

## ACCORD WORKSHOP SUMMARY

The ACCORD (Atmospheric Chemistry Center for Observational Research and Data) is a partnership between NCAR's Atmospheric Chemistry Observations and Modeling (ACOM, formerly ACD) Laboratory, NCAR's Earth Observing Laboratory (EOL), NSF Atmospheric Chemistry, and the University community. Briefly, the mission of ACCORD is to build a better alliance between ACOM and University partners to address important, critical, and emerging questions in *in situ* observational atmospheric chemistry, and to provide a vehicle for community input into ACOM's role in answering these questions. The basic structure of ACCORD was agreed upon in Autumn 2013, and a first meeting of the ACCORD Science Committee (ASC, consisting of 6 University and 3 NCAR members, <http://www2.ACOM.ucar.edu/accord/science-committee>) was held in Spring 2014. A major activity decided upon by this committee was a community workshop, designed to obtain a bottom-up consensus of major science questions facing our field of endeavor, and facilities and instruments needed to answer these questions.

To that end, an open community workshop was held in Boulder, March 30-April 1, 2015. To help structure the workshop, a survey was first distributed to the community, in which scientists were asked to present their ideas regarding important atmospheric chemistry problems that can be addressed via *in situ* observations, and measurements, instruments, and related activities that should be carried out to address these problems. Results from the survey were used to generate the workshop discussion themes, and to provide a starting point for discussions. The ASC used the surveys to define seven central workshop themes. This included five science themes centered on the following topics – Secondary Organic Aerosol, Aerosol Optical and Physical Properties, Reactive Nitrogen, Biosphere-Atmosphere Interactions, and Regional and Global Oxidants. A major goal of the workshop was to bring early-career scientists (junior faculty, post-docs) to the workshop to allow them a platform to present their ideas, and to further connect them with the broader community – thus, a separate theme on early-career scientists was included. Finally, a general facilities discussion topic was included as part of the workshop. The workshop consisted of a series of breakout discussions, and plenary presentations and discussions. Some central themes identified in the discussions, and possible readily-actionable activities are identified below. This is followed by a list of potential activities brought forward at the workshop that are associated with the seven themes.

### **Central Themes:**

- 1) The desire for a community focus on re-analysis of previous field campaigns was prevalent, and associated with multiple themes. Scientific issues associated with these 'virtual campaigns' included (for example) global HO<sub>x</sub> budgets, ozone production in biomass burning plumes, the evolution of Arctic composition, BVOC fluxes, and SOA formation. There was overwhelming support by the community for this type of activity, and a desire to convey this message to NSF. These activities provide an excellent opportunity for inclusion of students, early-career scientists and newcomers to our field, including under-represented groups.
- 2) A field campaign in a terpene-dominated landscape was put forward as part of multiple science themes (HO<sub>x</sub> budgets, biosphere-atmosphere exchange and carbon cycling). The campaign would also have obvious connections to SOA formation as well.
- 3) There was a desire to develop a chamber collaboration network. In particular, the desire for a centralized data repository was put forward.
- 4) The need for training (particularly for early-career scientists) on all aspects of instrumentation use and development, and field deployment (particularly aboard aircraft) was communicated. This should clearly include under-represented groups.
- 5) The continuing (and expanding) need for standards, calibration, and intercomparison exercises was prevalent across most science themes.
- 6) Associated to a degree with items (4) and (5), the need for well-characterized ground site(s) for scientific study and instrument testing, etc, and/or a mobile laboratory that can be deployed at a ground site, was expressed.

### **Readily actionable items:**

- 1) Plan a measurement-model workshop, to 'kick-start' the activities associated with item (1) above. With well-established connections between modelers and measurement scientists, ACOM would be a logical host and coordinator for this activity.
- 2) A feasibility study on steps forward regarding maintenance of a long-term measurements at a ground site, and/or the need for a mobile laboratory;
- 3) The development of an ACCORD community web site, that becomes a go-to location for all relevant information (links to campaign data; information on upcoming field campaigns, and opportunities for participation; connector for mentors/mentees; repository for training videos; availability of standards and calibration capabilities at NCAR and in the community; etc.)
- 4) Development of a chamber collaboration network, with a central data repository.
- 5) Develop plans for a training workshop on instrument design and deployment. This should be directed toward early-career scientists, newcomers to the field, and should specifically include under-represented groups.

## **SCIENCE TOPIC #1 – Secondary Organic Aerosol**

**Introduction:** Issues related to SOA formation/loss and impacts were prevalent in survey responses. A number of sub-themes and scientific questions were identified, including the following needs: to speciate and quantify semi-volatile VOCs, and to understand their partitioning between gas- and condensed-phases; to determine the impact of multi-phase chemistry, particularly regarding extremely low volatility species; to quantify the relative impact of daytime versus nighttime chemistry in SOA production; and to understand oxidative cascades for VOC, particularly isoprene and terpenes.

It was recognized that great progress has been made over the past five years in understanding the complexity of the processes involved in SOA formation. Much of this progress has been due to rapid developments in Chemical Ionization Mass Spectrometer (CIMS) techniques, which are now able to identify thousands of compounds in ambient and lab-generated particles. With these new technical developments, the community is now in a position to make significant advances, but challenges remain, notably:

- How do we deal with the chemical complexity of SOA in our efforts to understand the species and mechanisms by which they form?
- In addition, do current measurements inform us properly on the impacts of SOA on climate and health?

Two over-arching science questions motivate our current research priorities on SOA:

- What are the processes involved in the formation, transformation, and loss of SOA and how does this impact aerosol composition, health, weather, and climate?
- What are the most important VOC sources of SOA, and where are they important in different environments?

The instruments, instrument-related activities, and facilities required to address these questions are similar whether we are exploring VOC precursors or SOA transformations. Therefore we consider these all to be essential activities. Specifically, we have identified field and chamber related activities, associated with specific questions that have arisen from these overarching questions.

