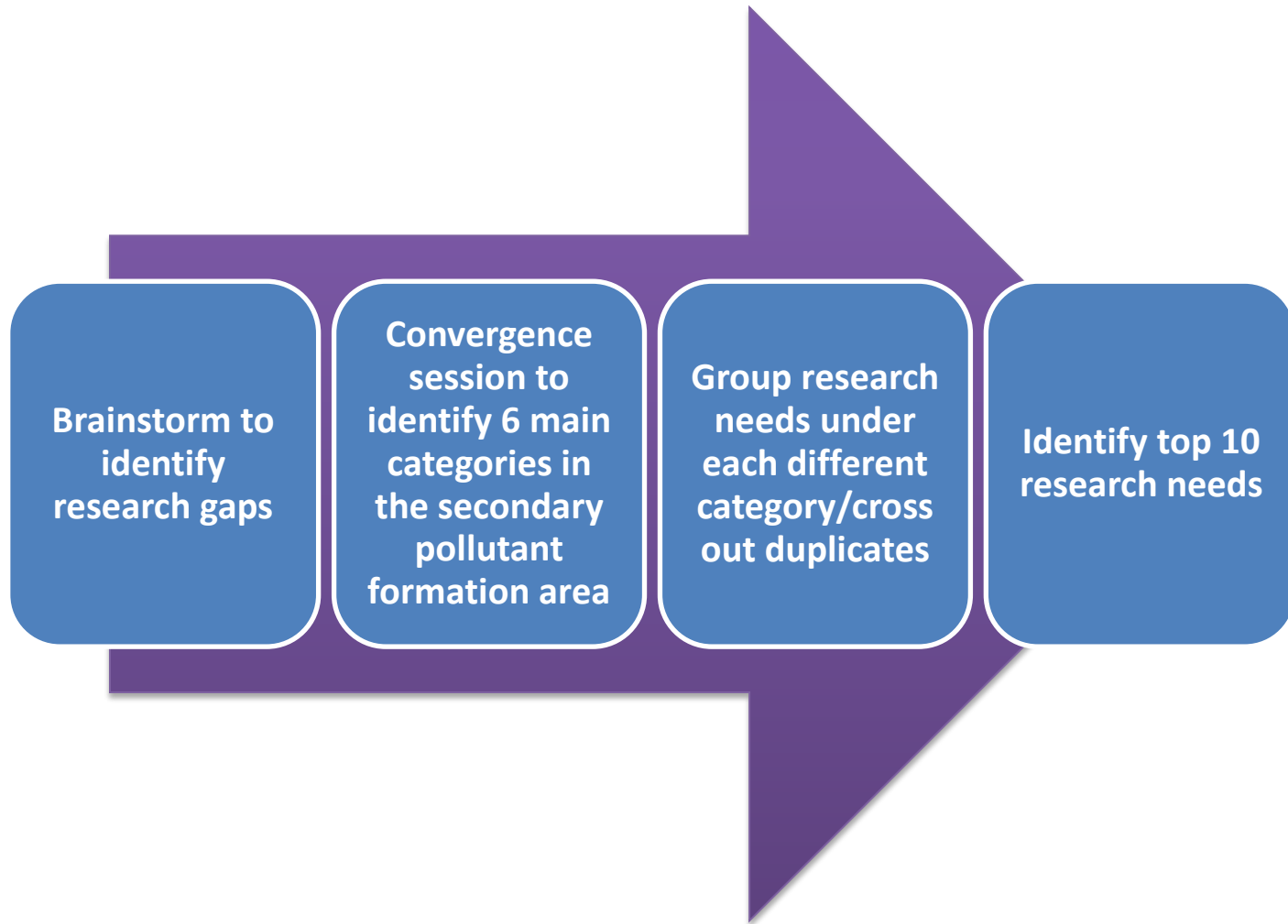


# **Top 10 Research Needs**

## **Secondary Pollutant Formation**

**CRC A-98 AQRN Workshop  
Atlanta, GA  
February 10<sup>th</sup>, 2016**

# Process and Outcome



# Top 10 Research Needs

## Chemistry

### **1. Influence of NO<sub>x</sub> on SOA/PM formation and ozone**

- (1) Evaluate ozone and SOA/PM formation at current and future VOC-NO<sub>x</sub> conditions
- (2) Identify the importance of daytime and nighttime nitrate radical oxidation
- (3) Evaluate the fate of organic nitrates and their impacts on NO<sub>x</sub> cycling and ozone formation
- (4) Update predictive models for SOA/PM and ozone formation as a function of ambient NO<sub>x</sub> levels
- (5) Use chamber studies to test chemical mechanisms and evaluate relative reduction factors

# Top 10 Research Needs

## Chemistry

### 2. Role of Water

The proposed research attempts to fill scientific gaps to help enhance our scientific understanding of the role of water in the atmosphere. The proposed research will conduct controlled studies (with respect to water content) to:

- (1) Quantify differences in secondary pollutant formation due to changes in RH
- (2) Collect new data on the hygroscopicity of secondary pollutants and the ability of secondary pollutant to act as seeds for cold and warm clouds
- (3) Model interactions of secondary pollutants in aerosol-cloud interactions and cloud processes
- (4) Dry and wet deposition effects
- (5) Water role for Henry's Law Constant for highly oxidized compounds

