PAUL SCHERRER INSTITUT

PSI

Volatility of biomass burning organic aerosol

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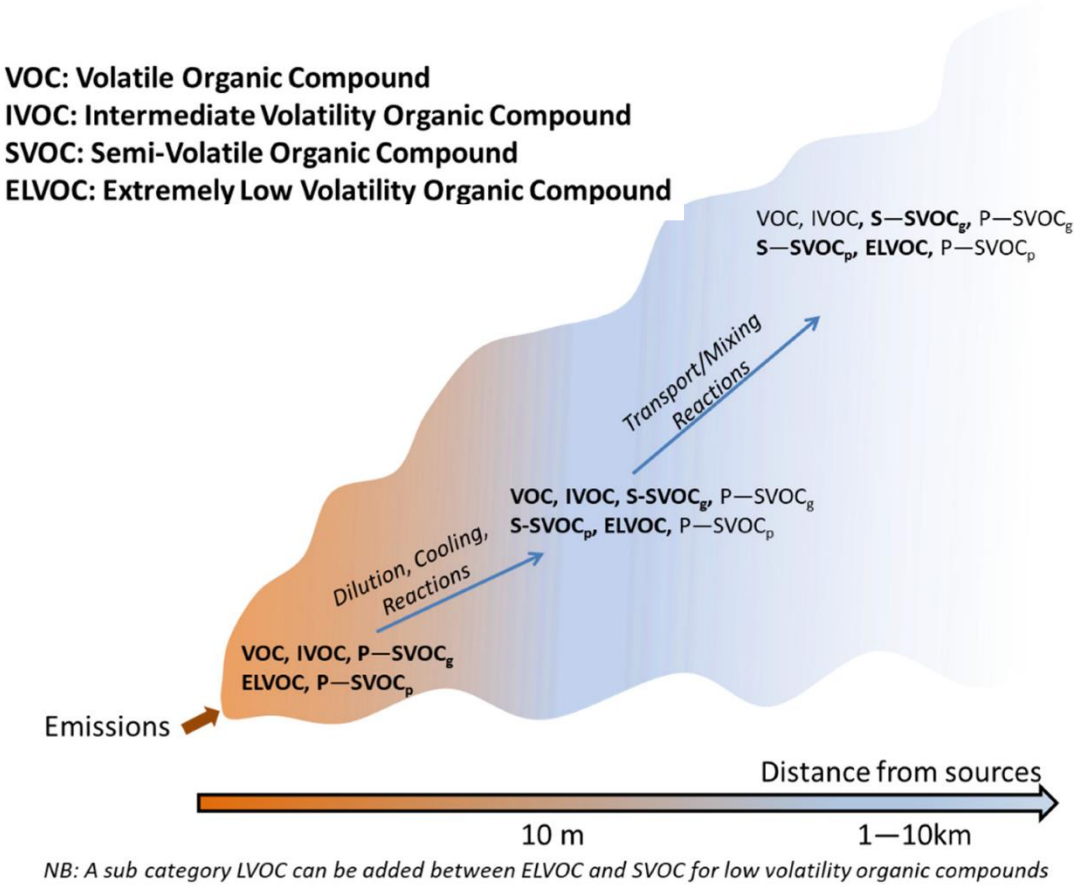
The importance of volatility in organic aerosols

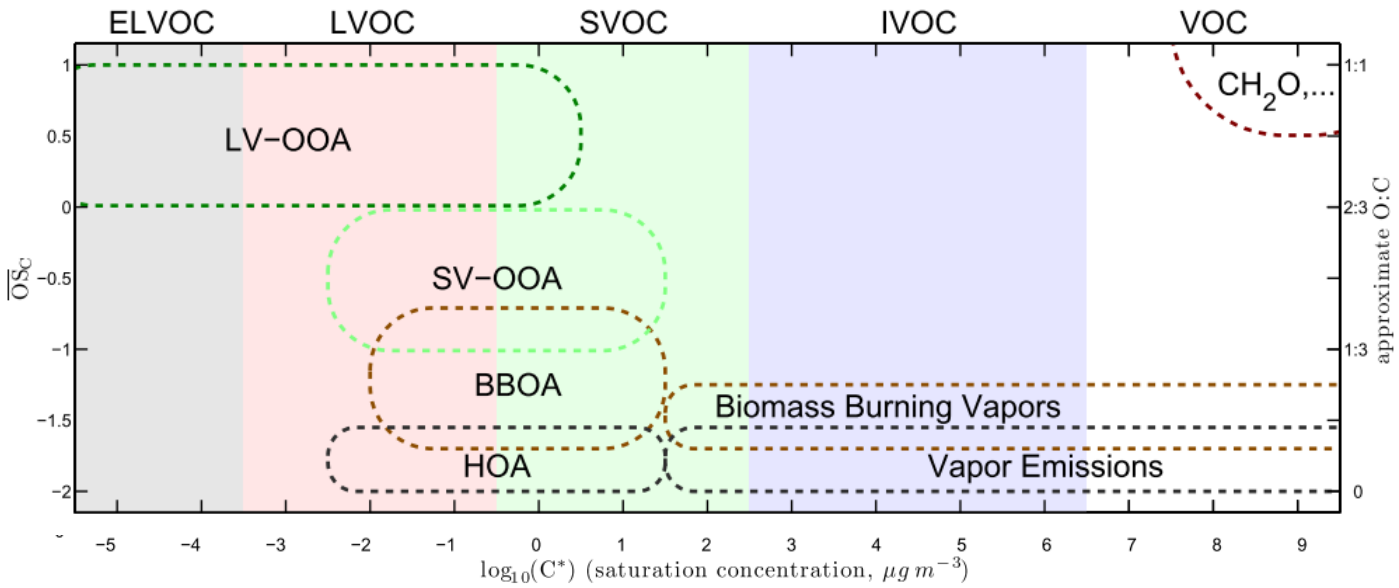
- Primary organic aerosol (POA) emitted from biomass burning contributes a large fraction of carbonaceous aerosol.
- Volatility is an important property of aerosols because it dictates the partitioning of compounds between the gas and particle phase, thereby affecting their atmospheric fate.

