The Coordinating Research Council (CRC) conducted an Air Quality Research Needs Workshop on February 9–10, 2016, at the Georgia Institute of Technology, in Atlanta, GA. The workshop brought together researchers from academia, government, and industry to brainstorm and prioritize a short-list of high-priority research needs in the areas of mobile source emissions modeling, regional air quality modeling, and secondary pollutant formation. Highlights from the workshop are presented below; detailed results and conclusions are available via the CRC website (http://crcao.org/workshops/2016%20A-98%20AQMRN%20Workshop/A-98index2016.html).
Regional air quality models are employed in developing and implementing the National Ambient Air Quality Standards (NAAQS) and related regulations, and evaluating and selecting cost-effective emissions control policies. For the past 25 years, regional air quality models have been designed, developed, and continually improved. For instance, the U.S. Environmental Protection Agency's (EPA) Community Multiscale Air Quality (CMAQ) modeling system is designed using interactions of atmospheric chemistry and physics. CMAQ is an Eulerian (i.e., three-dimensional gridded) transport and atmospheric chemistry modeling system, which simulates ambient concentrations of ozone, particulate matter (PM), and toxic air contaminants throughout the troposphere. The chemical and physical processes are represented by state-of-the-art modules, which calculate initial aerosol concentrations (primary organic aerosols, or POAs) and subsequent aerosol concentrations (secondary organic aerosols, or SOAs). To simulate the complex atmospheric processes, CMAQ requires meteorological information and emission rates from sources of emissions that affect air quality in time and space. Hence, CMAQ relies on emissions modules to provide pollutant input estimates (magnitude, chemical speciation, location, and temporal variability of pollution sources). Input emission rates for CMAQ are estimated using the Sparse Matrix Operator Kernel Emissions (SMOKE) system, where SMOKE uses EPA’s Motor Vehicle Emissions Simulator (MOVES) to estimate mobile source emissions. Figure 1 illustrates the building of regional air quality estimates.

To help identify the most critical modeling processes or modeling data inputs that could be improved, CRC sponsored the Air Quality Research Needs Workshop. The workshop was attended by 50 invited technical experts on mobile source emissions and air quality simulation models. The main objective of the workshop was to generate a list of priority research needs.

Held over one-and-one-half days, the workshop began with an invited presentation for each of the three areas: regional air quality modeling, MOVES and emissions inventories, and secondary pollutant formation. These three speakers summarized the state of the science, identified ongoing research, and suggested initial areas where improvements could be made. The workshop participants were then separated into the three breakout groups to brainstorm research needs for their area. After the brainstorming, each group worked to clarify and consolidate the ideas and voted on their breakout group’s top 10 priorities. The three groups developed 30 research needs statements. The process is illustrated in Figure 2. The next morning, all workshop participants met.
together to discuss the top 10 priorities from each group and participants voted to identify the overall top 10 priorities for the workshop. The overall top 11 priorities are presented below. Two of the final top 10 were very similar—and thus combined for this write up—and three tied for tenth place.

### Top Research Needs

1. **Improved Spatial and Temporal Allocation of Emissions**
   (This is a combination of two top 10 priority items; from MOVES and Regional topics.)

   Spatial and temporal allocation of on-road and non-road mobile emissions is critically important to achieving accuracy of emission inventories and air quality model results. Currently, mobile source and nonroad emissions are distributed to counties using activity data and then to air quality model grid cells using spatial surrogates. Spatial allocation and activity distribution need improvement because modeling is being performed more frequently at finer scales, such as 4 km and 1 km. Presently, disparate data sources are used to develop vehicle activity data. In addition, vehicle miles traveled and vehicle population data are not developed consistently throughout the country in such a way that meshes with MOVES source type and road type definitions. The start and end of trips should also be considered as it is important to properly allocate off-network emissions.

