#### **SOA Formation and Properties**

# **Big Picture**

- Goal: Need to understand the sources of SOA
  - Anthropogenic, Biogenic, Biomass Burning
  - Need to understand anthropogenic influence on biogenic SOA
- Method: Need to understand these processes under different seasonal and source dominance conditions
  - Mimic in lab
  - Field studies in different locations, seasons.
- **Tool/Outcome:** Need a reliable model to capture all of the above
  - Detailed, more physically and chemically based model
  - Reliable parameterization for use in regional and global models

# Lab Studies

- Phase state of aerosols: liquid / solid / mixed-phase
- Effect of coatings on SOA (evaporation)
- Closure on gas-phase organics
- Interaction between anthropogenic precursors, oxidants on biogenic SOA formation
- What level of details are needed in models to explain laboratory data
- Detailed "master" models to serve to understand what's going on and aid the parameterization (can't extrapolate from empirical parameterizations)
- SOA formation in clouds: Need a cloud chamber?

#### Field Measurements

- C14 measurements at high time resolution
- Molecular tracers (e.g., Jamie Schauer work)
- Closure of gas-phase organics
  - Total amount
  - Speciation
  - Volatility
- Diverse locations and seasons
  - GVAX
  - Phoenix (anthropogenic only)
  - Amazon (biogenic)
- New instruments for long term measurements

# **Discussion Points**

- Which level of detail is needed in the models?
  - DW: we need to figure out what level of detail is needed to capture SOA formation into a model
- PD: it would be useful to look at SOA under diverging sets of conditions
  - E.g. region where biogenics are minimized; SOA formation in biomass burning plumes
- LK: anthropogenic-enhancement of biogenic SOA. Also partitioning theories need some revision (Alla's talk)
- SM: not clear on how many families of precursors need to be considered. Some precursors may not be receiving attention
- Which measurements?
  - SM: O/C, N/C, H/C, functional groups (FTIR), aromatics, PAHs.
  - PZ: Measurements of molecular tracers (Kleindienst, Schauer).
  - PD: closure is not feasible (PZ: not even in lab)

# **Discussion Points II**

- Which measurements?
  - LK: 14C with high time-resolution
  - DW: time-resolution is everything (15min to 1-hr @ ground site). Otherwise the details get blurred
  - JLJ: need measurements of gas-phase and semivolatiles, including volatility, some composition, with high time-resolution, even 14C
    - SP: did these measurements a while back (total gas-phase), could do again w/ some effort. Typically a factor of 2 more than speciated (vs regular GC). Could get some volatility resolution with a cooled inlet
    - LK: total OH reactivity produces similar information
    - JW: hi-res PTRMS (LK: this will be at MAOS in SGP starting next summer)
- Which field studies?
  - GVAX: polluted
  - BNL IOP: downwind of NYC & East Coast
  - Amazon 2014
  - PD: other locations with little biogenics? Phoenix: isoprene was x100 lower than in Southeast. Also go somewhere in the wintertime (less biogenics, also different partitioning of semivolatiles)
  - SM: Wyoming high winter O3 (gas drilling, snow cover, high NO2). Don't know if it makes SOA. They have 2000 wells, expect 10000 in a few years.
  - Other sources of energy: oil sands, but not in the US

#### **Discussion Points III**

- SM: what about removal processes in models?
  - JF: removal is even more uncertain than formation. Dry deposition needs a second look
  - JLJ: second comment on dry deposition. European study shows big effect
  - JF: mixing state may also play a role
  - SM: OH reaction or photolysis? JLJ: Abbat's experiments showing 10-20% mass loss in 1 week. Also lab experiments w/ ambient particles. Alla: coating with hydrophobic layers will make a difference
  - LK: long-range transport over Pacific or Atlantic to see if there is a loss of OA/ $\Delta$ CO
- Need more vertical profiles to see whether predictions of high SOA on free trop are realistic
- Clouds? BE: they form some SOA. There is also precipitation that causes loss. BE: believes that small acids are mostly due to cloud formation.
  - PZ: study of cloud SOA showing that it is important? BE: Sooroshian et al. showing oxalic acid formation, but it is a few percent of OA. JLJ: unclear whether it is important, it would be useful to have a field study to go after that.
- SP: there is a lot going on on particles themselves in the dark. Some stored chemical potential from the photochemistry

## **Discussion Points IV**

- Laboratory studies?
  - SM: anthropogenic-biogenic interactions have big implications on the radiative forcing (preindustrial vs. present). Not just look for small effects, but for big effects.
  - AZ: effect of PAH coatings on biogenic SOA (stops evaporation)
  - SM: detailed "master" models are an important piece but not whole story. They can serve to understand what's going on and aid the parameterization (can't extrapolate from empirical parameterizations)
- Emission inventories?
  - SM: constrain box model w/ ambient measurements, still see SOA gap
  - JF: if there are missing emissions that we are not measuring, that will be important
  - RZ: emissions are probably within the scope of this program (may not have the resources). PD & RZ: can be analyzed in field studies using ratios to CO. Need partners in other agencies.
- JW: additional measurements at long term facility? (Have hi-res PTMRS, mini-AMS, PILS)
  - JLJ: if those were operated with high-quality and long term, that would already be a lot. Focus
    on that first.
  - JW: would welcome suggestions of additional measurements
  - SM: spectroscopy of OA in UV-Vis range? JW, RZ: absorption at UV wavelengths would be useful.
  - JF: are SGP long-term measurements the best way for breakthrough in SOA? Maybe not.
     Maybe Eastern US where there is more of a mixture of anthropogenic & biogenic
- PZ: what about nitrate and sulfate? RZ, JLJ: amount and size distribution of ammonium nitrate are still uncertain.
- RZ: SOA formation is strongly linked to new particle formation and growth. JLJ: a nano-SMPS at SGP or other long term sites would be useful

## Discussion Points V

- JW: discussion can be continued
- JF: we would need to have an SOA model with similar complexity of an O3 model. We know what makes O3, we don't know what makes SOA
  - SM: we can get O3 to 20% with the different models. But we don't know if we can predict the changes to future emissions or climate. Gross differences in models
- SP: different types of SOA have different refractive indices that they'd change the backscatter by up to 25%. So models may need to keep track of different types of SOA separately. (n ~ 1.4 to 1.6, but only starting)
- PD: some GCM folk perceive that direct effect is not uncertain enough to merit working on it

# Objectives

• Focus on critical processes and properties related to SOA formation to improve global and regional models.

#### Look for opportunities to:

- Build collaborations
- Bring critical areas of research to the attention of the community and program management
- Advance your own ideas and interests commensurate with program objectives for continued success within the program

#### **Discussion Points**

- Need more physically / chemically based SOA models to guide the development of reliable parameterized models
- Need to demonstrate that detailed SOA models provide right answers for the right reasons
- Need to sufficiently constrain the models to properly evaluate them
  - Laboratory experiments under realistic conditions
  - Focused field studies

# Laboratory Studies

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