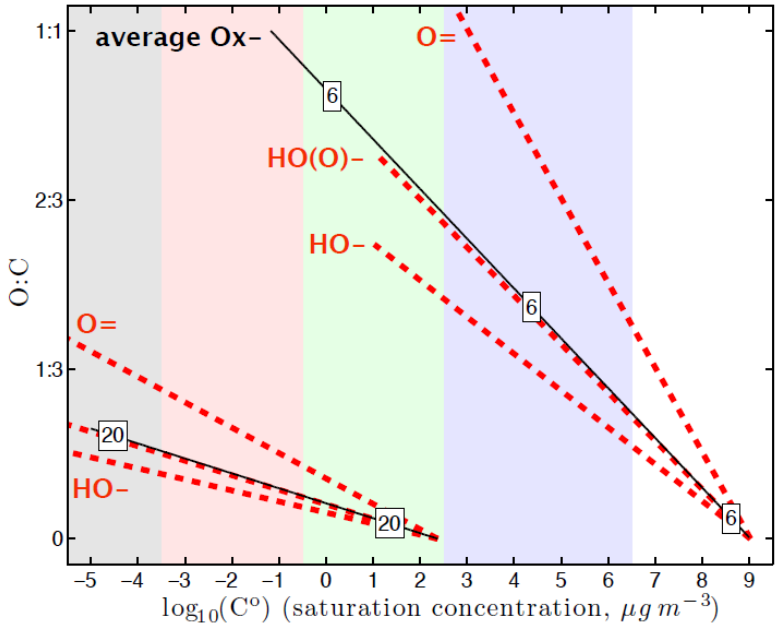
Crop residue



Volatility description

- The volatility can be described by saturation concentration (C*)
- The volatility basis set has been used as a framework to represent the volatility and the oxidation state
- Different oxygenated functional groups reduce on volatility at different levels

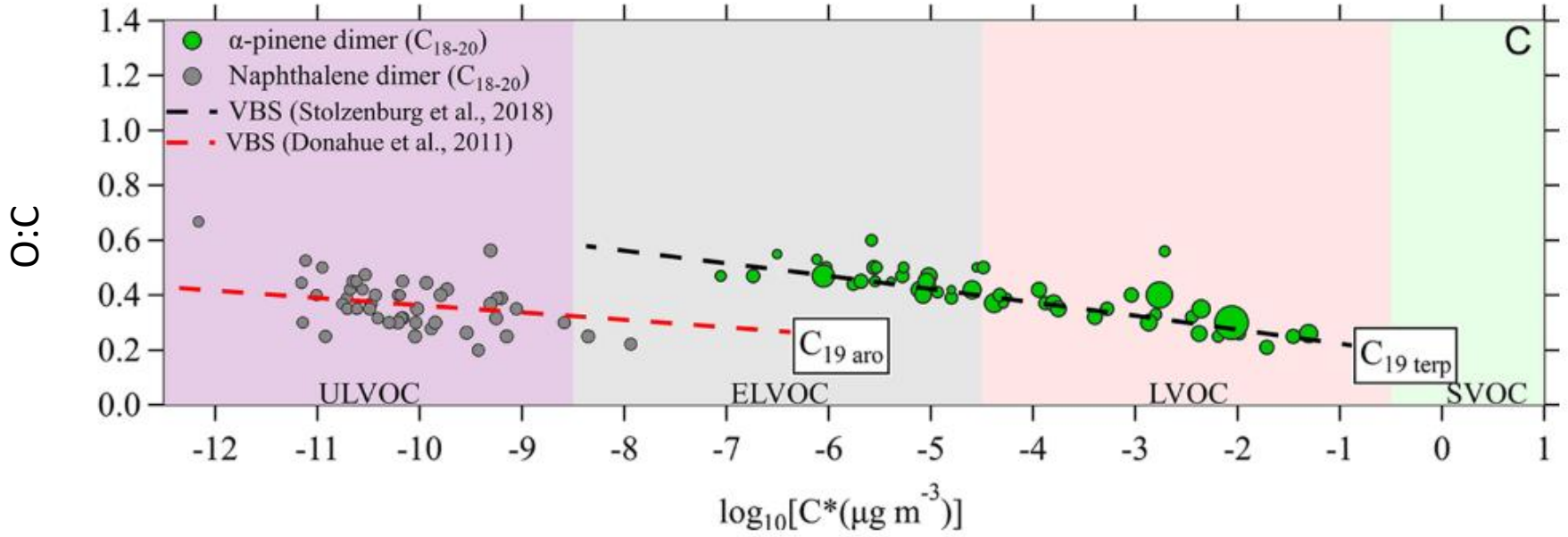




N. M. Donahue, 2011

Uncertainty of volatility estimation

- Estimating the volatility using parameterization could have large discrepancy because of the complexity of particles, e.g., chemical structure, size, viscosity…
- Volatility of POA from BB on molecular level is not available

