Geophysical Research Abstracts,
Vol. 10, EGU2008-A-12294, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-12294
EGU General Assembly 2008

Detection of Gas Phase Oxidation Products of Limonene, α-pinene, α-terpinene, ocimene and β-caryophyllene within an Atmospheric Simulation Chamber using Chemical Ionisation Reaction Time-of-Flight Mass Spectrometry

Timo K. Carr (1), Kevin P. Wyche (1), Rebecca L. Cordell (1), Andrew M. Ellis (1), Paul S. Monks (1), Gordon McFiggans (2), Fiona Turner (2) and Martin Irwin (2)

(1) Department of Chemistry, University of Leicester, Leicester, UK,

(2) Department of Chemistry, University of Manchester, Manchester, UK

(tc59@le.ac.uk / Phone: +44 116 2525681)

Atmospheric aerosols are known to have a profound effect on the local, regional and even global environment. They are responsible for reduction in visibility, cloud formation, and have also been implicated with climate change due to their light scattering and absorbing properties altering the Earth's radiative budget. In addition, aerosols have been determined to impose various adverse health impacts on human life.

Formation of the Secondary Organic Aerosol from the oxidation of various volatile organic compounds (VOCs) constitutes a major source of total aerosol. Atmospheric oxidation of VOCs is known to yield an array of low volatility products which are able to undergo gas-to-particle partitioning *via* nucleation or condensation to pre-existing seed particles. SOA has sources both anthropogenic and biogenic with the total annual global emissions estimated at approximately 100 Tg C yr^{-1} and 825 Tg C yr^{-1}, respectively (Alfarra *et al.*, *Atmospheric Chemistry and Physics*, 2006, **6**, 5279)

The photooxidation systems of 5 different biogenic precursors to SOA, (limonene, α-pinene, α-terpinene, ocimene and β-caryophyllene), have been investigated utilising the indoor atmospheric simulation chamber facility at the University of Manchester (UK). As part of the study the University of Leicester Chemical-Ionization Reaction Time-of-flight Mass Spectrometer (CIR-TOF-MS) was utilized to provide the first comprehensive, "*real-time*" measurements of the organic gas-phase component of the SOA forming matrix. During the experiments the CIR-TOF-MS employed H_3O^+ ions to initiate proton transfer to the analyte volatile organic compounds. The CIR-TOF-MS operates with sensitivities of the order 100 ncps $ppbV^{-1}$, has detection limits around 10 ppbV min^{-1}, records data with a resolution ($m/\Delta m$) of approximately 3000, and has the ability to capture the entire VOC/OVOC mass spectrum in any one instant.

The tropospheric oxidation pathways of 135 different atmospheric VOCs have been mapped within the Master Chemical Mechanism (MCM). The work presented will discuss preliminary results of the examination of the oxidation of VOCs that are currently not incorporated into the MCM and will consequently help in the validation of the mechanism, as well as addition to the MCM database itself. In total 20 experiments were conducted, both at high and low initial VOC concentrations (250 ppbV and 50 ppbV respectively), getting close to actual atmospheric concentrations. For example, for limonene, 90% of the precursor was oxidised in the chamber with a total of 45 ions detected at high concentrations with 9 ions higher in mass than that of the precursor. At low concentrations, 99% of the limonene was oxidised, resulting in a total of 20 ions detected with 4 of those heavier than the precursor. Similar total oxidation and detection of ions was established with all 4 other VOC precursors. This work presents the first analytical observation of the oxidation products from the precursor VOCs themselves at such low and realistic concentrations.