A Summary Report on

2022 Air Quality Research Needs Workshop

November 8 and 9, 2022, Davis, California

Co-Sponsored by:

Coordinating Research Council

California Air Resources Board

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1. INTRODUCTION

To identify the needs of the air quality research community, the Coordinating Research Council (CRC) and the California Air Resources Board (CARB) co-sponsored an Air Quality Research Needs (AQRN) Workshop that was held on November 8 and 9, 2022 at the University of California, Davis. The main purpose of this workshop on AQRN was to bring together researchers from academia, federal and state agencies, industry, and other stakeholders to brainstorm and develop a focused research agenda that can be used by CRC and CARB and other organizations to help guide future air quality research. The CRC organized the first AQRN in 2016, which resulted in 11 top research needs (see Appendix A for details and for research projects that were sponsored by CRC to address those needs). This was followed by the Southern California Ozone Research Symposium (SCORES) in 2018, also sponsored by CRC, to develop research needs focused primarily on ozone in southern California (see Appendix B for details). The drivers for air quality research may have changed since those workshops, warranting a fresh deliberation of the research needs. Some of the drivers that may impact future AQRN include:

- Revision of National Ambient Air Quality Standards (NAAQS) that may result in new non-attainment regions, test the ability of models to predict concentrations more accurately at lower levels, or require new modeling tools.
- Greater emphasis on environmental justice issues may require refined tools at local scales.
- Availability of more and more data (e.g., sensor data and newer satellite data) leading to increased use of machine learning tools that use observations and model estimates for data fusion, especially for developing exposure metrics for health studies.
- Potential new policies on climate, energy, and infrastructure that may impact what data are needed, including emissions inventory data, and require new modeling capabilities.
- Future of mobility – autonomous vehicles, goods movement, vehicle electrification.
- Global issues, such as the impact of climate change on air quality and/or global shifts in transport.
- Advances in computer capabilities.

The air quality community is always looking to improve air quality models (AQM) together with the underlying emissions and meteorological models. While many advances have been made over the years in physics and chemistry in these models that also take advantage of advances in computational resources, major gaps and uncertainties still remain. Given that and the evolving research drivers, there was value in bringing together the scientific community to reflect on the status of AQMs and brainstorm on future research needs to further improve the models to meet the ever-growing needs. The research needs identified as part of the 2022 AQRN Workshop will be made available to the broader research community for use, hopefully leading to synergies across different subject areas, fostering collaboration among different stakeholders, and leveraging resources to address the research gaps. This report provides an overview of the 2022 AQRN Workshop as well as a summary of breakout session prioritizations and full group prioritization results that identified knowledge gaps and future research needs.

2. WORKSHOP OBJECTIVES AND ORGANIZATION

The two main objectives of the 2022 AQRN workshop were to:

- Brainstorm on key research issues related to future air quality model development needs and identify research gaps in air quality;
- Anticipate future air quality research needs for use by the research community.

The workshop was organized around four major themes to facilitate discussions:

1. Emissions
2. Meteorology
3. Chemistry
4. Regional and local air quality modeling.

The detailed workshop agenda is shown in Appendix C. The workshop was structured to first have three speakers for each theme to provide background information on the topic. The speakers provided an overview of the current state of science, research gaps, and initial thoughts on future research needs to serve as background information and to stimulate discussion and brainstorming during the breakout sessions. All the speaker presentations were held in the plenary session. This was followed by a plenary brainstorming session to identify and discuss big picture issues/needs. The purpose of the plenary brainstorming was to allow all participants to share their thoughts on all themes before dividing into four breakout sessions. The ideas gathered during the plenary brainstorming were sorted into the four main themes and discussed further during the breakout sessions.

The workshop participants self-selected which of the four breakout sessions they wanted to attend. The session facilitators guided the discussion during the breakout sessions with the objective of identifying specific research issues/needs under each theme. After a list of research issues was developed, each participant in the breakout session was allowed to pick the top five issues from that list during “voting”. All the votes were then totaled to determine the top five (or six/seven in case of a tie) research issues for each theme. The breakout session participants also discussed specific research needs to address the research issues that were identified.

The session facilitators presented both the research issues and research needs to the whole group in a follow-up plenary session for further discussion. After presentations and discussion from each session, each participant voted for their top ten issues. The votes were tallied to determine the overall top ten research issues.

3. TOP RESEARCH ISSUES/NEEDS

Tables 3.1 through 3.4 show the list of top research issues identified under different themes. The issues that made it to the overall top ten list are highlighted in bold. The specific research needs to address those issues are discussed later. The overall top ten research issues that were identified during the final brainstorming and voting are listed in Table 3.5 (in the order from top to bottom).