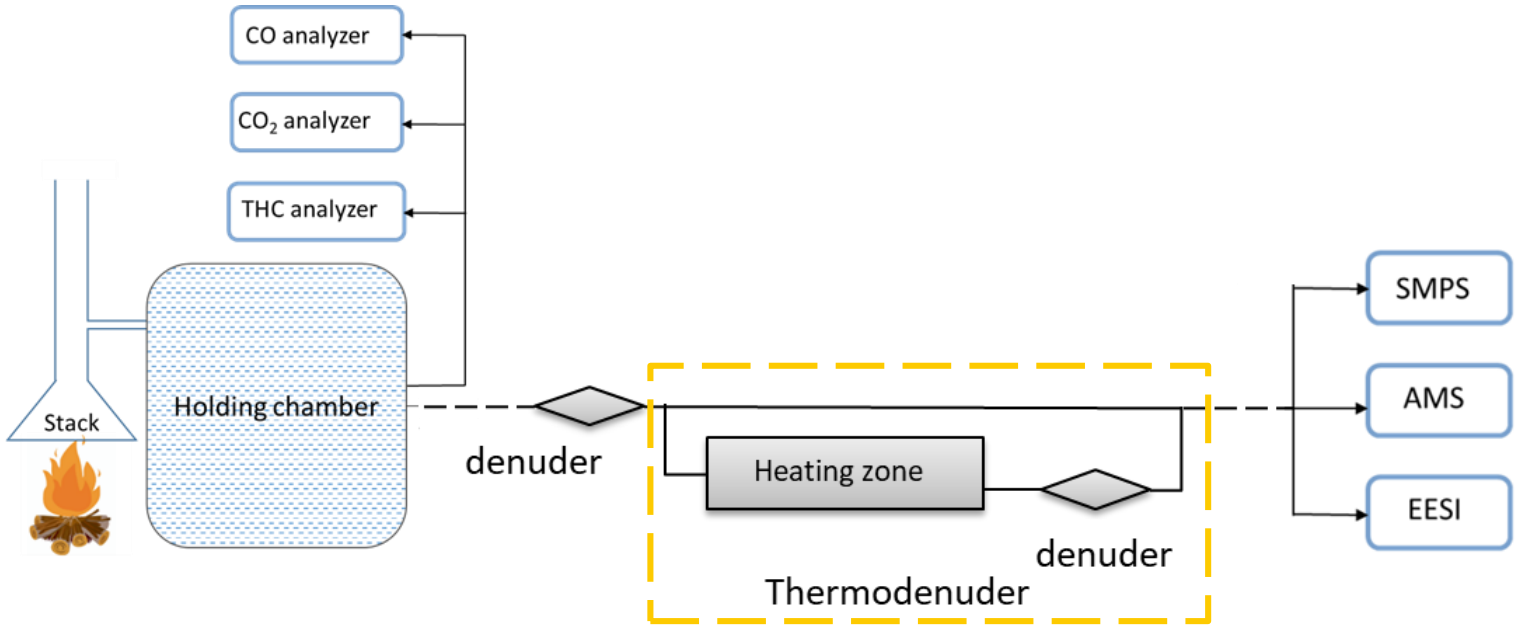


M. Wang, 2020

Questions

- What affects the volatility of BBPOA from the observation?
- What is the volatility distribution of BBPOA on molecular level?

Experimental setup



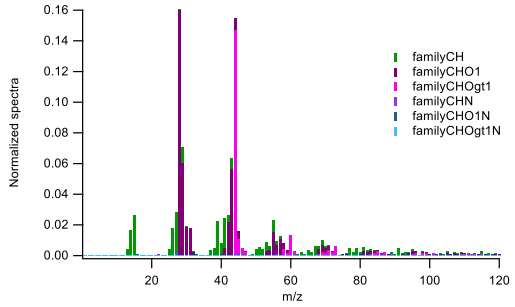
Beech Spruce Straw Cow dung

SMPS: scanning mobility particle sizer
AMS: aerosol mass spectrometer
EESI: extractive electrospray ionization time-of-flight mass spectrometer