**Activity #1: A chamber collaboration network and data archive is proposed. This can be accomplished quite readily.**

Recent laboratory chamber studies performed at Caltech (FIXCIT) have demonstrated the importance of chamber studies performed in close coordination with field campaigns. Chamber studies can also be critical for instrument intercomparisons and provide crucial input for models. In addition, the variety and specialization of

existing chambers adds value to the community. In view of this and limits in existing funding, we recommend the creation of a website with information on existing chambers in the US and links to data repositories where scientists can access data from past experiments. Scientists who would like access to a chamber may connect with those with chambers at the proposal stage. Chambers at NCAR and elsewhere can be used for proposed "boot camps" for best practices, training, etc.

**Potential Leaders:** Jim Smith (UC-Irvine), possibly others with chambers (Surratt, Ng, Shilling, Jimenez) or interests (Cappa, Russell, Barsanti, Fry).

**Facilities needed:** Website developers, data archiving (if needed), intercomparisons.

**Other instrumentation or related needs:** Funding linked to participation?

**Other potential participants:** SOAS community.

**Potential Role for ACOM in this activity:** Planning and organization, intercomparisons, education and training.

**Activity #2: Data mining exercises (using data from previous campaigns such as SOAS and GoAmazon 2014/15) are proposed to address issues related to biogenic SOA formation and transformations. The activity could be implemented on roughly a 1-year time scale.**

There is a feeling that those in the community who have recently participated in field campaigns need to prioritize data analysis: What have we learned about SOA from recent campaigns such as SOAS and GoAmazon 2014/15? This type of data mining may substantially increase the findings from past investments in field measurements. This secondary analysis should likely focus on merging, integrating or inter-comparing data sets from multiple groups or multiple campaigns and with specific comparisons to models so as to clearly differentiate the efforts from initial measurements and analyses.

**Potential Leaders:** Existing project leadership (SOAS, GoAmazon 2014/15, etc.).

**Facilities needed:** Data mining support, archives, networking opportunities.

**Other instrumentation or related needs:** Data workshops, announcement of opportunities.

**Other potential participants:** SOAS and other project communities, not limited.

**Potential Role for ACOM in this activity:** Workshops and visits, dissemination of data mining tools (links to NCL and other graphical tools).

**Activity #3: To improve speciation and quantification of SOA and its precursors, a centralized organic synthesis facility is proposed. The timescale for potential implementation of this facility is ~ three years.**

There is clear need for accurate standards of many types of gas- and particulate phase compounds that are observed to participate in SOA formation and evolution. This includes precursor VOC, highly oxidized, low volatility organics, multifunctional organics containing sulfur and nitrogen, and oligomeric compounds that may form within particles. Due to the unstable nature of these species (thus the need to produce these compounds just prior to use), and because of the special skills and experience required, it stands to reason that this may be an important activity to have housed in a National Center. Recognizing that a substantial commitment of resources are required, we propose to initially work with university partners who have expertise in the creation of these standards to provide information for those who are interested in creating their own standards.

**Potential Leaders:** TBD (interest from Keutsch, Surratt).

**Facilities needed:** Centralized synthesis facility.

**Other instrumentation or related needs:** Distribution and standard practices.

**Other potential participants:** Organic synthesis community.

**Potential Role for ACOM in this activity:** Possible location for a centralized synthesis facility, although the view that this may be better housed at a University was also expressed.

**Activity #4: To examine issues related to aerosol formation and transformations in an urban-rural transition, an urban-based field campaign is proposed. The timescale for preparation for this campaign would be on the order of 5 years.**

Recent advances in analytical techniques (e.g., CIMS) should be applied to an urban environment along with parallel efforts to link SOA chemistry to health impacts. This can be performed along a gradient of emissions changes from urban to rural. Links with activities proposed by other breakouts (e.g., oxidants group) will be made where possible. There needs to be better collaboration between the atmospheric chemistry community and biologists and health scientists who are concerned about linking composition to impacts. Such questions arise as “what information is required about SOA in order to understand health and climate impacts?”.

**Potential Leaders:** Ng (interest from Surratt, Jimenez, Carlton, Weber).

**Facilities needed:** Urban setting, partners from health sciences.

**Other instrumentation or related needs:** Instruments are available. Study should include vertically resolved observations of precursors and SOA properties.

**Other potential participants:** EPA centers, SOAS community, ...

**Potential Role for ACOM in this activity:** Planning and organization, aircraft instruments.

**Activity #5: To examine cloud water processing of SOA, an aerosol- cloud-chemistry campaign is proposed. The timescale for preparation for this campaign would be (at least) 5 years.**

The chemical processes that lead to SOA formation through aqueous phase reactions in cloud droplets and aqueous phase particles are poorly understood. Such measurements are a challenge for current research instrumentation. Techniques for directly measuring the amount of water in ambient particles are challenging, as are sampling techniques that allow us to directly probe water droplet chemical processes. Ground-based cloud sampling allows for techniques requiring longer sampling times and more sample handling.

**Potential Leaders:** Barth, possibly others (Sorooshian, Collett, Hawkins, Turpin).

**Facilities needed:** Research site with access to cloud water like Storm Peak, La Jolla (Trinidad Head, Look Rock?).

**Other instrumentation or related needs:** Aqueous-phase composition, inter-comparison pre-campaign (ARISTO/Rapid?).

**Other potential participants:** Cloud physics community.

**Potential Role for ACOM in this activity:** Project leadership, instruments, expertise.

## **SCIENCE TOPIC #2 – Biosphere / Atmosphere Interactions (Emission and Deposition)**

**INTRODUCTION:** The biosphere plays a major role as both a source and a sink for a suite of reactive trace gases and particles. Despite this, the process and impacts of surface-atmosphere exchange are poorly understood. A number of overarching questions were identified from the survey responses; these formed the basis for preliminary discussions:

1. What are the controlling parameters for surface-atmosphere exchange?
2. How do ecosystems affect regional to global atmospheric chemistry?
3. What is the role of pollution and nutrients in biogeochemical cycles?
4. How will land-atmosphere fluxes of trace gases and particles respond to changes in land cover, climate, and air quality?

