Deriving physical properties of SOA by using isothermal evaporation experiments under varying conditions and model optimization

Taina Yli-Juuti, Zijun Li, Olli-Pekka Tikkanen, Angela Buchholz, Eetu Kari, Liqing Hao, and Annele Virtanen
University of Eastern Finland, Department of Applied Physics, Finland

Secondary organic aerosols (SOA) are complex mixtures and their physical and chemical properties vary depending on ambient conditions. Volatilities of the SOA constituents and viscosities of the mixtures are among the most important properties for gas-particle partitioning. Both of these properties depend on the chemical composition of the particles, i.e., the SOA precursors and oxidation conditions. However, for even the same organic particle composition, volatilities of the constituents depend on temperature, while viscosity is expected to depend on both temperature and relative humidity. While these physical properties for SOA are uncertain, even less is known about their variation with ambient conditions. In this study, we derive volatility distributions, i.e., the saturation concentration distributions, of SOA particle constituents and particle viscosities based on isothermal evaporation experiments. By repeating the experiments under different temperature and relative humidity (RH) conditions and by applying numerical models together with an optimization method, we investigate also the enthalpies of vaporization and the temperature and RH dependencies of viscosity.

SOA particles were formed either by photo-oxidation or ozonolysis of alpha-pinene (apinOH and apinO$_3$, respectively) in a flow reactor. After size selecting 80 nm particles and diluting the gas phase in a differential mobility analyzer, the evaporation of the particles in a stainless steel residence time chamber (RTC) was followed over up to 8 hours. Particle size was measured with a Scanning Mobility Particle Sizer (SMPS) and particle composition was characterized with a High Resolution Time of Flight Aerosol Mass Spectrometer (HR-ToF-AMS). The temperature and RH during size selection and in the RTC were controlled and varied between the experiments. For each initial particle composition (apinOH and apinO$_3$), experiments were repeated at temperatures of 10 and 20 degrees Celsius and at RH between dry and 80%.

The measurements were interpreted by using two numerical models to simulate particle evaporation: a liquid-like particle evaporation model and a kinetic multi-layer model KM-GAP. These models were optimized to measured particle size change with a Monte Carlo genetic algorithm using the SOA properties as the fitting parameters. Estimates for the SOA properties in focus were obtained by fitting the models simultaneously to the measured evaporation of particles of same initial composition at two different temperatures and at different humidity conditions.

For both systems (apinOH and apinO$_3$) evaporation was slower under dry conditions compared to high RH and slower at 10 degrees Celsius compared to 20 degrees Celsius. However, the intensity of the temperature effect as well as the RH effect at intermediate humidities differed between the two systems. In this presentation, we will present SOA properties derived from the isothermal evaporation as well as discuss the potential and limitations of such methods for determining the unknowns among SOA properties.