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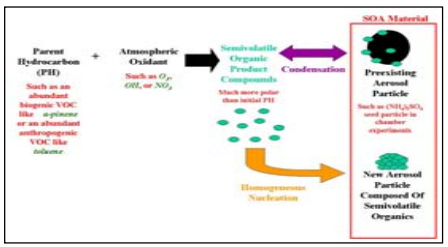
Next Generation Scientists—Next Opportunities

Chemical Speciation of Secondary Organic Aerosols

Environmental Issue

- **Purpose: To conduct a detailed investigation of the chemical composition within secondary organic aerosol (SOA)**
- **SOA are formed by essentially two steps:**

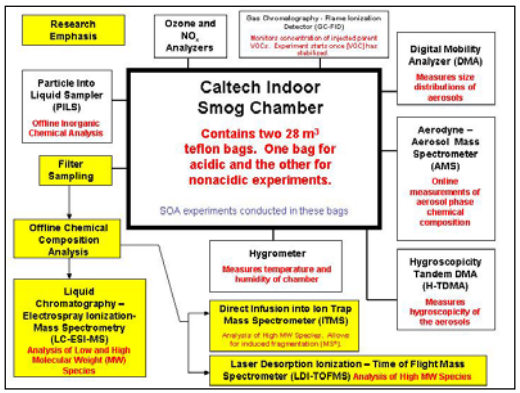
1. Volatile organic compounds (VOCs) are emitted directly into the atmosphere via biogenic and anthropogenic sources and are oxidized by atmospheric oxidants such as ozone (O_3), nitrate radical (NO_3), and hydroxyl radical (OH).
2. The products of the above gas phase oxidation reactions can either be highly volatile (such as glyoxal or formaldehyde) or semivolatile (such as some dicarboxylic acids or ketoacids). The semivolatile compounds will likely partition to preexisting aerosol via condensation due to their lower volatility compared to their parent VOC or create new particles by nucleation.



- **SOA significantly contributes to the fine particulate matter burden within the ambient atmosphere, especially in urban areas.**
- **Understanding chemical composition within SOA will help unveil important chemical reaction mechanisms (which are important for chemical and climate models), physical properties of the aerosol (such as hygroscopicity, albedo, and cloud activation ability), and adverse human health effects.**

Scientific Approach

- **Caltech Indoor Smog Chamber Studies:**



1. Chamber experiments allow the study and isolation of single systems such as important biogenic and anthropogenic VOCs present in the highly mixed atmosphere. Systems such as the ozonolysis of α-pinene (biogenic) and C_5-C_8 cycloalkenes have been studied.
2. These experiments enable the investigation of aldehydes and ketones as possible monomers that are expected to polymerize via heterogeneous chemistry (Kalberer et al., 2004; Gao et al., 2004).*
3. Aerosol generated during chamber experiments will be collected w/ Teflon filters.

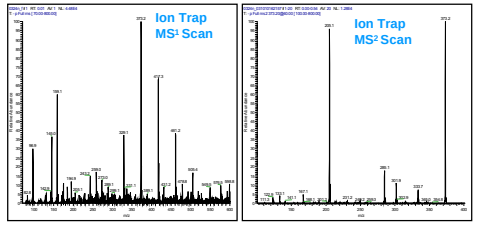
- **Ambient Aerosol Field Study: Southeastern Aerosol Research and Characterization (SEARCH)**

1. Major goal for ambient sampling of aerosol in this locale is to determine source contributors to SOA.
2. Quartz and Teflon filters are used at rural and urban sites in FL, GA, MS, and AL. These filters are sent back to Caltech for offline chemical analysis.

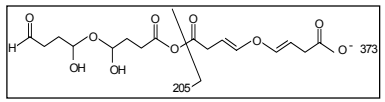
Impact

- **Example Result from Smog Chamber:**

Ion Trap Mass Spectrum of SOA in Cycloheptene-O_3 System (Direct Infusion)



1. MS^1 scan above shows monomeric species (e.g., 131, 145, and 159 m/z). These result from the breakdown of the cycloalkene through multiple oxidation steps.
2. MS^1 also shows high MW species (e.g., 329, 373, and 416 m/z) that are very likely oligomers possibly generated via *gem*-diol, aldol condensation, acid dehydration, or any combination of the 3 reactions. MS^2 scan of the 373 m/z suggests the following structure; it results from *gem*-diol reactions of ketoacids & dialdehydes as well as acid dehydration:



3. Implications: Due to important current important issues facing the aerosol community for climate modeling and understanding aerosol physical proprieties we seek to answer: Are these high MW species being generated in the gas phase, aerosol phase, or heterogeneously, and how abundant are they?

*Citation: Kalberer et al., *Science*, 303, 1659-1662, 2004; Gao et al., *J. Phys. Chem.*, in print, 2004.

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