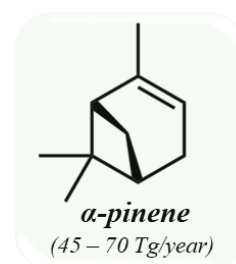


Aqueous Phase Photo-oxidation of α -Pinene Oxidation Products - Kinetics, Mechanism and Product Studies

The Earth's atmosphere is a chemical mixture with a very complex composition. It is estimated that about 2000 Tg*/year of organic compounds are emitted into the atmosphere as gases and another 300 Tg/year as suspended particulates (aerosols). The formation of aerosol particles in the atmosphere have been intensively studied owing to their tremendous impact on the human health, air quality and climate change. A significant portion of aerosols contained in the troposphere is represented by secondary organic aerosol (SOA).¹



α -pinene (C₁₀H₁₆) is considered as a one of the most important global SOA source, since it is the second foremost released non-methane compound with an estimated yearly emission rate of ~70 Tg. Reactions of α -pinene with different atmospheric oxidizing reagents results in more hydrophilic and polar compounds formation, which can undergo aqueous-phase processing. A large amount of water dispersed in the atmosphere (i.e., cloud, fog, and aerosol liquid water) makes it an important reaction medium for α -pinene oxidation products (Figure 1). However, reactions of aqSOA formation are very poorly recognized. One of the reason is the lack of the clean standards of atmospheric relevant compounds (not commercially available), which synthesis and purification is often complicated and consist of several steps. Therefore, aqSOA formation is becoming a challenging topic of interest in the field of atmospheric chemistry.

In presented project, in order to reduce some of the uncertainties in aqSOA formation mechanisms, **I focus on the kinetics, mechanism and product studies of cis-pinonic acid (PA), diaterpenylic acid acetate (DTAA) and cis-norpinic acid (NPA) in reaction initiated by OH radicals**, see structures on the left. Studied compounds are widely known as important tracers for α -pinene oxidation (later-generation products) and are of interest of a number of important fields studies. As ambient biogenic SOA is highly complex in nature investigating the behavior of individual compounds helps to detangle the chemical complexity. **A detailed study of the transformations of the**

investigated compounds in the aqueous-phase will provide a number of significant information about aqSOA formation from the investigated compounds. Moreover, obtained results will serve useful in extending the models for prediction of atmospheric processes, which are currently insufficiently developed making the ambient aerosol budget underestimated. In the presented study, **the composition of the generated aqSOA compounds will be also conducted using advanced mass spectrometry techniques (including high-resolution spectra).** At this step possible structure of selected products will be proposed.

Considering that global annual production of aqSOA closes in the range of 20-30 Tg, the aqueous-phase oxidation by OH can be an important removal mechanism of water-soluble monoterpene oxidation products. Therefore, the aqSOA studies are becoming the big challenge in the atmospheric chemistry field.

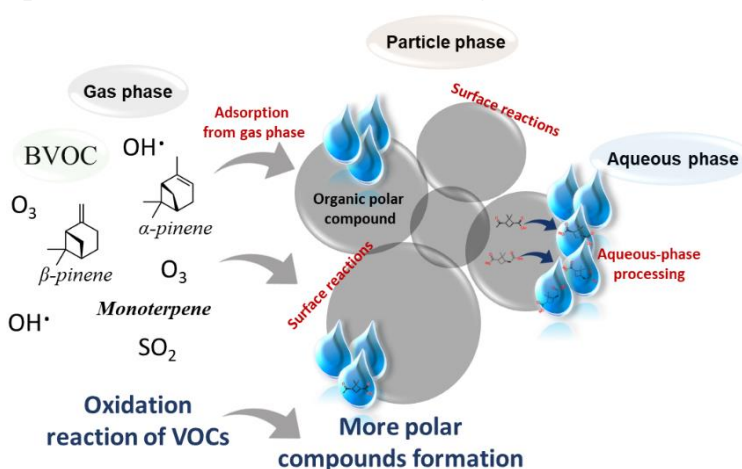


Figure 1 An illustrative scheme of the participation of aqueous phase processes in the formation of SOA particles.

1. Hallquist, M., et al., The Formation, Properties and Impact of Secondary Organic Aerosol: Current and Emerging Issues. *Atmospheric Chemistry and Physics* **2009**, *9*, 5155-5236.

*Teragram - 10¹² g