Thermal properties of secondary organic aerosols

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Secondary Organic Aerosols (SOA) has a complex chemical composition and cannot easily be described in terms of vapour pressures or heat of vaporisation. Consequently several different volatility measures are used to describe their thermal properties. However, it is a challenge to clearly present and compare volatility data. To overcome this we have developed a method that makes it easy to compare volatilities and gain more information about the thermal properties of SOA.

Methods

The thermal properties of SOA can be obtained with a Volatility Tandem Differential Mobility Analyzer (VTDMA). The VTDMA measures how much size selected particles evaporate at a certain temperature.

The volatility of the particles can be presented in several different ways. Volume Fraction Remaining, VFR(T), is derived from the measured particle modal diameter (D_p) at a certain evaporation temperature T and nomalised to the selected diameter (D_{pRef}).

$$VFR(T)=(D_p/D_{pRef})^3$$

Typically, VFR(T) has been derived for several temperatures e.g. from 298 K up to 483 K. To obtain more information over the full range of evaporation temperatures, a sigmoidal curve was fitted to the full range of VFR data versus evaporation temperature.

$$VFR_T=VFR_{max}+\frac{(VFR_{min}-VFR_{max})}{1+\left(\frac{T_{position}}{T}\right)^{S_{VFR}}}$$

The slope factor S_{VFR} and $T_{position}$ define the shape and the mid-position of the curve. VFR_{max} and VFR_{min} define the boundaries of the highest and lowest VFRs, respectively. To more strictly define the most volatile and the non-volatile fraction, the equation was used to derive VFR_{298K} and VFR_{523K}. In addition, $T_{VFR0.5}$, the temperature where half of the particles volume is evaporated was calculated. $T_{VFR0.5}$ is a general measure of the volatility. The slope factor, $S_{VFR,}$ is a qualitative measure on the distribution of the volatility of the major components of the particles.

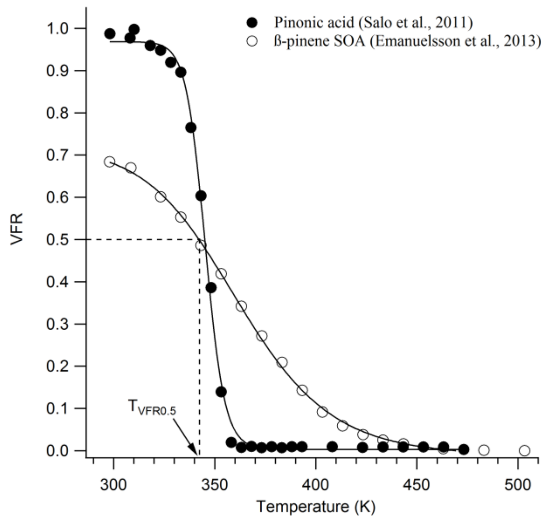

Figure 1. Pinonic acid and SOA from β-pinene charaterised over several evaporation temperatures.

In Figure 1, pure pinonic acid and SOA formed from ozonolysis of β-pinene are compared. A less steep slope (increased S_{VFR}) indicates a wider distribution of volatilities e. g. a more complex chemical composition. Pure pinonic acid (S_{VFR} = -72.4) has a steeper slope than the β-pinene SOA (S_{VFR} = -15.6). $T_{VFR0.5}$ for pure pinonic acid and β-pinene SOA was 342.2 K and 364.6 K, respectively.

Conclusions

The parameters $T_{VFR0.5}$ and S_{VFR} derived from the Sigmoidal fit have been shown to be valuable for comparing volatilities measured using a VTDMA instrument. An increase in $T_{VFR0.5}$ corresponds to less volatile aerosol particles and a decrease in S_{VFR} corresponds to a more complex volatility distribution.

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