Instruments

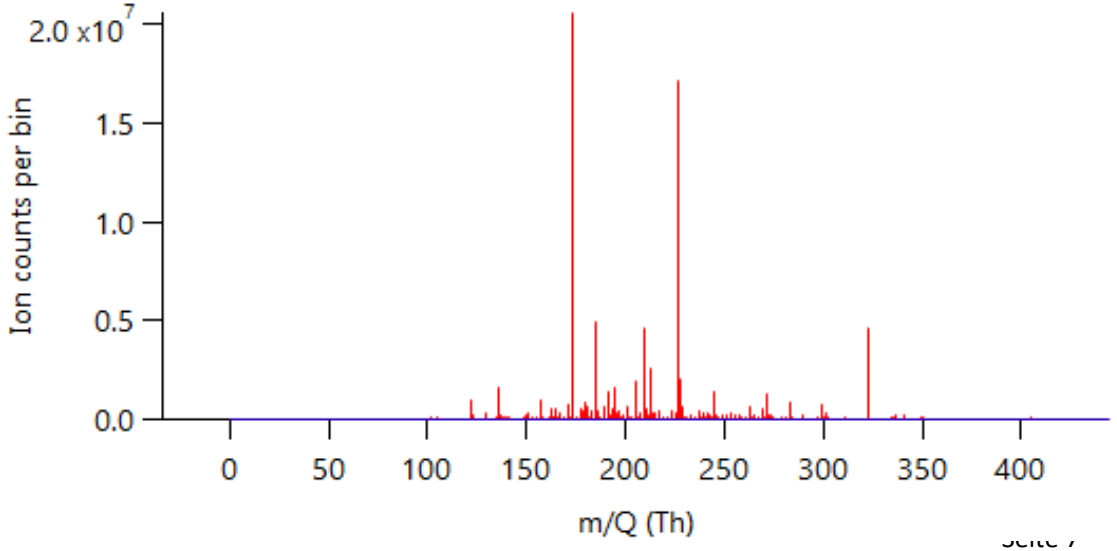
AMS-HTOF

- Can be quantitative
- For non-refractory compounds
- Electron Impact Ionization: extensive fragmentation
- Difficult to retrieve molecular information



