ASR
Atmospheric System Research

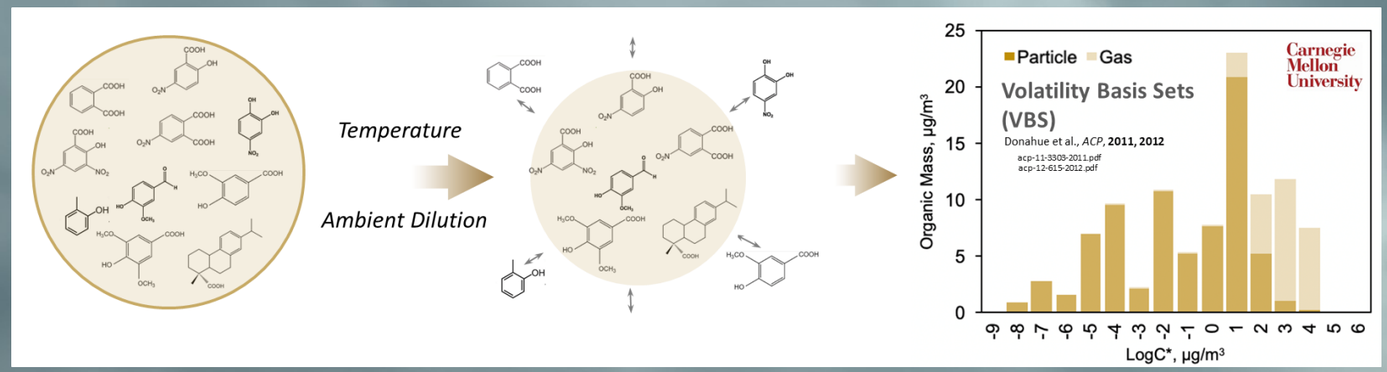
Atmospheric Aerosol Chemistry Group

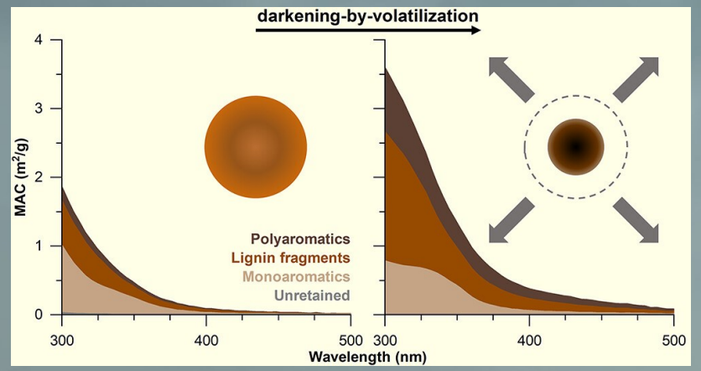
Molecular Insights into OA Optical Properties, Gas-Particle Partitioning, and Viscosity Assessment

