Modelling evaporative behaviours of secondary organic aerosol from α-pinene and TMB

YU MORINO*, KEI SATO, KIYOSHI TANABE, SATOSHI INOMATA, AND YUJI FUJITANI

National Institute for Environmental Studies, Ibaraki, Japan (correspondance: morino.yu@nies.go.jp)

Volatility determines gas-particle partitioning of organic compounds, thus volatility is a key factor to understand atmospheric behaviours and to simulate concentrations of organic aerosol (OA). Various studies had been conducted to experimentally measure and numerically simulate volatility distributions of OA, and over the last decade, it was found that evaporation of OA was slower than that expected by equilibrium models [1,2]. It had been suggested that formation of low volatility compounds, such as oligomers [3], or particle phase diffusion [2,4] could limit the evaporation of OA, though contributions of these factors are not clarified.

In this study, we experimentally evaluated volatility of secondary organic aerosol (SOA) from α-pinene ozonolysis and 1,3,5-trimethylbenzene by external dilution chamber experiments and chemical composition analysis. Volatility distributions were estimated from compositions observed by Proton Transfer Reaction Mass Spectrometry (PTR-MS) and Electrospray Ionisation Mass Spectrometry (ESI-MS). In addition, we conducted model simulations based on two-dimensional volatility basis set (2D-VBS) with processes of kinetic gas-particle partitioning and formation/dissociation between monomers and dimers.

Experimental results showed that low volatility compounds had important contributions to SOA, and their contributions were reproduced by the SOA model with high dimer formation rates and low dimer dissociation rates. Slow dissociation of dimers had significant contributions to reduce SOA evaporation rates as compared to equilibrium model. However, this process alone cannot explain slow SOA evaporation and particle phase diffusion also should be considered to reproduce the observed slow SOA evaporation.

[1] Grieshop, et al. (2007) *Geophys. Res. Lett.*, **34**, L14810. [2] Vaden et al. (2011) *Proc. Natl. Acad. Sci.*, **108**, 2190-2195. [3] Trump and Donahue (2014), *Atmos. Chem. Phys.*, **14**, 3691-3701. [4] Yli-Juuti (2017) *Geophys. Res. Lett.*, **44**, doi:10.1002/2016GL072364.