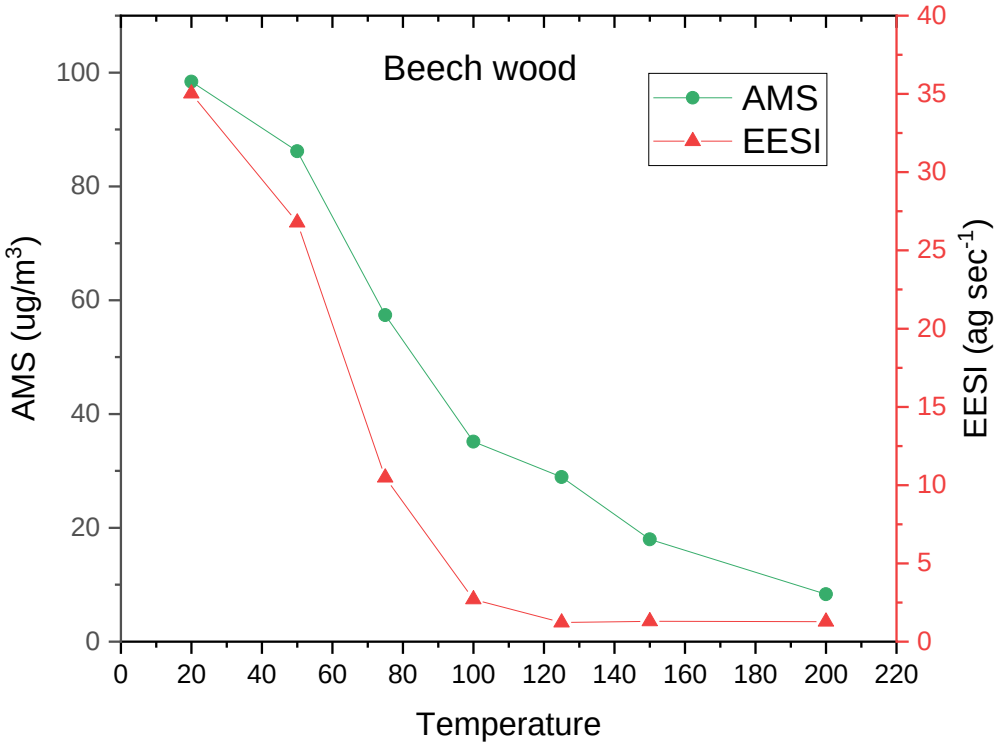
EESI-TOF

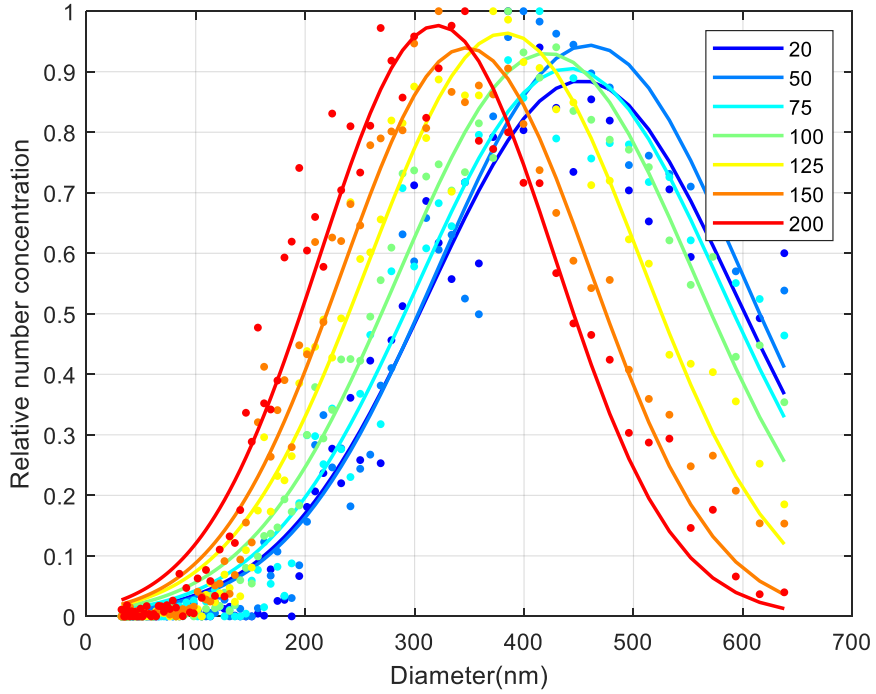
- No thermal decomposition
- Extractive Electrospray Ionization: limited fragmentation
- Can obtain molecular formula
- Only for water-soluble species here



Evaporation from SMPS, AMS, and EESI

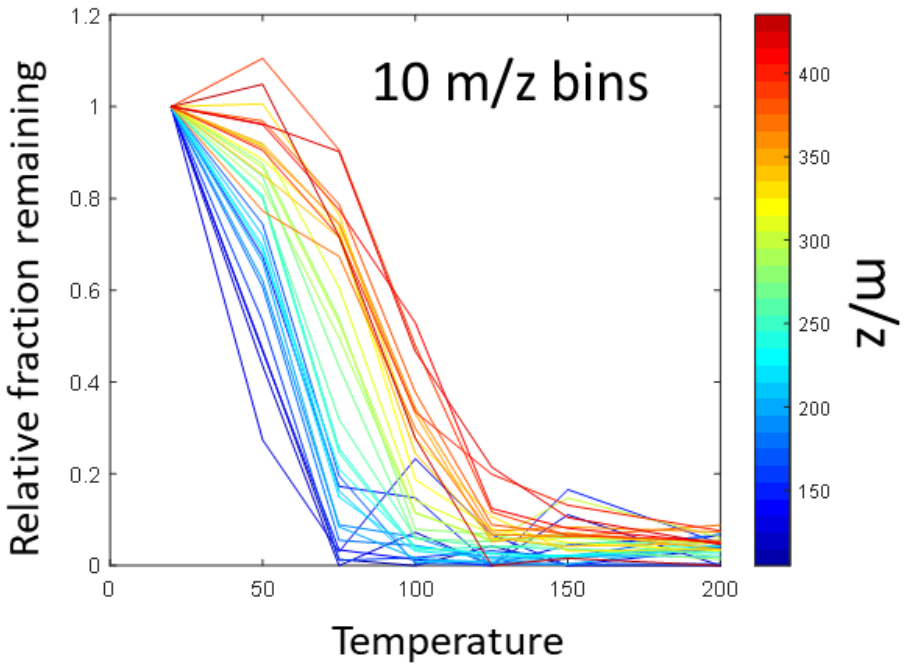
- EESI only observes the soluble fraction (and those that bind to Na^+) , most of which evaporates before 100 C
- Particle size decrease from ~ 450 nm to 300 nm by number concentration





Evaporation data from beech wood

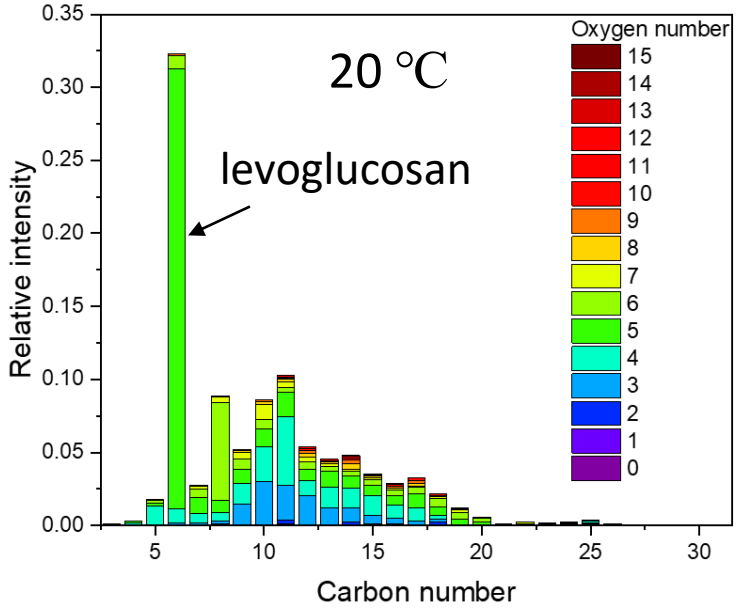
- In general, there is a trend of m/z dependence for compounds measured by the EESI