   The proposed research would develop sources of data that track the movement of vehicles throughout each day (e.g., using GPS systems). Onroad mobile sources could be more properly spatially allocated using these data. Locations of trip starts could be identified, along with the movement of vehicles between counties. Means of identifying short- and long-haul trucks versus passenger vehicles should be considered. Truck stop locations and time spent at those stops could be identified. Similarly, nonroad engine use would be monitored and allocated. Methods to develop spatial surrogates for very fine grids and irregular grids should be developed. These new and enhanced data sources should be applicable nationwide.

2. **Enhance the Use of Measurements to Evaluate Emission Inventories and Models** (MOVES Topic)

   Several recent studies have claimed that one of the primary sources of bias between modeled and measured air pollution concentrations is inaccuracies in the emission inventories, particularly for mobile sources. Because there are many sources of inherent uncertainty in emission inventory development and air quality model formulation, it is often difficult to confidently attribute the magnitude and sources of error.

   As such, it is important that emissions rates are evaluated on a regular basis using methods that can remove the additional uncertainty introduced by chemical transport models.

   Real-world emission measurements (including on-road, roadside, plume sampling, and tunnel studies) are needed to evaluate MOVES onroad vehicle emission rates on a regular basis. Each type of measurement has strengths and weaknesses in capturing the full range of real-world emissions from the wide diversity of vehicles on the road, so emission evaluations need to consider information from multiple studies. Comparisons should account for transformation and losses of emissions in the near-road environment (such as PM and reactive nitrogen compounds). Additional work is needed to evaluate real-world emission rates other than on-road running emissions, such as starts, extended idling, evaporative, and...
brake and tire wear emissions and emissions from nonroad equipment. This emission data should be collected in ways that can be used to inform updates to MOVES and other emission inventory models.

3. Understand the Influence of NOx on SOA/PM Formation and Ozone (Secondary Pollutants Topic)
The formation of secondary pollutants (e.g., ozone, SOA) is highly dependent on oxidation chemistry in the atmosphere. Reductions in oxides of nitrogen (NOx) emissions through emerging control technologies will push ambient NOx levels lower. These future reductions will challenge the ability of current chemical models to estimate changes in relative SOA formation from precursor volatile organic compounds (VOCs) in an increasingly peroxide-rich environment. Further, NOx–VOC interactions can lead to additional secondary products (e.g., organic nitrates), which directly influence ambient NOx loadings and secondary pollutant formation.

Additionally, reactions between nitrogen dioxide (NO2) and atmospheric ozone produce nitrate radicals, which are also involved in VOC oxidation and secondary aerosol formation. Research is needed to evaluate the ability of the chemical mechanism to properly predict changes in secondary pollutant formation at lower NOx concentrations. Applicable research should: (1) evaluate ozone and SOA formation under current and future VOC–NOx conditions; (2) identify the importance of daytime and nighttime nitrate radical oxidation; (3) evaluate the fate of organic nitrates and their impacts on NOx cycling and ozone formation; (4) update predictive models for SOA and ozone formation as a function of ambient NOx levels; and (5) use chamber studies to test chemical mechanisms and evaluate relative reduction factors.

4. Undertake Air Quality and Emission Trend Analysis (Regional Topic)
Emissions are in a declining trend in the United States, but man-made emissions in East and South Asia have increased. Ambient data analyses show that mid-tropospheric ozone concentrations in remote areas, within the United States and globally, have been increasing over the past two decades. Therefore, it is necessary to assess air quality trends at locations that are not directly influenced by local anthropogenic emissions and evaluate the implication of global emissions on future air quality and environmental policies.

Long-term trend analysis of ozone and other photooxidants is needed at locations such as global background sites, upstream of urbanized areas, over the ocean, and at remote mountain sites. In addition to spatial variability, the analysis should consider temporal variation. Satellite-retrieved data, long-term ground-based measurements, and radiosonde data at background sites can be utilized for this work. The analysis should include concentration and emission trends, and identify mechanisms that drive these trends. Separate meteorological effect, such as inter-annual and inter-decadal variations, is desirable so that the impact of human activities associated with the trends can be isolated and extrapolated to future scenarios.