Further discussion at the workshop identified the following, more specific science questions that needed to be addressed:

1. What are the controlling parameters for BVOC emissions?
  - a. Short-term parameters: How do we up-scale leaf-level measurements, what are short-term drivers?
  - b. Long-term: How will these emissions change with climate, land use, and chemical composition of the atmosphere (CO<sub>2</sub> and O<sub>3</sub>)?
  - c. Importance of the emission of unknown compounds
2. Can a better understanding of deposition processes of trace gases and particles be obtained?
3. How can we disentangle emissions, chemistry, and deposition of BVOC, SVOC, and particles?
4. What are the sources and impacts (on aerosols, clouds, hydrology) of biological particles (pollen, etc.)?
5. How important is the role of the ocean as a source of trace gas and particle emissions and removal?
6. Do biogenic emissions have a significant role in ecosystem-atmosphere coupling? (i.e. can we observe the impact of biogenics on climate, and then the feedbacks on ecosystems?)
7. What is the role of fire emissions on down-wind atmospheric chemistry and climate forcing? Key questions: composition of emissions as a function of combustion process and ecosystem type; chemical evolution; aerosol properties; how to connect remote sensing with predictive fire modeling?
8. What are the processes controlling soil emissions of NO<sub>x</sub>, ammonia, and amines?

Four specific activities were proposed to address some of these issues:

#### **Activity #1: A multi-scale regional BVOC field campaign targeting reactive carbon mass closure**

The goals of this campaign would be: (1) to develop a process-based understanding of BVOC emissions from biochemical leaf-level processes to regional canopy fluxes, and (2) to achieve reactive carbon closure (emissions, canopy transformations, deposition). The focus would be on a terpenes-dominated region (e.g., boreal forest, Pacific NW, with no significant MBO emissions), to differentiate from recent campaigns focused on isoprene chemistry. Note also that strong coupling to forest ecology, biology, and remote sensing (land use, vegetation) communities would be required. There could also be coupling / connections with plant chamber work.

**Interested participants:** Frank Keutsch, Alex Guenther, Delphine Farmer, Dylan Millet, Colette Heald, Louisa Emmons, et al.

**Facilities needed:** leaf-level measurements, ground sites, towers, aircraft (C-130 & twin otter), EOL micromet (energy fluxes, turbulence), tethersondes?

**Other potential participants:** biology, forest ecology, remote sensing communities; connect to modeling on variety of scales; some members of SAS community

**Potential Role for ACOM:** requestable chemistry instruments, modeling

#### **Activity #2: Explore the feasibility and approach to making long-term flux measurements**

A strong need for more systematic long-term BVOC flux measurements was identified. This activity would establish a network of people interested in better understanding the feasibility of different approaches. Two possible approaches are as follows:

- Make use of existing supersites (UMBS/PROPHET, Blodgett Forest, UNC, etc.) to carry-out a rotating series of year-long state-of-the-art flux field campaigns (e.g. 5 sites, 1 year each). These could be selected for regional diversity, and have the advantage of known climatology.
- Make use of existing network sites (LTER/NEON), to incorporate inexpensive BVOC samplers (e.g. REA system with OPC) at multiple sites. This approach has the advantage of possible longer-term deployments in numerous locations, however, there is a need to better understand power limitations at these sites.

Both of these approaches would capitalize of the extensive ancillary information on forest composition, etc. from existing sites.

**Interested participants:** Alex Guenther, Glenn Wolfe, Delphine Farmer, Rob Rhew, Gunnar Schade

**Facilities needed:** low-cost, low-power isoprene and VOC instruments, REA system for sampling BVOC emissions, OPC, personnel to run sites/data collection

**Other instrumentation or related needs: (new instrumentation; calibration etc):** better simple isoprene and VOC instruments; connection to models

**Other potential participants:** TBD

**Potential Role for ACOM:** coordination, calibrations, QA/QC, data archiving, modeling

#### **Activity #3: Assess and compile current measurements of ocean emissions and deposition of VOCs, primary organic, DMS, NH<sub>3</sub>, and ozone.**

The goals of this activity would be to explore what data is available, to develop collaborations with the oceanography community, and to identify gaps in measurements.

**Interested participants:** Tim Bertram, Glenn Wolfe, Oliver Wingenter, Rob Rhew

**Facilities needed:** Access to data

**Other potential participants:** The oceanography community

**Potential Role for ACOM:** provide link to existing data

#### **Activity #4: Re-analysis of past data in connection with models**

The goal of this activity is to coordinate analysis of observations from all relevant past field campaigns, including measurement and modeling groups, focusing on specific science questions in a “virtual campaign”. Note that this type of activity was identified in other discussion groups. Possible topics for ‘virtual campaigns’ consistent with the Biosphere-Atmosphere theme include (but are not limited to) the following:

- Fires: find all data that sampled fire plumes from all past campaigns, look at emission factors, ozone production from fires, etc. Keep abreast of progress on FIREX and other future campaigns as well
- BVOC fluxes: to test biogenic emissions model and look for trends, historical changes

**Interested participants:** Emmons, Orlando, Bob Yokelson (biomass burning)

**Facilities needed:** Collocated/coordinated data repository

**Other potential participants:** grad students, post-docs, EC scientists, including those from under-represented groups.

**Potential Role for ACOM:** Hosting 1-2 week visits of grad students and post-docs (from measurement groups) to get introduction to using model output with observations, running box models, improving emissions inventories, etc., as a mechanism of connecting observations and models (capitalize on ACOM strengths here)

## **SCIENCE TOPIC #3 – Reactive Nitrogen**

**Introduction:** This topic was defined by survey responses that related to the sources and impacts of ammonia and amines, and their effects on particle formation and growth; the quantification of agricultural emissions of these species (and N<sub>2</sub>O); the formation and loss of organic nitrates, particularly from biogenics, and their impacts on NO<sub>x</sub> removal and cycling; and the role of NO<sub>3</sub> radical in biogenic oxidation, and the concomitant effect on NO<sub>x</sub> budgets.

Workshop discussions were centered on two main themes, ‘reduced’ reactive nitrogen species (ammonia, amines and amides), and the more traditional ‘oxidized’ reactive nitrogen (NO<sub>x</sub>, NO<sub>y</sub>, organic nitrates and NO<sub>3</sub> chemistry). Discussion groups at the workshop discussed the following major issues and identified the following questions as being central to progress.

Reduced Nitrogen:

- What is distribution of ammonia on regional to continental scales?

