Status and problems of numerical simulation of secondary organic aerosol formation

Makoto Koike[1]; Hitoshi Matsui[1]; Nobuyuki Takegawa[2]; Yutaka Kondo[3]

[1] Earth and Planetary Sci., Univ. of Tokyo; [2] RCAST, Univ of Tokyo; [3] RCAST, Univ. of Tokyo

Quantitative evaluation of the performance of one of the most advanced mechanistic secondary organic aerosol (SOA) modules/models Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution 2 (MADRID2) in the three-dimensional Models-3/Community Multiscale Air Quality (CMAQ), in urban air is made. Model calculations were compared for the Tokyo, Japan, metropolitan area with measurements made using an Aerodyne quadrupole aerosol mass spectrometer (Q-AMS) at an urban site for nine days in July and August 2003. In general, model calculations reproduced absolute values and temporal variations of meteorological parameters, C2-C8 volatile organic compounds (VOCs), NOx (NO + NO2), inorganic aerosols, and O3 concentrations reasonably well at this site. However, model calculated SOA concentrations are a factor of five smaller than observed oxygenated organic aerosol (OOA) concentrations, and calculated total organic aerosol (OA = SOA + primary organic aerosol) concentrations are smaller by a factor of two, indicating missing processes or sources in the current organic aerosol model calculations. On the other hand, observed features of diurnal and day-to-day variations of OOA are captured by our model calculations. Because of the large quantity of unidentified total non-methane VOCs (NMVOCs) in urban air, a possible contribution of SOA formation from high-molecular-weight VOCs is examined through simple sensitivity studies, in which emissions are increased to account for unidentified NMVOCs. It was found that they have potential to be one of the missing SOA sources, demonstrating the importance of reliable measurements of high-molecular-weight VOCs and total NMVOCs. Relationships between SOA and O3, including regional enhancements (150x150 km2) around the Tokyo metropolitan area, also are discussed.