Ultimately, the analyzed trends should be applied to future projections by utilizing a meteorology–emission–chemical transport modeling platform. While projecting future trends is highly uncertain, various climate change mitigation strategies and clean-technology deployment options could be accommodated in scenario development. Additionally, it would be useful to revisit traffic growth projections used to develop air quality management, transportation and state implementation plans. While such projections have been made for a wide-range of applications, there has been little effort to revisit the projections developed in the past and assess the accuracy by utilizing available data.

5. Characterize Emissions and Composition of Secondary Pollutant Precursors from Gasoline and Diesel Nonroad Sources (Secondary Pollutants Topic)
A significant number of mobile sources, powered by gasoline and diesel engines, are operated off highways and local roads. These non-road sources contribute significantly to NOx and PM emissions. As a result of less-stringent regulations compared to those applied to motor vehicles, and the absence of emissions controls systems for many engines, non-road sources have much higher emissions rates per unit activity for precursors of ozone and SOAs. Further research is needed to better characterize precursors and formation processes for secondary pollutants from non-road sources.

Research also is needed to identify and better quantify the contributions of non-road sources to the atmospheric formation of ozone and SOAs. For the non-road sector, research outcomes are needed for: (1) chemically-resolved emissions profiles that include the most important ozone and SOA precursors; (2) ozone-forming potential and mass yields for SOA formation; and (3) experimentally-constrained mechanisms and/or parameterizations to model secondary pollutant formation in regional/global air quality and chemical transport models.

6. Improve Big (and Small) Data for Nonroad Activity (MOVES Topic)
Non-road engines such as lawn maintenance equipment, farm equipment, marine, aircraft, and construction equipment contribute significantly to the overall emissions inventory. This contribution is growing as emissions from other sources
heterogeneous chemistry. Water also modifies particle physical pathway for small molecules contributing to SOAs through mechanisms and therefore impacts the formation, evolution, and fate of secondary pollutants. Water modifies the reaction

Research is needed to update, improve, or generate non-road engine activity for use with MOVES. This would entail inventorying engine populations, performing and obtaining survey data on equipment use patterns, and developing alternative methods to collect or generate data. Research needs also include performing instrumented activity and emissions data collection to measure relevant activity, such as fuel use or engine-hours of operation per day.

7. Address Transfer Line and Chamber Wall Losses (Secondary Pollutants Topic)
Laboratory “smog chambers” often provide the fundamental data for understanding and predicting SOA formation. One major challenge in translating results from chamber experiments to robust parameterizations for models is evaluating the various wall effects on SOA formation and mass yields. While particles lost to chamber walls are often accounted for, there is limited understanding regarding the loss of organic vapors, reactive intermediates, and oxidants to chamber walls, which could lead to substantial underestimation of SOA formation. It is critical to thoroughly evaluate vapor wall loss in experimental setups to ensure the SOA yield parameterizations derived from laboratory experiments are robust and relevant to atmospheric conditions, where there are no wall effects.

Additional organic vapor-surface interactions during transfer of exhaust through constant volume sampling (CVS) and sampling lines may also bias measured PM emission rates and exhaust gas composition. Research is needed to investigate the effects of vapor loss in different parts of the emission measurement system, including the transfer lines, the CVS, and associated sampling lines. Research would include a systematic evaluation of organic vapor loss to environmental chambers to evaluate wall loss for organic vapors formed from different VOCs under various oxidation conditions. The extent of reversible vapor-wall partitioning should also be examined. In terms of chamber walls, experiments should also be designed to probe the effects of chamber use history on vapor wall loss.

8. Assess the Role of Water on SOA (Secondary Pollutants Topic)
The presence of water influences atmospheric reactions and mechanisms and therefore impacts the formation, evolution, and fate of secondary pollutants. Water modifies the reaction pathway for small molecules contributing to SOAs through heterogeneous chemistry. Water also modifies particle physical states and subsequent interactions of aerosols with clouds. Water uptake of secondary aerosol is complex and contributes significant uncertainty to our understanding of visibility, fogs, and clouds. The role of water in the atmosphere is not well understood and thus rarely incorporated in current air quality measurement and modeling schemes. New data and models are needed to constrain the impact of ambient relative humidity (RH) for secondary pollutant formation, evolution, and fate.