- What is the diurnal distribution of NH<sub>3</sub>?
- What is the partitioning of reduced nitrogen species?
- What are the atmospheric distributions of organic amines? Are they mostly in particle phase?
- Similarly, what are the atmospheric distributions of the organic amides? Are they mostly present in the gas phase?

Oxidized Nitrogen:

- What is the fate of organic nitrates (photolysis, deposition, hydrolysis), particularly those of biogenic origin?
- How much knowledge of organic nitrate speciation do we need?
- What is the role of the NO<sub>3</sub><sup>•</sup> radical in oxidative chemistry and nitrate formation?
- What is the (potential) role of alkyl peroxy nitrates in the transport of reactive nitrogen?
- Can closure of the nitrogen budget be obtained in the biosphere (possibly a study at a ground site such as UMBS could address this question)?
- What is the source strength of soil NO<sub>x</sub>?
- What are the sources and impacts of HONO?

Three activities were proposed, two related efforts centered on ammonia/amines, and one related to organic nitrates.

#### **Activity #1: Ammonia (Amines) Standardization**

It was thought that a calibration / intercomparison exercise regarding ambient measurements of ammonia and organic amines would be useful, in advance of a field experiment (see next activity). The goal is to intercompare ammonia measurement techniques in chambers and at a field site. Given that techniques for amines are at an earlier stage of development, comparisons and testing of available techniques would be done at a more informal level. Plenary discussions raised awareness of previous ammonia intercomparisons that have taken place recently - the intercomparison proposed here should build on (and include relevant parties from) these previous studies.

**Potential Leaders:** J. Smith/F. Flocke/D. Hanson

**Facilities needed:** Chamber, Field site (Boulder area)

**Other instrumentation or related needs:** Calibration, standards, inlet

**Other potential participants:** Both commercial and custom instruments, Aerodyne, Texas A&M...

**Potential Role for ACOM in this activity:** Leadership, standards, inlets, supporting measurements, logistics

#### **Activity #2: Ammonia Emissions Experiment**

This experiment would take advantage of lessons learned in the intercomparison described above. A deployment in the Midwest / central US, where agricultural emissions are large and isolated, would be desirable possibility.

**Potential Leaders:** C. Stanier, F. Paulot, V. Aneja

**Facilities needed:** CIRPAS Twin Otter (?) if payload suitable; Mid West deployment

**Other instrumentation or related needs:** Instruments, inlets, standards, etc. developed in Activity #1 above.

**Other potential participants:** TBD

**Potential Role for ACOM in this activity:** Calibration, inlet design, supporting measurements

#### **Activity 3 - Organic Nitrates/Partitioning**

A large flux of reactive NO<sub>x</sub> is cycled into/through organic nitrates, particularly those of biogenic origin. Thus, the ultimate fate of these species is critical to our understanding of ozone production in BVOC-dominated regions. The goals of this activity are: to develop/intercompare techniques for measurement of (speciated) multifunctional nitrates, to determine the partitioning of these species between gas and aerosol phases, and to determine their ultimate removal pathways from the atmosphere, and thus their role in permanently removing or recycling NO<sub>x</sub>.

**Potential Leaders:** J. Crounse, Sally Ng, Rob Griffin

**Facilities needed:** Chamber; Field Site (Pasadena; Biogenic area – PROPHET?)

**Other instrumentation or related needs:** speciated multifunctional nitrates, total nitrates, aerosol measurements

**Other potential participants:** TBD

**Potential Role for ACOM in this activity:** Calibration, inlet design, supporting measurements, coordinating standards

## SCIENCE TOPIC #4 – AEROSOL OPTICAL AND PHYSICAL PROPERTIES

**Introduction:** This topic was built around survey responses that related to the need to understand the role of tropospheric aerosol on radiative forcing; the need to understand budgets of black / brown / organic carbon aerosols; sources of CCN, and impacts of aerosols on clouds; and impacts of aerosols and aerosol toxicity on human health.

Discussions at the workshop led to the identification of three key science questions that future in situ activities should focus upon:

- What processes drive changes in aerosol size distribution and composition? How do these processes vary vertically in the atmosphere thereby affecting cloud properties?
- How is aerosol scavenging a function of chemical composition and storm type? What are implications on aerosol lifetime which is important for climate studies?
- How do aerosol optical properties vary as a function of chemical composition for multiple wavelengths? How does aerosol optical lifetime differ from aerosol lifetime?

Three potential activities were identified, as described below.

### Activity 1: Monitoring Climate-Relevant Aerosol Properties

Existing monitoring networks across the U.S. and globe have been sampling the atmosphere during a period of historic environmental regulation and changing climate. The emphasis for most routine measurement networks has traditionally been to understand acid deposition and surface air quality. Determining the extent to which existing datasets can be used to understand climate-relevant aerosol properties, such as CCN and IN concentrations, is critical to develop better models that more accurately project our changing world.

**Activity 1a:** Investigate how to capitalize on existing datasets (identified below) to analyze in the context of understanding climate-relevant aerosol properties over the long term.

**Activity 1b:** Design, develop and implement infrastructure (can be communication infrastructure) to support routine monitoring of climate-relevant aerosol properties, e.g., CCN & IN measurements, alongside existing measurements of aerosol composition, size distributions, multiplex measurements, Kappa and chemical composition at different sizes. Measurement strategies may find that a Lagrangian perspective facilitates investigation of aerosol “aging”.

**Potential Leaders:** Jesse Creamean, Annmarie Carlton

#### Facilities Needed:

**Activity 1a:** Catalog existing data sets with short descriptions in one location (with links). Of particular interest are existing mountain top sites, such as Storm Peak Lab, Whiteface Mtn., Mt. Mitchell, Mt. Soledad, Mt. Bachelor, CalWaters Study, because they occasionally experience clouds. Investigate other locations including other continents.

**Activity 1b:** Identify existing monitoring locations that can support (e.g, space, data management, etc) additional measurements of climate-relevant aerosol properties.

