Gas-phase products and secondary organic aerosol formation from the ozonolysis and photooxidation of myrcene

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Terrestrial vegetation releases a great variety of volatile organic compounds (VOC) into the atmosphere. Monoterpenes, like myrcene, contribute significantly to this global biogenic VOC emission. In the atmosphere, monoterpenes rapidly undergo oxidation reactions by OH radicals (mainly during the daytime), NO₃ radicals (mainly during the nighttime) and O₃ to form multifunctional oxidation products. The products of these reactions are likely to be of low volatility and hence might lead to secondary organic aerosol (SOA) formation.

In the present study, we report results from a series of chamber experiments performed in the LEAK chamber at TROPOS in which the gas-phase products and SOA yields obtained from myrcene O_3 reactions with and without an OH radical scavenger as well as from the myrcene OH radical reaction in the presence of NO_x have been measured. During the experiments the consumption of myrcene as well as the formation of gas-phase products was monitored using a proton transfer reaction mass spectrometer (PTR-MS). Ozone concentration was measured by an O₃ monitor and the mixing ratios of nitrogen oxides were measured by a NO_x monitor. Particle size distributions between 3-900 nm were monitored every 11 min using a differential mobility particle sizer (DMPS) system. In addition to the products observed by means of the PTR-MS by their m/z values, an identification of carbonylic compounds by their DNPH derivatives was performed.

Beside low molecular mass products the formation of 4-vinyl-4-pentenal with a yield of 55 % in myrcene ozonolysis has been observed. The further oxidation of this major first generation product lead to the formation of two dicarbonylic products with m/z 113 and to SOA formation. The influence of the continuing oxidation of 4-vinyl-4-pentenal on SOA formation will be discussed in detail. The emergence of the gas-phase product hydroxyacetone as direct result of the myrcene ozone reaction will be mooted, because hydroxyacetone seems to be formed directly from the Criegee radical (dimethyl carbonyl oxide). Such a rearrangement of a Criegee radical is different from the currently discussed reaction pathways.