Research is needed to fill scientific gaps to help enhance our scientific understanding of the role of water in the atmosphere, specifically to: (1) quantify differences in secondary pollutant formation due to changes in relative humidity; (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) investigate dry and wet deposition; and (5) assess the role of water on Henry’s law constants for highly oxidized compounds.

9. (3-way tie) Improve Future Emissions Inventory Projections (MOVES Topic)
MOVES relies on the U.S. Energy Information Administration (EIA) annual publication, Annual Energy Outlook, to establish many of the future year on-road vehicle activity and fuel use projections. These input data are not updated with each Outlook release, and the default MOVES model assumptions for future projections can become out of date. There is a need for regular, periodic updates to the national-level future activity projections of the MOVES model that are more frequent than official MOVES model releases.

Research is needed to develop guidance for the implementation of periodic updates to future-year vehicle activity projections incorporating regularly published resources. Updates to projection data include vehicle miles traveled (VMT), vehicle class sales/populations, vehicle technology implementation, and activity among fuel type. In addition, because future-year activity data for air quality modeling is required at the county level, research is needed to develop methods to forecast differential activity growth that varies geographically, with higher vehicle activity growth in areas with higher than average human population growth.

9. (3-way tie) Condensation Rules for Chemical Mechanisms (Regional topic)
Air quality models typically use chemical mechanisms to represent the wide variety of atmospheric constituents and their interactions. These equations can vary depending on the model application, which will dictate how complex the mechanism needs to be. For example, regulatory modeling may have different needs than research applications; similarly,
it may be practical to model more detailed chemistry when modeling only a few grid cells than when modeling thousands of cells.

Chemical mechanisms are updated to incorporate new information and understanding of atmospheric chemical reactions such as NOx cycling, marine effects, and the impacts of nighttime meteorology and chemistry. Current tools do not support easy updates to the mechanisms, and condensing from explicit mechanisms to ones suitable for practical use and specific purposes can be difficult. Research is needed to investigate options to develop an automated approach for updating chemical mechanisms. This research could include a better approach to linked gas-aqueous-aerosol phase chemistry and integration with SOA and heterogeneous chemistry.

9. (3-way tie) Fires: Wild and Prescribed (Regional topic)
Fires are a significant contributor to PM emissions in the United States, accounting for 35 percent of PM2.5 mass in the 2011 National Emissions Inventory. Historically, national-level information has been used to estimate emissions from fires, but information at the state, regional, and local level can improve emissions inventories. Unlike other anthropogenic sources, fire emissions vary widely from year to year, making them difficult to model and especially difficult to project for the future. Research would be helpful to resolve questions such as the magnitude and speciation of fire emissions, their spatial and temporal allocation, plume rise, in-plume chemistry, relation of emissions to fuel types and burning stage, and the prediction of fire activity using soil moisture, satellite data and weather. Research is also needed on the interaction of fire emissions with emissions from other sources (e.g., fires near roadways).

Conclusion
There are many opportunities for improving air quality modeling through research. This list of prioritized needs compiled from the 2016 Air Quality Research Needs Workshop can serve as a guide for agencies that are considering funding or conducting air quality modeling research. A total of 30 research need topics were identified and discussed at the workshop, and they can be found on the CRC website (http://crcao.org/workshops/2016%20A-98%20AQM%20Workshop/A-98index2016.html). Universities and graduate students are encouraged to review the longer list to identify research topics for integration into unsolicited research proposals and dissertation work. By identifying this short list of research needs, the conference attendees hope to better focus resources toward improving the models that are used in air quality planning efforts. In some cases, data do not exist and new methods are needed to obtain the data. In other cases, data exist and new strategies are needed to analyze the data. In any case, the proposed research projects would help evolve air quality modeling over the next five years.

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