# Top 10 Research Needs

## Chemistry

### **3. Source Apportionment of Organic Aerosols**

- (1) New receptor-oriented approaches to quantify the contributions of known sources to SOA in ambient air
- (2) New methods for measuring components of SOA and apply statistical and optimization methods such as CMB and PMF to estimate sources making significant contributions to ambient levels
- (3) Other information in constraining estimates, including gas measurements, fast-response instruments, and nonparametric information such as wind fields
- (4) Single and multiple site analytical methods
- (5) Bayesian approaches to combine information across sites
- (6) Relative importance of POA and SOA

# Top 10 Research Needs

## Technology

### **4. Contribution of Fossil and Non-Fossil Sources to Secondary Organics Aerosol**

- (1) Perform radiocarbon analysis to distinguish fossil and nonfossil sources of carbonaceous aerosol.
- (2) Combine filter-based radiocarbon measurements with collocated organic aerosol source apportionment results to determine fraction of modern carbon in different types of SOA.
- (3) Develop and apply novel analytical techniques to distinguish fossil and non-fossil sources

These measurement results can be compared with model simulations to evaluate our estimated SOA sources and the representation of biogenic-anthropogenic interactions in the atmosphere. They can also help estimate sources of “anthropogenically influenced SOA” and estimate how this influence has changed since pre-industrial period.

# Top 10 Research Needs

## Inter-comparisons

### 5. Transfer line and chamber wall losses

**Factor of 4~5 fold impact on mass yields**

- (1) Investigate the effects of vapor loss in different parts of the emission measurement system including the transfer lines, the CVS, and associated sampling lines
- (2) Conduct systematic evaluation of organic vapor loss to Teflon environmental chambers to evaluate wall loss for organic vapors formed from different VOCs under various oxidation conditions.
- (3) Examine the extent of reversible vapor-wall partitioning
- (4) Design experiments to probe the effects of chamber history on vapor wall loss

# Top 10 Research Needs

## Composition

### **6. Anthropogenic VS biogenic interactions**

- (1) Need to do molecular-level characterization (including need of organic synthesis) of the interactions in both the gas and condensed phases in order to develop explicit models
- (2) Need kinetic measurements of important processes that result from anthropogenic-biogenic interactions, especially for explicit models
- (3) Need to test explicit models which capture these interactions against both lab and field studies in order to identify shortcomings that need further fine tuning/examination
- (4) Needed to evaluate if these interactions lead to changes in aerosol optical properties (e.g., brown carbon) and whether they increase the ability of aerosol to act as cloud condensation nuclei (CCN)



# Top 10 Research Needs

## Composition

### **7. Quantifying the contribution of intermediate volatility organic compounds to secondary organic aerosol formation**

- (1) Need to measure IVOC emissions from important source classes (non- and on-road mobile sources, fires, cooking, etc.)
- (2) Need to develop methodologies to incorporate IVOC emissions into inventories, including implementation of these methodologies in inventory tools such as SMOKE and MOVES
- (3) Need to conduct laboratory measurements of SOA production/yields from strategically selected set of IVOCs that span a range of molecular size and structure
- (4) Need to develop updated parameterizations for SOA production from IVOCs and implement these in chemical mechanisms (SAPRC, CB05) and SOA modules (VBS, SOM) used in chemical transport models
- (5) Need to evaluate predictions of updated models/inventories against ambient measurements of IVOC concentration and SOA production
- (6) Need to evaluate measurement

# Top 10 Research Needs

## Composition

### **8. Assessing Impacts of Changes in Fuels on Formation of Secondary Pollutants**

The goal of this work shall be to identify and quantify precursors of gas and aerosol pollutants from various fuels and fuels and fuel mixtures, fuel blends, and fuel additives using a broad variety of analytical instruments and method

- (1) Need to conduct experiments to determine impacts of changes to fuels using representative, standard and non-traditional, combustion technologies to generate exhausts that are introduced into controlled environmental reaction chambers under simulated atmospheric conditions
- (2) Need to perform comparisons of conventional, reformulated, bio-based and non-traditional fuels, and their resulting exhausts in order to improve understanding of the relationships between fuels, fuel evaporates, exhausts, and produced secondary products

# Top 10 Research Needs

## Composition

### **9. Emissions and Composition of Secondary Pollutant Precursors from Gasoline and Diesel Driven Non-Road Sources**

- (1) Need to study chemically-resolved, emissions profiles that include the most important O<sub>3</sub> (e.g., alkenes) and SOA (e.g., intermediate volatility organic compounds) precursors
- (2) Need to study ozone-forming potential (e.g., maximum incremental reactivity scale) and mass yields for SOA formation
- (3) Need to investigate experimentally-constrained mechanisms and/or parameterizations to model secondary pollutant formation in regional/global air quality and chemical transport models

# Top 10 Research Needs

## Modeling

### **10. Long-term measurement from closure, SOA models with ambient observations**

There is a pressing need for closure studies in three contexts.

- (1) Multi-generational aging of a single precursor, where organic aerosol levels will change progressively as the mixtures ages
- (2) Source-specific emissions and oxidation from rich sources such as biomass burning or vehicles in smog chambers, where complete speciation of the emissions may be lacking and thus complete enumeration of the extent of oxidation may also be lacking
- (3) Ambient, where the full range of precursors are processed and aerosol properties are tracked over time

An SOA closure program would focus on these three elements across multiple laboratories and campaigns. It would include support for focused research efforts dedicated exclusively to closure, and also supplemental augmentations designed to add closure to more expansive efforts (i.e. field campaigns).