PA24) Effects of NOx on the Molecular Composition of Secondary Organic Aerosols Formed by the Ozonolysis and Photooxidation of α-pinene

박준현 · 자임빈바바 · 임호진 경북대학교 환경공학과

Introduction

The molecular composition of Secondary Organic Aerosols (SOAs), obtained from the ozonolysis and photooxidation of α -pinene, was investigated using an ultrahigh-resolution Fourier Trasnsform-Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) system. SOA formation was performed in an indoor smog chamber.

2. Materials and Methods

The molecular formulae of individual species were identified on the basis of the measured ionic mass using guidelines, such as number of atoms, elemental ratios, and the nitrogen rule. In each of the SOAs obtained, 815-3501 monomeric and oligomeric (mainly dimeric) species were identified below m/z 800.

Results and Discussion

From ozonolysis, mainly 95% of the typical oxygenated species (CHO) were detected, whereas from photooxidation under high NOx concditions, 32% of nitrogen-containing species (CHON) were detected. Several common abundant species (e.g., $C_9H_{14}O_6$, $C_{10}H_{14}O_6$, $C_{10}H_{16}O_5$, $C_{17}H_{26}O_7$, $C_{19}H_{28}O_9$, $C_{10}H_{15}NO_8$, and $C_{10}H_{15}NO_9$) could be listed as candidate tracers for the conventional tracers for α -pinene SOA. The increased percentage of CHON as a primary effect of NOx on the SOA composition evidently affected other physicochemical parameters, such as elemental ratios (i.e., O/C, H/C, and N/C), the Double-Bond Equivalent (DBE), the Carbon Oxidation State (COS), and the organic-mass-to-carbon ratio (OM/OC). The O/C, OM/OC, and COS for CHON were apparently greater than those observed for CHO, indicating that nitrogen preferentially exists in the oxidized form (e.g., -ONO₂). The complexity of oligomerization was observed in DBE and OM/OC according to the number of carbon atoms.

4. References

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