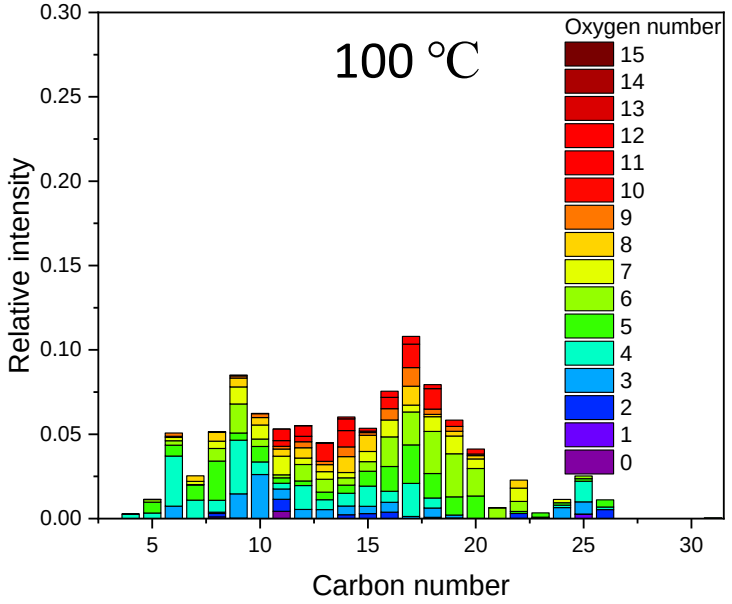


EESI

Evaporation data from beech wood

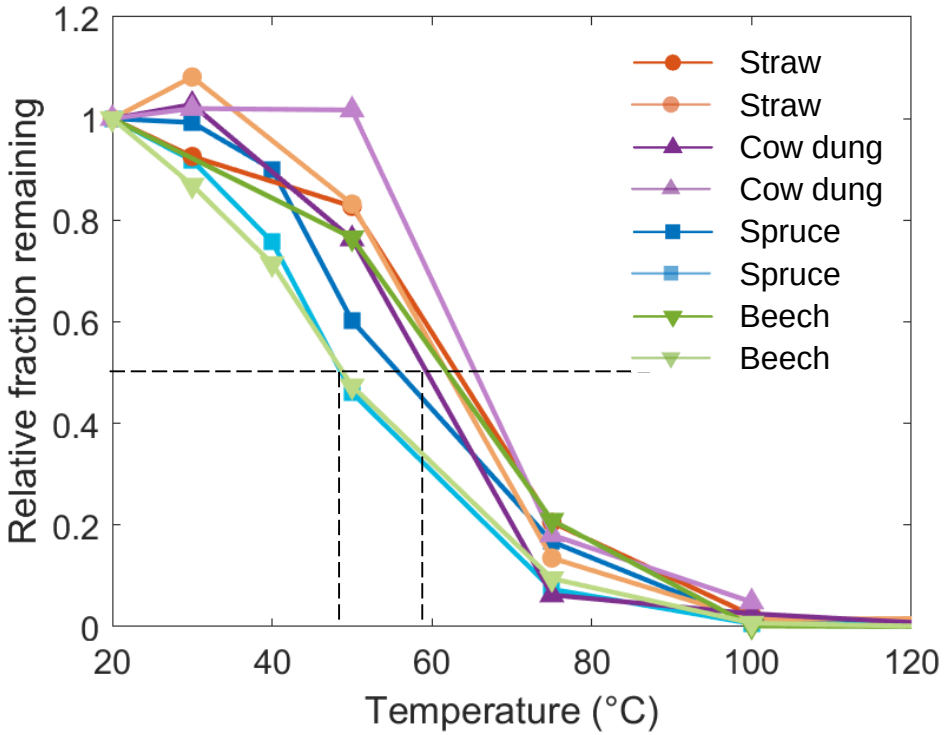
- The composition changes correspondingly
- At higher temperatures, the remaining compounds have more oxygen and carbon number