ALEX LASKIN

PURDUE UNIVERSITY

U.S. Department of ENERGY



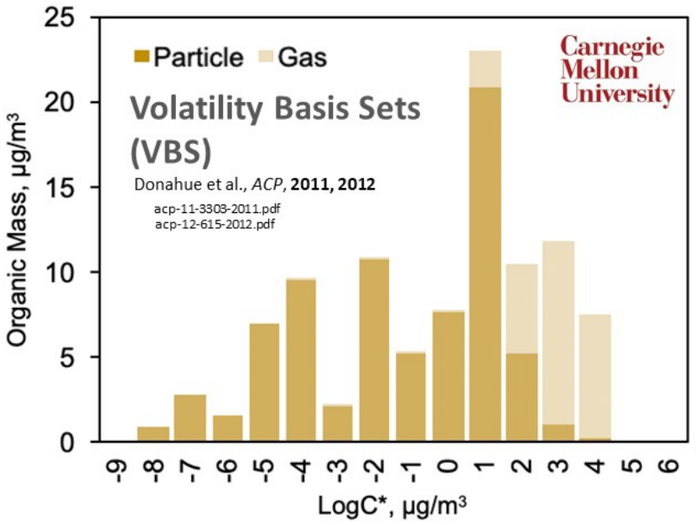


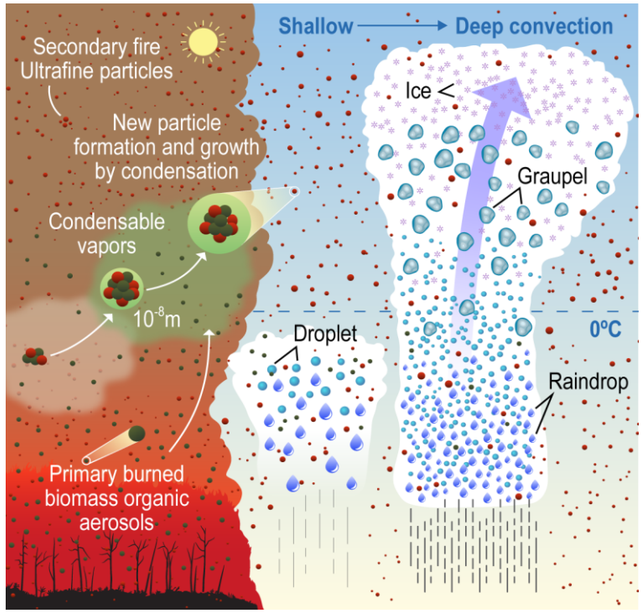
D. Calderon-Arrieta, et al ES&T, **2024**
https://doi.org/10.1021/acs.est.3c10184

2025 Joint ARM-ASR meeting

WRF-Chem modeling of OA

- Current modeling incorporates VBS based on laboratory data assumed to represent real-world conditions
- VBS of real-world, source specific OA is essential to improve model fidelity

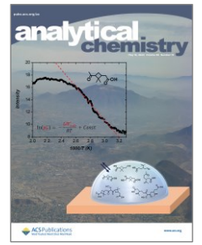




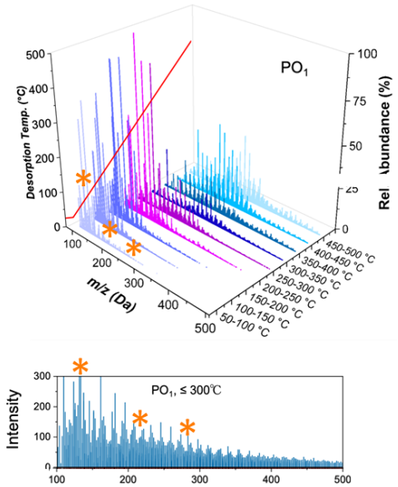
M. Shrivastava, et al OneEarth, **2024**
https://doi.org/10.1016/j.oneear.2024.05.015

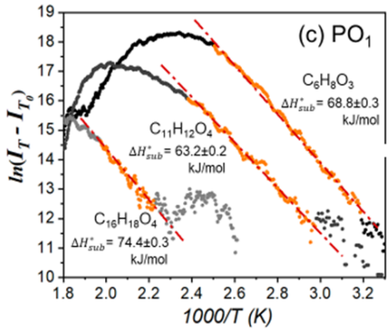
Molecular-based VBS Construction

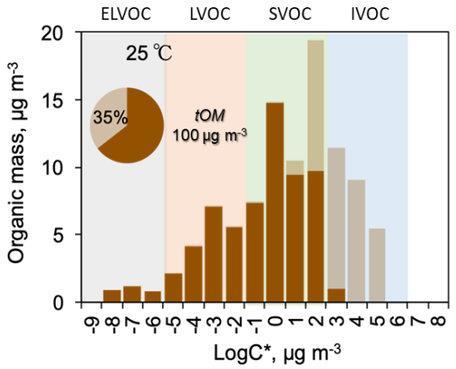
- TPD (temperature programmed desorption) → separates compounds by volatility
- DART (‘direct analysis in real time’) → chemical ionization source
- HRMS (high resolution mass spectrometer) → mass analyzer



West et al., *Anal. Chem.* **2023.**
https://doi.org/10.1021/acs.analchem.3c00923





