Atmos. Chem. Phys. Discuss., 12, C7777–C7779, 2012
www.atmos-chem-phys-discuss.net/12/C7777/2012/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Analysis of secondary organic aerosol formation and aging using positive matrix factorization of high-resolution aerosol mass spectra: application to the dodecane low-NO_x system" *by* J. S. Craven et al.

Anonymous Referee #2

Received and published: 4 October 2012

Overall: The presented manuscript describes the application of positive matrix factorization to high resolution - AMS data for an SOA experiment involving dodecane and OH radicals. The results include the findings of 3 factors that are assigned to the gas-phase partitioning of initial oxidation products, particle phase oxidation, and partitioning of the extended oxidation products. The results are very interesting but lack molecular level detail which is disappointing since the authors used a chemical ionization mass spectrometer with high resolution.

Comments: âĂć The composition of the factors 1-3 are not described. Thus, it's very

Full Screen / Esc
Printer-friendly Version
Interactive Discussion
Discussion Paper

difficult to conservatively interpret the meaning of the factors. âĂć What is meant by elemental analysis, do the authors refer to elemental ratios O/C and H/C or rather the fragment ion elemental compositions CcHhOo? âĂć Interestingly, the AMS community has adapted the van Krevelen diagram for bulk characterization of the mass spectra by plotting O/C and H/C which are determined from just a few characteristic fragmention ions. However the van Krevelen diagram (van Krevelen, 1963) was designed to elucidate the elemental compositions of many individual molecular formula. Since the authors write, "Elemental analysis of the PMF factor mass spectral profiles elucidates the combinations of functionality that contribute to the slope on the Van Krevelen diagram" it would be helpful to show the detected fragment ions representing each factor in a van Krevelen diagram at a few specific points over the experiment. âĂć The motivation for the current work – a study of alkane oxiation – is based on a description of UCM from GC/MS methods from more than 10 years ago. What is the evidence of alkane components; does this contridict the observations from several recent papers which have referred to an aliphatic or terpenylic character in ambient aerosol? Is the oxidation of alkanes suspected to be more significant than terpenes as the source of aliphatic or terpenylic character. âĂć Please provide at least a short summary of the CIMS instrument and its general operation (St. Clair et al., 2010; Paulot et al., 2009; Crounse et al., 2006). âĂć Please detail the resolving power with respect to a specific mass and provide the mass range of the observed ions with chemical ionization. Examples of the well resolved molecular ions would nicely complement this work. âĂć PHA is an unnecesary acronym, potentially leading to confusion. Please write out peroxyhemiacetal formation. âĂć The term amu is not an SI unit for mass. It pertains to the mass scale where the mass of oxygen was fixed to 16.0000000. Please see "Units in Mass Spectrometry" by KENNETH L . BUSCH (http://www2.chemistry.msu.edu/courses/cem832/units_of_mass.pdf). âĂć The caption for Figure 4 appears to be incorrect, "...early C18 SOA formation." âĂć Seed particles were dried or wet? âĂć What were the desired gas-phase concentrations?

ACPD

12, C7777–C7779, 2012

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 16647, 2012.

ACPD

12, C7777–C7779, 2012

Interactive Comment