**Other instrumentation or related needs:** multiple wavelength instruments

**Other potential participants:** cloud physics colleagues (PDM at NSF); NSF-DOE intercomparison of IN at AIDA cloud chamber and then at Storm Peak (Dan Cziczo, MIT) – measurements and models

**Potential role for ACOM in this activity:** ACOM could host the web site for cataloging existing data sets.

**Activity 2: Exploit Current Datasets Examining Aerosol Scavenging and Plan Future Studies**

Recent campaigns, e.g. DC3, GO-Amazon, SEAC<sup>4</sup>RS, potentially can give information on scavenging of inorganic, organic, black carbon, and dust aerosols. To our knowledge, one DC3 case has been analyzed for aerosol scavenging, but many other cases have yet to be studied. Further, measurement of black carbon in DC3 and SEAC<sup>4</sup>RS in clouds was not possible because of the inability to separate the aerosol from cloud particles. Thus, coordinated field studies can further our understanding of atmospheric processing of aerosols.

**Activity 2a:** Continue analysis of DC3 and SEAC<sup>4</sup>RS datasets to determine aerosol scavenging of inorganic and organic aerosols as a function of storm type. Producing vertical profiles of CCN, IN, and their chemical composition would also be beneficial. Identify potential other field studies for same analysis.

**Activity 2b:** Design future studies, via community workshops, to investigate cloud processing of aerosols based on 'lessons learned' from past campaigns.

**Potential Leaders:** Mary Barth, Andy Ault, Rebecca Sheesley, Annmarie Carlton

**Facilities Needed:** Workshop discussions of field campaigns in marine, urban, downwind of urban regions, coastal regions and just inland should identify needed facilities. Of interest would be to ensure good aircraft inlets for aerosol sampling in clouds, the storm penetrating aircraft, and radars.

**Other instrumentation or related needs:** The main need is to have adequate aircraft inlets for sampling in cloud.

**Other potential participants:** Aircraft aerosol, CCN, and IN measurement investigators

**Potential role for ACOM in this activity:** Coordination of field activities and hosting any workshops

**Activity 3: Development and Application of Multi-wavelength Instruments**

Scattering, absorption and extinction of solar radiation across a spectrum of wavelengths impact regional climate. However, measurements are often made at a single wavelength. For example, separation of absorption into contributions from black and brown carbon, each with distinct climate-relevant properties, typically occurs at a single wavelength, with extrapolation used to fill in the gaps. The relative contributions between black and brown carbon depend on source and chemical processing, and the implication in a climate model can be substantial.

**Activity 3a:** Develop and utilize multiple wavelength instruments in field studies, such as a prescribed fires field campaign. Develop more sensitive multiple wavelength instrumentation with lower detection limits and well-established accuracy to allow measurements in more remote locations (e.g. the free troposphere). Develop Lagrangian process models to represent various aerosol optical properties at multiple wavelengths in order to design strategic sampling of these properties in field campaigns and learn how they change over an aerosol (both single particle and aerosol population) lifetime.

Activity 3b: Use instrumental tools described above to address some of the following questions, using a combination of laboratory and field measurements: How are radiative properties of BC impacted by morphological factors? How does the mixing of BC and BrC with other aerosol components impact radiative properties? How do optical properties of BC/BrC change with atmospheric aging? And how can these complex processes be best represented in climate models?

**Potential Leaders:** Chris Cappa, Rebecca Sheesley, Sasha Madronich (suggested), Bob Yokelson, Solomon Bililign

**Facilities Needed:** Multiple wavelength instruments of aerosol optical properties; for field deployment, small aircraft to find transitions, and mobile surface facility for detailed measurements

**Other instrumentation or related needs:** aerosol composition, aerosol size distribution, VOCs, trajectory models

**Other potential participants:** Christine Wiedinmyer (NCAR/ACOM) for biomass burning emission studies, NOAA/CSD who is planning a biomass burning emissions field experiment and who have excellent aerosol optics instrumentation.

**Potential role for ACOM in this activity:** aircraft, mobile facility

## SCIENCE TOPIC #5 – REGIONAL AND GLOBAL OXIDANTS

**INTRODUCTION:** Regional and global oxidants encompass a broad range of gas-phase chemistry with its links to multi-phase chemistry. The problems can be viewed either as the unique atmospheric chemistry of places, such as forests or cities, or as unique but connected chemical systems. Survey responses were most concerned with places: forests, where the measured oxidant levels are inconsistent; megacities, a local-to-global atmospheric chemistry problem of the future; and regions with hydraulic fracking, a potential air quality problem related to energy extraction. Several responses referred to the atmospheric chemistry of the transition between “ecosystems”, such as megacities and their surrounding rural and forested areas. From the atmospheric chemistry point-of-view, survey responses focussed on the following “chemical systems”: changing reactive nitrogen levels and their impact on other pollutants; VOC oxidation mechanisms, particularly for multi-functional VOC oxidation products in low NO<sub>x</sub> environments; multi-phase chemistry; halogen chemistry, which can have global implications; and unknown chemistry, particularly the importance of missing OH reactivity. Additional survey responses noted that the global oxidation capacity was poorly understood, making it difficult to predict future changes.

Survey responses regarding activities needed to answer these scientific questions were diverse, but can be grouped into a few categories. Field campaigns and studies included intensive field campaigns with knowledge of the vertical structure of the chemistry, aircraft campaigns over wide areas, and long-term dispersed field measurements. Instruments included new measurements of multi-functional oxygenated VOCs and speciated organic peroxy radicals, inexpensive network sensors, and routine sensors for reactive nitrogen species. Instrument activities included building confidence in HO<sub>x</sub> measurements through intercomparisons, developing calibrations for CIMS measurements, and artifact checking of all instruments. Facilities included unmanned aerial systems (UAS) for treetop flying and for global flying, miniaturized sensors, a standards laboratory particularly for oxygenated VOCs, and a community chamber for calibrations and atmospheric chemistry studies. The respondents pointed out the many recent, ongoing, and planned field campaigns that can answer some but not all of these science questions.

It was recognized in these discussions that the topic included discussions on all oxidants (OH/HO<sub>x</sub>, O<sub>3</sub>, NO<sub>3</sub>, Criegee, Halogens), and that the questions and themes presented below were to take into account all of these oxidants. After consideration of numerous science questions raised during workshop discussions, three major themes were identified:

- Transitions in chemical regimes and oxidants both vertically, horizontally and temporally (from megacities to regional and global scale, and between other “ecosystems”).
- Structure activity relationships: do mechanisms based on them adequately predict VOC oxidation pathways and partitioning in the atmosphere, especially for low-NO oxidation pathways, of VOCs and multifunctional products?
- What are the roles of VOCs and multiphase chemistry in local-to-global oxidation chemistry?