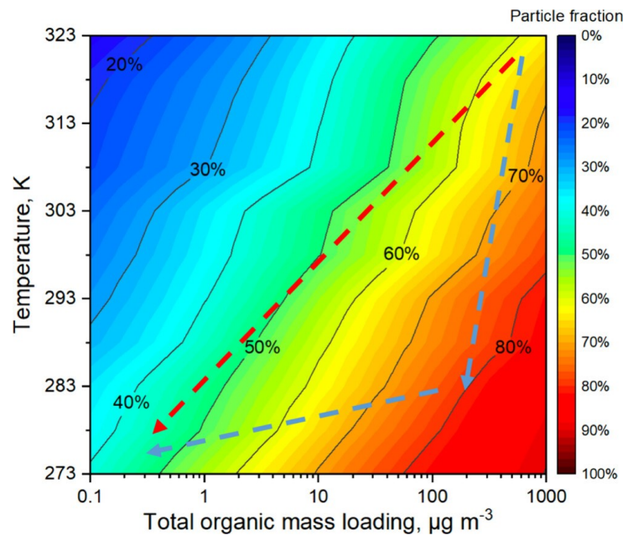


- list of $C_cH_hO_oN_n$ species (*i*)
  - $^{i}\Delta H^{*}_{sub}$ (kJ/mol)
    enthalpies of solid→gas transition
  - $^{i}C^{*}_{T}$ (µg m^{-3})
    saturation mass loadings

- species *i* grouped in **Volatility Basis Set (VBS)** $\log C^{*}_{j}$ bins
- heights (H_j) of VBS$_j$ $\quad H_j = \frac{[\sum_i {}^{i}C^{*}_{T}]_j}{\sum_j [\sum_i {}^{i}C^{*}_{T}]_j}$
- particle-phase mass fractions X^{p}_{j} $\quad X^{p}_{j} = H_j \times \frac{C_{tOM}}{C_{tOM} + {}^{i}C^{*}_{T}}$