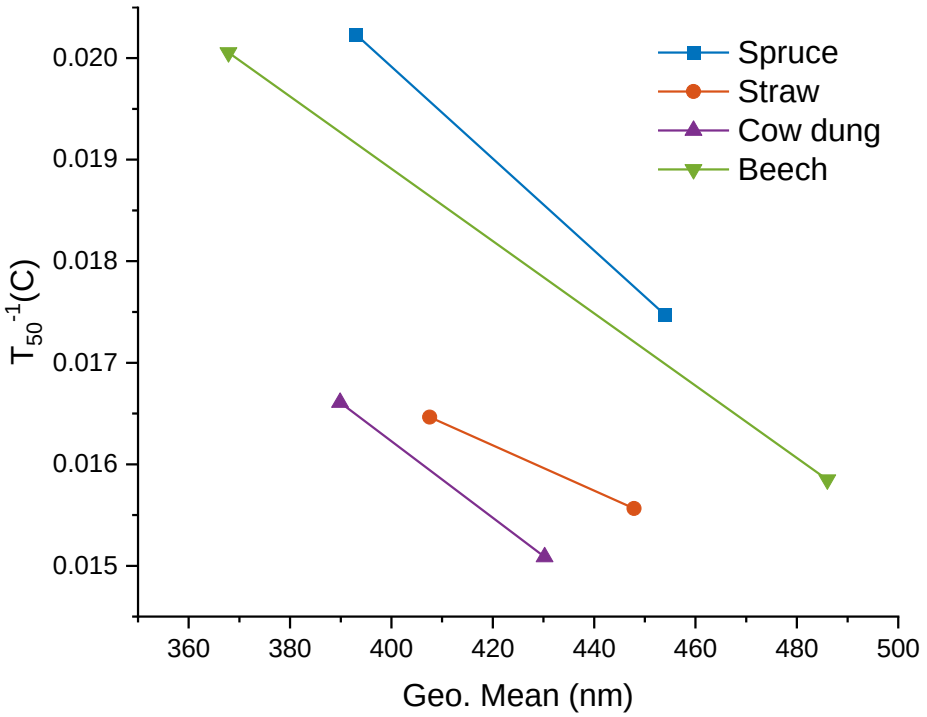


Influencing factors on evaporation: size

- The evaporation of levoglucosan is slower in bigger particles in the burning emission from the same fuel