The group identified a number of potential activities, as presented below. The activities were grouped according to the resources required to do them (analysis vs. chambers/models vs. large field campaigns), and the timescale on which they would likely occur.

### A) Activities already in the planning stages:

**Activity 1: Conduct a complete OH/HO<sub>2</sub>/RO<sub>2</sub> intercomparison study, conducted over ranges of conditions (VOC, NO<sub>x</sub>) and multiple platforms / locations (chamber, ground-based).**

Planning for this activity is already in the works and it will likely occur over the next three years.

**Potential Leaders:** HO<sub>x</sub> measurement groups (e.g., Brune, Stevens, Cantrell, Mauldin, ...)

**Facilities needed:** SOAS - like tower capability and chamber (SAPHIR?)

**Instrumentation needs:** ongoing advancements in existing HO<sub>x</sub> instrumentation / characterization; ancillary instruments, VOCs, OVOCs, peroxides, etc.

**Other potential participants:** process modelers

**Potential Role for ACOM:** tower, supporting measurements (NO, VOCs, PANs, etc.)

## B) Activities requiring no further experimental work.

### Activity 2: Analysis campaigns, using existing field data sets.

This activity and the one below it could happen without any need for further experimentation. Science topics addressed could be multiple, related to ozone production rates, HO<sub>x</sub> budgets and recycling mechanisms, global OH distributions, etc.

**Approach:** Data from both individual and community efforts need to be considered. Coordination of efforts is needed to ensure different groups use the same data set for different scientific efforts. As alluded to earlier, there is overall community support for these types of 'analysis campaigns' across multiple topics.

**Interested parties:** Many

**Potential Role for ACOM:** archive of many of these data sets (EOL), modeling support, enable connections between modelers and measurements groups.

### Activity 3: Achieve a good constraint on global OH.

The global distribution of OH is not well constrained. Global models frequently use methane and methyl chloroform lifetimes as a diagnostic for OH, but these values are not well known. This activity would make use of existing data to develop an OH climatology. Perhaps this would include an update to the Spivakovsky OH climatology, using a box model constrained by the much more numerous VOC measurements available now. Available OH measurements would be used, as well as consideration of indirect methods.

**Potential Leaders:** Bill Brune, Jingqiu Mao, Louisa Emmons

**Facilities needed/approach:** Involves analysis of existing data (see previous activity). There is a need to consider both direct and indirect methods of [OH] determination; analysis of past campaigns; development of a model testbed; which chemical context works best to expanding local HO<sub>x</sub> measurements to the globe. Coordinated analysis activities – first step: a virtual workshop.

**Other instrumentation or related needs:** Access to data.

**Other potential participants:** TBD

**Potential Role for ACOM in this activity:** data set logistics (although many at NASA)

## C) Activities requiring modest resources (chamber work, small-scale field studies)

### Activity 4: Where does the oxygenated carbon go?

The general idea is to do FIXCIT-like studies of (B)VOCs, OVOCs, tracing oxidative cascades in chamber experiments, perhaps coordinated with concurrent field campaigns.

People of interest: John Crounse, Frank Keutsch, Delphine Farmer, collaborate with developers of EPA type mechanisms

**Facilities needed/approach:** like SOAS FIX@CIT

- (i) characterize current state of instruments by doing calibrations/comparisons of CIMS/PTR-MS/GC
- (ii) mechanistic chamber studies for calibration, artifact studies and mechanism development and evaluation of structure reactivity concepts;
- (iii) complementary field work;
- (iv) make previous and new chamber data available to modelers working on mechanisms.

**Other instrumentation or related needs:** synthesis of standards

**Other potential participants:** reach out to European groups

**Potential Role for ACOM:** chamber, assistance with laboratory standards; facilitate interactions between modelers and experiments; structure-reactivity evaluations.

**Activity 5: Develop structure reactivity relationships (for peroxy radicals, epoxides, other multi-functional species)**

A need to get structure-reactivity rules for reactions of multifunctional organics, and peroxy/alkoxy radicals derived from them was expressed. The scope of the activity would include reactions of oxidants (OH, O<sub>3</sub>, NO<sub>3</sub>, ...) with OVOCs, and unimolecular and bimolecular reactions of peroxy and alkoxy radicals derived from the OVOCs. Key to this will be to develop quantitative understanding of the interactions between the multiple functional groups on these reaction rates. Coordinated theoretical and laboratory studies will be needed to develop these relationships.

**Potential Leaders:** Deborah Luecken

**Facilities needed/approach:**

- (i) organize small workshop of experts in this area – suggest that this be held as part of an existing meeting (The Davis Atmospheric Chemical Mechanisms meeting in Fall 2016 was specifically suggested);
- (ii) review existing mechanisms and recommend new relationships;
- (iii) theoretical and laboratory studies to fit data to these new relationships.

**Potential Role for ACOM :** large participation; laboratory work; collecting existing data

**D) Larger scale field studies, or projects otherwise requiring significant resources.**

**Activity 6: Asian monsoon - transitions from (local) megacity to regional and global scale**

The Asian summer monsoon anticyclone is a dominant feature of the circulation in the UT/LS during Northern Hemisphere (NH) summer. This system is coupled to a region of Asia that is experiencing a significant increase in anthropogenic emissions. Persistently enhanced pollution in the UT during this period, linked to rapid vertical transport of surface air from Asia, India and Indonesia in deep convection, and confinement by the strong anticyclonic circulation is clearly seen in satellite observations. These observations point to the unique and high impact of the Asian monsoon system. In situ observations are essential in providing key process information for constraining and evaluating global chemistry-climate models.

**Potential Leaders:** Laura Pan - great interest - leader TBD

**Facilities needed:** GV, NASA aircraft? Modeling simulations to predict the impact of reductions in air pollution and precipitation etc.