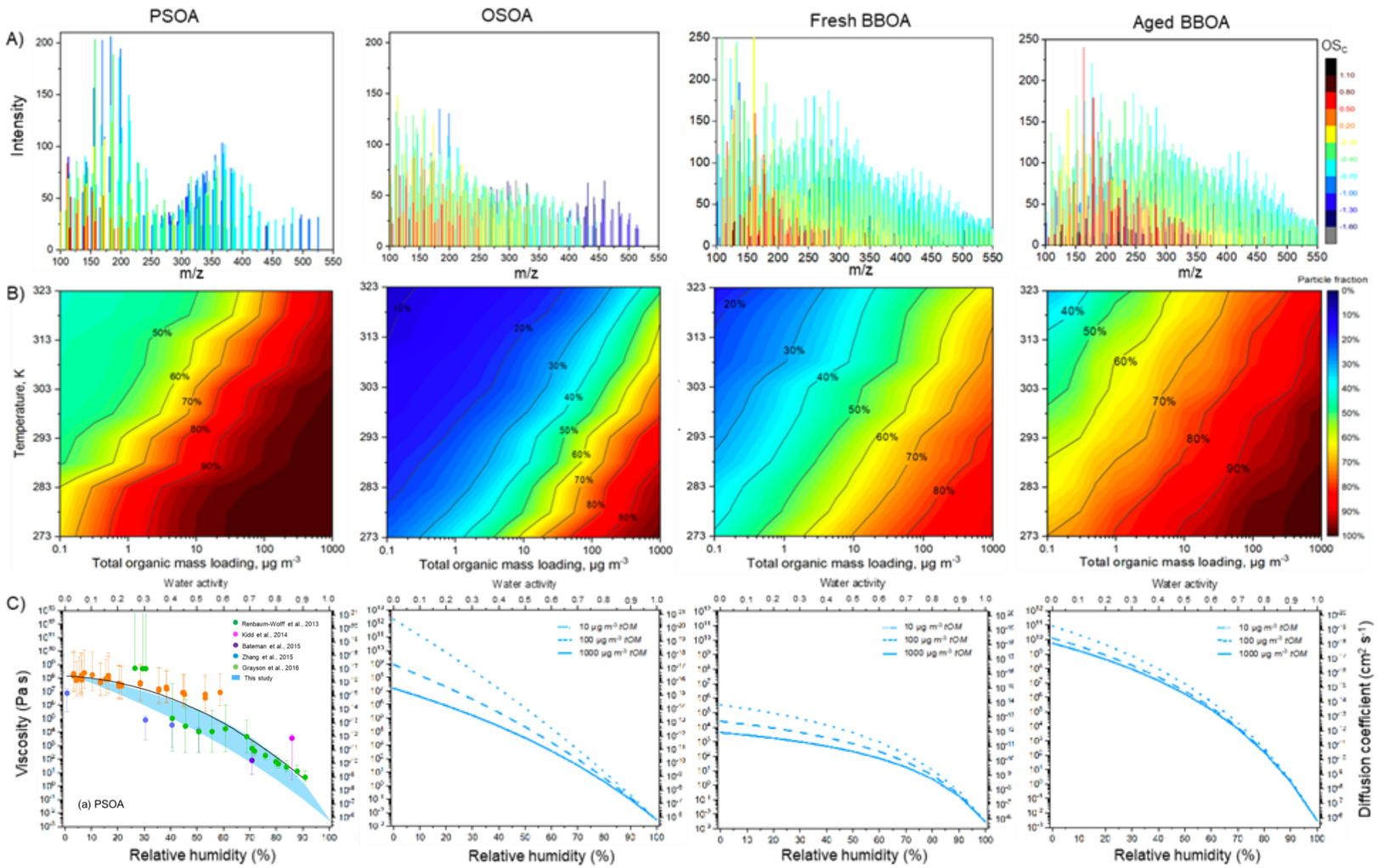
C_{tOM} - total organic mass loading

Q. Xie et al., *Anal. Chem.* 2024,
https://doi.org/10.1021/acs.analchem.4c01003



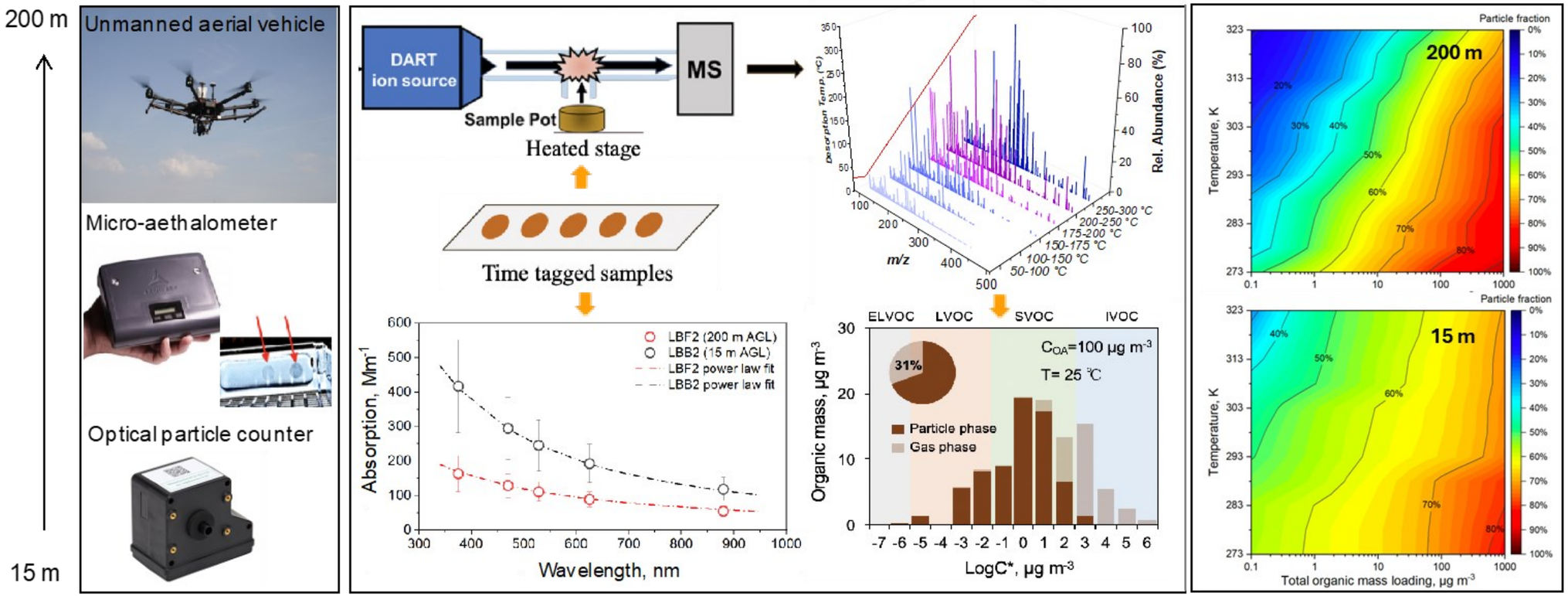
Distinct OA Composition and Properties

- Molecular Composition & Volatility
- Gas-Particle Partitioning
- Viscosity Calculations



Work with UAV Collected Samples

- measurements require >25 ng OA on substrate, with no additional sample preparation
- feasible to collect OA samples on UAS and TBS operated by the ARM AAF.



Acknowledgements

Qiaorong Xie

Dori Nissenbaum

Eli Windwer

Yinon Rudich

Nealan Gerrebos

Allan Bertram

Katherine Hopstock

Luis Ruiz Armenta

Sergey Nizkorodov