

Semivolatile gas-phase compounds and organic aerosol composition measured by thermal-desorption proton-transfer-reaction mass-spectrometry (TD-PTR-MS)

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A thermal desorption denuder sampling device to measure semivolatile organic compounds (SVOCs) in the gas phase has been developed and combined with a PTR-TOF8000 instrument (Ionicon Analytik GmbH, Austria). The composition of organic aerosol (OA) has been measured with the same instrument according to Holzinger et al. (2010). The first deployment of the combined SVOC and OA setup took place during the Southern Oxidant Aerosol Study (SOAS) in Centreville, Alabama, United States in the summer of 2013.

About 50 semivolatile organic compounds (SVOCs) exhibited significantly enhanced signals with mixing ratios in the range of 0.5-20 pmol/mol. More than 400 organic species were detected in the aerosol samples and ~150 of these desorbed at temperatures of 200°C and below, and exhibited mixing ratios above 0.5 pmol/mol in ambient air. If these ~150 species had significant concentrations in the gas phase they should have been detected with the SVOC denuder inlet as well, and indeed, all SVOC in the gas phase were also in the group of the ~150 species detected in OA, however, ~100 OA species were not detected in the gas phase.

Figure 1 shows number of carbon atoms and the carbon oxidation state of the ~150 OA and ~50 SVOC species. The species not detected in the gas phase typically have fewer carbon atoms and cover a wider range of carbon oxidation states, many of these species contain nitrogen atoms. OA species with less than five carbon atoms are considered to be thermal decomposition products that are produced during desorption from the collection cell. The budget of the detected compounds suggests that less than 30% of the detected OA mass is due to gas/particle partitioning of SVOCs and that other formation pathways must contribute significantly to the measured OA burden. We will discuss (i) possible secondary organic aerosol (SOA) formation pathways associated with ammonium and nitrate chemistry, (ii) the diurnal cycle of the detected species, and (iii) the role of meteorology and mixing in OA budgets.

Holzinger, R., Williams, J., Herrmann, F., Lelieveld, J., Donahue, N. M. and Röckmann, T.: Aerosol analysis using a Thermal-Desorption Proton-Transfer-Reaction Mass Spectrometer (TD-PTR-MS): a new approach to study processing of organic aerosols, *Atmos. Chem. Phys.*, 10, 2257–2267, doi:10.5194/acp-10-2257-2010, 2010.

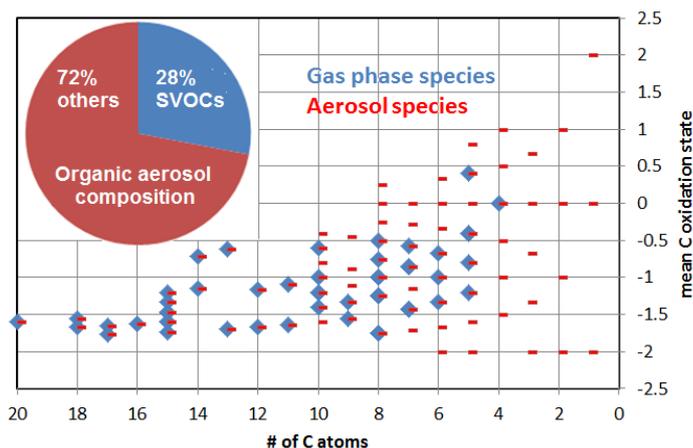


Figure 1. Detected organic species in the gas phase (SVOCs) and in organic aerosol. All species detected in the gas phase were also found in aerosol samples. OA species not present in the gas phase contain fewer C atoms and exhibit a wider range of carbon oxidation states. SVOCs constitute less than 30% of the detected OA mass.