**Other instrumentation or related needs:** full chemical payload, which requires instrument miniaturization; *GV needs oxidant measurements*; other platforms with HO<sub>x</sub>, other oxidants

**Other potential participants:** many local scientists, satellite community; Bob Yokelson

**Potential Role for ACOM:** similar to CONTRAST – requestable instruments, possible leadership role, forecasting and modeling activities.

**Activity 7: Sources, fates and impacts of halogens and other oxidants in the arctic (sea ice, snow cover, ocean emissions)**

The budget of halogens (Cl, Br, I), and their impacts (e.g., on ozone and mercury) are uncertain throughout the troposphere. Development in particular of CIMS techniques for determination of many inorganic halogen species places the community in a good position to make progress. The campaign would seek to understand these halogen budgets over a range of vertical scales, including over the first 10's of meters where significant vertical gradients could exist, to the free troposphere and lower stratosphere.

**Potential Leaders:** Greg Huey / Elliot Atlas, John Orlando

**Facilities needed:** aircraft (C-130; Twin Otter); ground based work also needed for sea-ice/snow measurements

**Other instrumentation or related needs:** Iodine measurements?

**Other potential participants:** to be identified

**Potential Role for ACOM:** contribution to leadership and organization; requestable facilities and instruments; modeling support

**Activity 8: SOAS-like field study with an extra emphasis on “new” oxidants, e.g., Criegee. (monoterpene-rich environment like the northwest?)**

There has been a large recent focus on isoprene chemistry. While these data are still being digested, the need to conduct similar types of experiments in a terpene-rich environment has been put forward. The campaign would take into account the renewed interest in and knowledge of Criegee radical chemistry, as well as techniques available for determining their concentration, and would benefit from coordinated chamber studies.

**Potential Leaders:** extended SOAS community

**Facilities needed:** tower and aircraft

**Other instrumentation or related needs:** measurement of Criegees

**Other potential participants:** TBD

**Potential Role for ACOM:** leadership participation, measurements, logistics (EOL), modeling and forecasting

**Activity 9: Field campaign associated with an African megacity - heavily polluted/tropical forest**

It is clearly important to consider conducting megacities studies in all areas of the developing world (including Africa, where there are a number of emerging megacities, and a dearth of air quality data). While a full-scale Megacity campaign (similar to MIRAGE or FRAPPÉ) may be some years away, continued development of partnerships, infrastructure, and ground-based data should be a focus. The leaders identified below would be responsible for keeping abreast of work going on in the community, and of developing partnerships and opportunities. The Megacity to be studied remains TBD.

**Potential Leaders:** Christine Wiedinmyer, Vernon Morris, Solomon Bililign – maintain awareness of NASA and UK-based activities, and coordinate with these folks on potential future activities

**Facilities needed:** rich complement of aerosol and gas-phase measurements; vertical structure of dynamics and chemistry (profiles). Mostly ground based (tower), treetop aircraft, tethered balloons. (similar to GoAmazon?)

**Instrumentation or related needs:** ceilometer, aerosol lidar, speciated VOC constituents, etc.

**Other potential participants:** local contacts, satellite community

**Potential Role for ACOM:** chemical measurements; modeling; forecasting; logistical support (EOL)

**Activity 10: (Topic 1) India - megacities and agriculture boom and local-to-regional scale.**

Much like the African megacity study discussed above, it was again recognized that this would be a long-term endeavor.

**Potential Leaders:** Viney Aneja

**Facilities needed:** Rich complement of measurements; vertical structure of dynamics and chemistry (profiles). Mostly ground based (tower), treetop aircraft, tethered balloons. (similar to Africa?)

**Other instrumentation or related needs:** ceilometer, aerosol lidar, speciated VOC constituents, etc.

**Other potential participants:** local contacts, remote sensing both lidar and satellite

**Potential Role for ACOM:** chemical measurements; modeling; forecasting; logistical support (EOL)

## DISCUSSION TOPIC #6 - GENERAL FACILITIES

**Introduction:** The scope of this discussion topic includes LAOF community-requestable facilities, other less formalized facilities available at NCAR, and general community needs for observational facilities. Informative introductory presentations were given by Linnea Avallone (NSF LAOF Program Director), who presented a status report on current LAOF facilities, and by Brigitte Baeuerle (NCAR EOL), who presented an overview of procedures involved in requesting these LAOF facilities. Survey responses were centered on a number of common themes, most notably the following: Community need for facilities related to instrument intercomparison, calibration and standards; a need to examine possibilities for the use of unmanned aircraft systems (UAS); the need for tower/sensor networks; the need for community engineering support; needs for community chamber facilities and

a dedicated ground site for measurements. Discussions at the workshop provided more focus and identified the following high priority community needs, and activities that could address them.

#### **Activity #1: Instrument intercomparison and calibration**

There is an ever-growing need for inter-comparison / calibration of instrumentation, particularly as the community's ability to measure larger numbers of, and chemically more complex, atmospheric constituents grows. Many examples were cited, including needs to: 1) inter-compare or evaluate instrument performance immediately prior to a field campaign; 2) determine comparability of different measurement techniques; 3) evaluate new sensors, and compare them with established methods; and 4) evaluate small sensors, particularly for possible deployment on UAS.

**Specific activity proposed:** The ACCORD Science Committee (ASC) determines annually a significant calibration/intercomparison /instrument evaluation issue, and a specific activity to address the issue. An AO is sent to the community by the ASC, community members fill in a short web-based form to express interest in participating. Depending on the scope of the project selected, ACOM leads the proposed activity (if sufficient funding is available) or initiates discussion with NSF regarding funding possibilities.

**Potential Lead:** ACCORD Science Committee, ACOM, facility owner, lead instrument group, EOL

#### **Activity #2: Establish a community atmospheric chemistry "engineering pool".**

The need for a community "engineering pool", in particular to provide support for aircraft instrumentation was strongly articulated. The engineer pool, centered at NCAR (ACOM and EOL), could eliminate inefficiencies by providing help in the following areas: articulating requirements for aircraft deployments, in particular to new/young investigators; providing assistance with software / DAQ / automation issues; helping with instrument design and certification issues; providing advice and assistance with inlet design, and providing an inlet 'library' for potential users; helping with automation / weight optimization / power requirements.

