10 aromatics, 3 biogenics, and linear/branched alkanes (C9-C24). UNIPAR simulations were compared with those produced by the Secondary Organic Aerosol Partitioning (SOAP) model, which employs simpler surrogate products for each precursor. Both UNIPAR and SOAP showed similar tendencies in SOA mass but were slightly underpredicted against observations at given five ground sites. The two models differed in terms of SOA composition and their sensitivity to environmental factors like sunlight, humidity, NOx, and SO_2. In CAMx-UNIPAR, SOA was primarily derived from alkanes, terpenes, and isoprene, and was significantly influenced by humidity, with higher SOA concentrations observed in the presence of wet inorganic salts that facilitated aqueous reactions of reactive organic products. NO_2 was positively correlated with biogenic SOA because elevated levels of nitrate radicals and hygroscopic nitrate aerosol effectively oxidized biogenic hydrocarbons at night and promoted SOA growth via organic heterogeneous chemistry, respectively. Anthropogenic SOA, which is formed mainly via daytime oxidation with OH radicals, was weakly and negatively correlated with NO_2 in urban areas. The reduction of NOx emissions could effectively mitigate SOA burdens in the Southern USA, where biogenic hydrocarbons are abundant. Furthermore, CAMx-UNIPAR found that the sensitivity of SOA to aerosol acidity was dominated by isoprene SOA.

Key words: SOA modeling, CAMx-UNIPAR, Air quality simulation