



Reasons for the Water Effect on Terpene Ozonolysis

Å. M. Jonsson and M. Hallquist

Department of Chemistry, Atmospheric Science, University of Göteborg, Sweden
(asajon@chem.gu.se)

Terpenes contribute significantly to the atmospheric secondary organic aerosol (SOA) load. One of the major pathways producing SOA is the reaction of terpenes with ozone. Still, after more than five decades of research on the ozone initiated degradation of unsaturated compounds, there is no established chemical mechanism that can explain the aerosol formation. It has for example been shown that presence of water can affect the aerosol production.

The way water comes into the mechanism is not clear even if a direct effect by the reaction of the produced Criegee Intermediate (CI) with water has been suggested. To elucidate the water dependence of aerosol formation from ozonolysis, the present study further reviews similarities and dissimilarities in the water dependence from previous studies. The study is restricted to the monoterpenes α -pinene, Δ^3 -carene and limonene.

The relative humidity can give variations in both mass and number of formed SOA. The difference in behavior between mass and number can be explained by that products formed are either nucleating, i.e. creating new particles, or condensing, i.e. causing an increase in mass. The disagreement in water dependence on SOA formation between studies can have several reasons and four of these reasons are covered.

1) **Radical chemistry:** In ozonolysis experiments an OH scavenger (e.g. 2-butanol, cyclohexane and CO) is often used to reduce the effect of OH radical chemistry on the ozone degradation mechanism. Obviously, using an OH scavenger will suppress the OH chemistry. However, it has been shown that e.g. 2-butanol gives more HO₂ radicals in the system than cyclohexane which might influence the SOA production.

2) **Experimental method:** One issue in experimental design in studies of aerosol formation is the way of mixing the reactants. Normally, there are high concentrations

in smog chambers during the initial mixing, while flow reactors avoid this by more or less developed systems for the initial mixing. Other relevant issues are static versus flow reactor experiments and the use of different conditions, e.g. time, temperature.

3) **Gas phase processes:** An example is the concentration of reactants used. If the aerosol formation is a non-linear process (which is most likely) then the concentration of reactants and the corresponding initial rate of production are crucial for the aerosol formation. Another example is that the (CI)-water reaction can proceed via the water-dimer. This will be important, especially at high water concentrations.

4) **Liquid phase processes:** In the literature, several liquid phase processes have been proposed that will influence the mass of aerosol formed. It is an open question how water will influence the rate of liquid phase processes.

This paper presents and elucidates the probability of each process and if the process is to be of importance in the “real” atmosphere.