#### **Specific activity proposed:**

- Hire an EE / systems engineer to replace recent retirees and to preserve ACOM strength and capability.
- Use this (enhanced) group to support community instrumentation needs (visits to universities to help with design issues and provide information; continue to provide support for aircraft structural analyses and fabrication services as required; etc.)
- Increase visibility / accessibility of these services. If a large demand develops for this group, a cost recovery model could be adopted in the future.

**Potential Lead:** ACOM / EOL / RAF

#### **Activity #3: Establish or enhance an existing ground site for long-term measurements and instrument testing**

The need was identified for a ground site that could be used as a proving ground for new instrumentation, for instrument testing, characterization and inter-comparison exercises, and for ground-based field campaigns. The site should be well characterized, with long term measurements of basic chemistry and meteorology in place.

#### **Specific activities proposed:**

- ASC forms a feasibility panel to further evaluate the need for this type of facility, and the level of support required. The panel would be charged with identifying suitable site(s) that offer a large variety of conditions. Examples include UMBS, BAO, Manitou, Storm Peak, Marshall, etc.
- If the process goes forward, provide instruments for basic tracer measurements, long-term monitoring, instrument testing, field activities, and data archiving.

**Potential Lead:** ACCORD to create feasibility panel; Respective field site operators; ACOM to potentially lead with site set up and instrumentation.

#### **Activity #4: Expansion of community requestable instruments and facilities**

Survey and workshop participants thought that there are many candidates for additional community resources that could be made requestable, either through LAOF or other processes. Many possibilities were discussed (e.g., ozone and particle LIDARs (ozone LIDAR network), other remote sensing / BL diagnostics instrumentation, tethered balloons, PTR-MS instruments). Recognizing limited NSF resources, adding new items may also require removing items that are currently requestable.

**Specific activity proposed:** ACOM / ACCORD solicits broad community input for potential facility instrumentation. ACCORD works closely with EOL and NSF LAOF and Atmospheric Chemistry to establish procedures for providing community input to NSF on suggested modifications to LAOF atmospheric chemistry relevant pool.\

**Potential Lead:** Asset owners / EOL / ACOM

**Other potential participants:** NSF LAOF and Atmospheric Chemistry program managers

#### **Activity #5: Chamber and small field project data archive**

**Specific activity proposed:** Create a central, open-access archive for data from smog chambers, and small ground-based field projects.

This database would expand upon the current EOL field campaign archive, would link to NASA and NOAA archives, solicit and assemble laboratory and chamber data, and provide data archiving for these data sets.

**Potential Leads:** EOL / NASA / ACOM

#### **Activity #6: Instrument calibration and standards**

There is a continued need in the community for instrument calibration and standards. It was thought that many resources are already available, in particular at ACOM, that could be made more readily available for community use.

#### **Specific activities proposed:**

- Advertise current capabilities in ACOM (kinetics chamber, aerosol chamber, radiation calibration and measurement support).
- Solicit community capabilities and resources, and compile a database.
- Investigate/compile standard synthesis capability in the community.

**Potential Lead:** ACOM / others TBD

### **DISCUSSION TOPIC #7 - EARLY CAREER SCIENTISTS**

**Introduction:** The ACCORD Science Committee thought it important that early-career scientists (including those from under-represented groups) be a major part of ACCORD, and that ACCORD provide a means for these scientists to get entrained into our science, to be aware of what is happening in the community (particularly regarding larger field programs and activities), and to get to know what NCAR/NSF resources and facilities are available to them, and how to access them. Thus, a survey question was posed to specifically address early career scientist needs. Prevalent themes among the survey responses were as follows:

- How can EC scientists be entrained into large (particularly aircraft) field campaigns?
- Can closer ties be established between measurement and model groups?
- Can connections between EC scientists and NCAR/ACOM be strengthened?

- Can more training for scientists in use and development of instrumentation be provided?

Workshop discussions were largely centered on these themes, and the following activities were proposed:

**Activity #1: Hold a (mostly) early-career measurement/modeling workshop.**

The idea of the workshop would be to provide a means for connecting observationalists (particularly those not involved in large field campaigns) with modelers, to learn of limitations of each, and to learn how best to make measurement/model comparisons.

**Potential Leads:** ACOM, Rob Griffin

**Potential Role for ACOM in this activity:** Workshop host, with participation of ACOM/University/Community Scientists. (Note possible connection here with the proposed measurement/model workshop on page 1/2).

**Activity #2: Create a library of training videos/manuals.**

These instruction tools would include modules on basic laboratory practices, basic instrumentation description and techniques, tools used in data analysis, etc. These could be assembled in an ACOM YouTube Channel and/or Wiki site. Others could contribute, as part of their NSF proposal Broader Impacts.

**Potential Lead:** ACOM; others TBD

**Activity #3: Visitor programs/Mentoring and Training**

Specifically, ACOM (and EOL) should inform the ACCORD constituency of existing visitor programs to/from NCAR (e.g., the UVisit program; ASP Graduate and Professor Fellowships; ACOM Visitor program; additional EOL opportunities), and tailor these existing programs (when possible) toward EC scientists (e.g., establish an ACOM/ACCORD Early-Career Seminar Series). Inclusion of under-represented groups should be a major consideration here.

**Activity #4: ACOM/ACCORD website as a 'clearing house' for opportunities and resources.**

The ACOM / ACCORD website could provide connections/links to useful resources for ACCORD constituency, including:

- Campaigns being planned, with contacts, and potential opportunities;
- Opportunities to participate in campaigns (e.g., some of more mature requestable instruments have opportunity/need for student help)
- Instruments and facilities that can be borrowed / used (e.g., chambers not in use)

The website could also provide a mechanism for connecting mentees and mentors (solicited on a volunteer basis) within the ACCORD community.

**Potential Lead:** ACOM; others TBD (e.g., R. Griffin, W. Stockwell as mentors)

**Activity #5: A training workshop on instrumentation use, and related items.**

This activity could be organized by NCAR (ACOM and EOL), with participation of University professors who teach relevant courses. The workshop could be considered along the lines of a pre-ARISTO activity, providing early advice on how to design and build an aircraft instrument, and all the issues that need to be considered. The workshop could be proposed as an ASP Summer Colloquium.

**Potential Lead:** ACOM and EOL; others TBD