



Gas/particle partitioning of oxidation products in simulation chamber experiments

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Simulation chamber studies on the atmospheric oxidation of VOCs have proven to be useful in helping to identify the chemical composition of secondary organic aerosol (SOA). However the large number and diverse chemical nature of the reaction products presents difficulties for sampling and analysis. Furthermore, many of the products are semi-volatile and can partition between the gas and particle phases. In this work, a new denuder-filter sampling system has been developed to collect gas and particle phase products arising from the atmospheric oxidation of VOCs. The denuder is coated with a mixture of XAD-4 resin and the derivatizing agent O-(pentafluorobenzyl)-hydroxyl amine (PFBHA) which reacts specifically with compounds containing aldehyde and ketone functional groups. The filter is also coated with PFBHA to derivatize the particle-phase products. The derivatized compounds are detected by GC-MS. The performance of the denuder was tested on a wide range of polar organic compounds including aromatic aldehydes, phenols, benzoquinones, furans and smaller carbonyls such as glyoxal and methyl glyoxal.

Once tested the method was successfully applied to simulation chamber studies of

p-xylene and isoprene photo-oxidation in order to investigate the gas/particle partitioning behaviour of the products formed. Experiments were carried out in a 6000 L FEP foil atmospheric simulation chamber equipped with online GC-FID and SMPS instruments. GC-MS was employed for the identification and quantification of derivatized species. Partitioning to the particle phase was observed to be orders of magnitude higher than expected for glyoxal and methyl glyoxal when compared to theoretical values based on vapour pressure alone. This may possibly be explained by a hydration/polymerization process occurring within the particles formed.