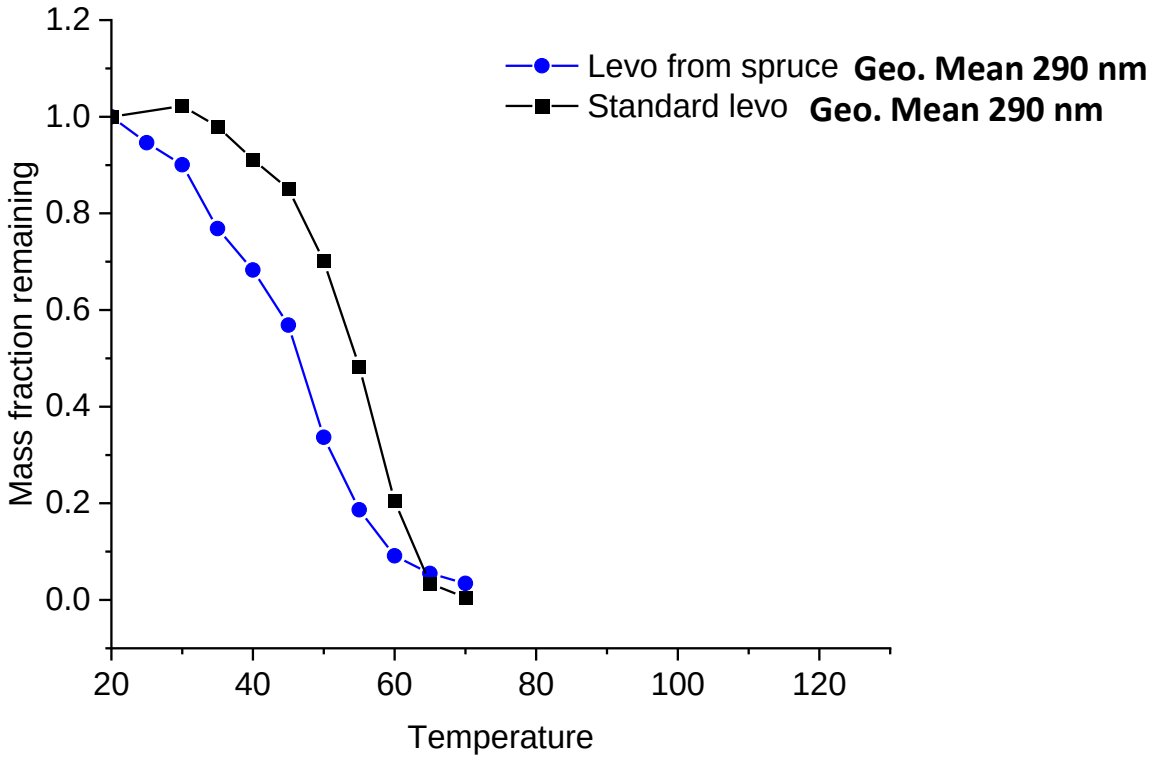


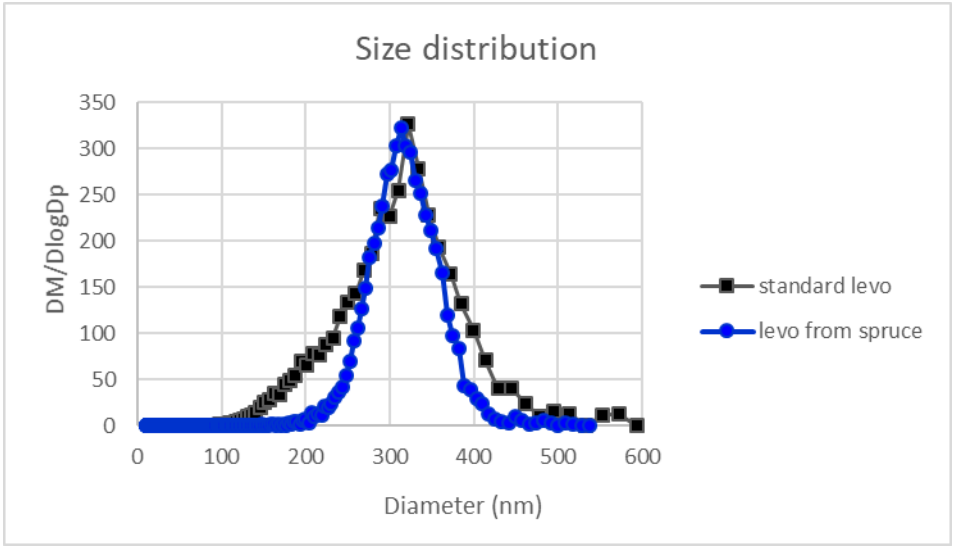
T_{50}^{-1}: 0.02 0.017
faster slower



Influencing factors on evaporation

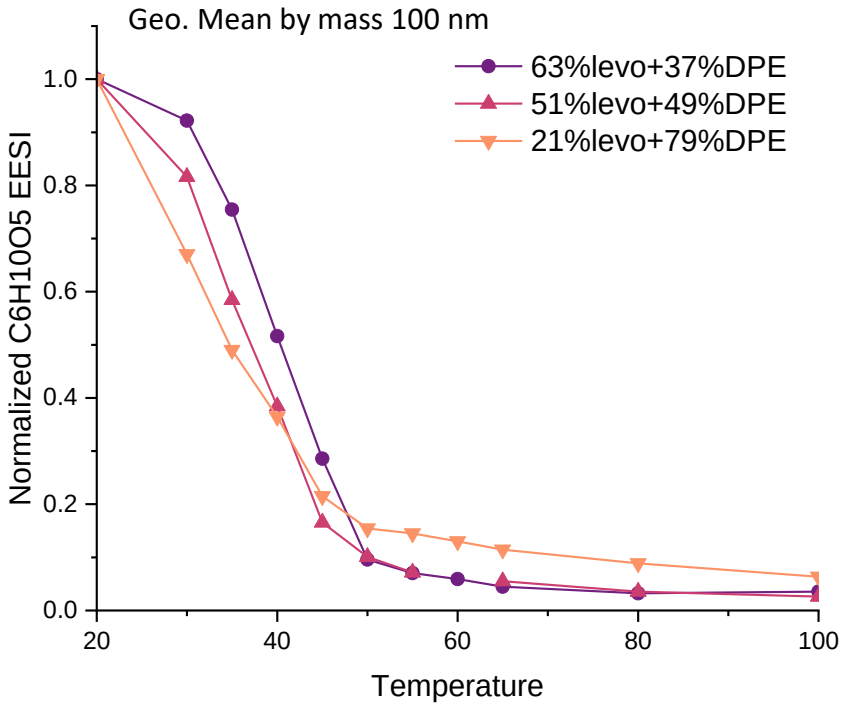
Levoglucosan from monodispersed POA evaporates faster than that from monodispersed standard

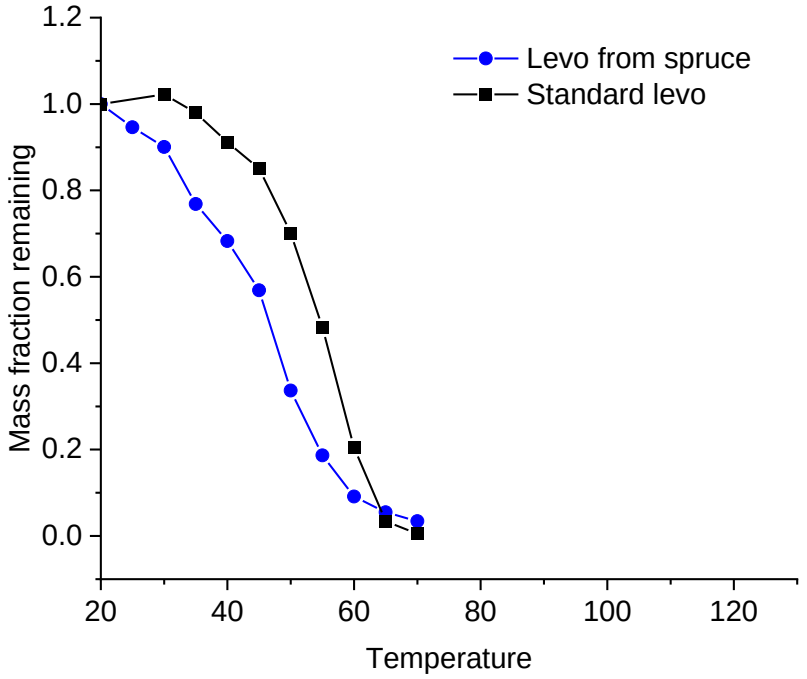




Influencing factors on evaporation: non-ideal activity

- The lower the fraction of levoglucosan, the faster the particle evaporates.
- The interaction between levoglucosan and DPE is repelling, and makes levoglucosan evaporate faster in the mixed system





DPE: dipentaerythritol

Further work

- Model the evaporation of each individual compounds to get the volatility distribution from different fuels

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Summary

- The larger compounds evaporated generally slower than compounds having smaller molecular weight.
- Size and chemical composition play important roles in evaporation of BBOA

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