Table 3.1: Top Research Issues Identified for Emissions

Issue #	Research Issue
1	**Emissions Inventories on Environmental Justice-Relevant Scales**
2	**Measure and Speciate N-containing and PM Emissions from Fuel Combustion**
3	**Urban Biogenic Emissions**
4	Evaluate Emissions from Sources other than Mobile Sources
5	PM Emissions: Dust, Tire & Brake Wear
6	Guidelines for Improving Inventories
7	Truck Emission Inventory Improvement

Table 3.2: Top Research Issues Identified for Meteorology

Issue #	Research Issue
1	**Consistent Implementation of Planetary Boundary Layer (PBL) Processes in Air Quality and Meteorological Models**
2	PBL & ASL Development and Assimilation Addressing Nocturnal Wind Speed Biases
3	Vertical Profile Measurements of Meteorology, Trace Gases, and Aerosols
4	Spatial Observations of Chemical Surface Fluxes
5.	Better Representation/Verification/Assimilation of Clouds and Lightning

Table 3.3: Top Research Issues Identified for Chemistry

Issue #	Research Issue
1	**Chemistry of Today and Tomorrow**
2	**OA (SOA) Temperature Dependence**
3	**Gas-Phase Mechanism Evaluation**
4	NH_3 – SOA Interaction
5.	Halogen Activation (Sources)
6.	Urban Sulfate Production

Table 3.4: Top Research Issues Identified for Regional and Local Air Quality Modeling

Issue #	Research Issue
1	**Multi-component Satellite / Ground Data Assimilation**
2	**Coupling + Feedbacks between Air Pollution and Meteorology**
3	**Characterization of Global Scale Processes that Act as Boundary Conditions for Cities**
4	Machine Learning + Explainable Artificial Intelligence (AI)
5.	Quantifying Uncertainty for Ensembles
6.	Decision Support Tools for Non-Technical Persons

Table 3.5: Top ten overall Research Issues Identified from the 2022 AQRN Workshop

Issue #	Research Issue	Theme
1	**Multi-component Satellite / Ground Data Assimilation**	Modeling
2	**Emissions Inventories on Environmental Justice-Relevant Scales**	Emissions
3	**Coupling + Feedbacks between Air Pollution and Meteorology**	Modeling
4	**Chemistry of Today and Tomorrow**	Chemistry
5	**Consistent Implementation of PBL Processes in Air Quality and Meteorological Models**	Meteorology
6	**Measure and Speciate N-containing and PM Emissions from Fuel Combustion**	Emissions
7	**OA (SOA) Temperature Dependence**	Chemistry
8	**Urban Biogenic Emissions**	Emissions
8 (tie)	**Gas-Phase Mechanism Evaluation**	Chemistry
10	**Characterization of Global Scale Processes that Act as Boundary Conditions for Cities**	Modeling

3.1. Emissions

Table 3.1 shows the top research issues identified under the emissions theme. Here are more details on each of those issues and specific research needs that were identified during the workshop to address each of the issues.

Emission Issue 1: Emissions Inventories on Environmental Justice-Relevant Scales

Environmental Justice (EJ) communities often experience degraded air quality, but our current inventories and models don't have the necessary spatial scales and chemical detail to resolve needed resolution for modeling in the EJ communities. In recent years, a lot of focus has been directed toward improving the air quality for EJ communities, but the emission inventories needed to be relevant for individual EJ communities lack the fine spatial scale and sectoral/compositional detail. If inventories do exist at the scale needed for EJ communities, they often are not consistent with larger scale inventories that are used for regional and regulatory modeling. The following research needs are identified to improve emissions inventories on EJ scales:

- Reconcile spatial scales of existing inventories for EJ communities and those used for regional and regulatory modeling;
- Compare top-down versus bottom-up inventories on EJ community relevant spatial scales;
- Develop appropriate surrogates for leveraging inventories from local scales to improve larger scale inventories;
- Develop spatial distribution of electric vehicle activity and future trends;
- Focus on “easily” controllable sources when prioritizing developing inventories.

Emission Issue 2: Measure and Speciate N-containing and PM Emissions from Fuel Combustion

Large uncertainties in NO_x and PM emissions from many in-use combustion sources exist. While there are still many uncertainties for N-containing and PM emissions, such as the NO/NO_2 emission ratio, on-road emissions are the best quantified. Emissions from other sources such as off-road, residential equipment and transportation with locomotive, marine, and aircraft emissions are less well understood. This is especially true for NH_3 emissions from NO_x control devices, which are likely to increase and are poorly quantified. The following research needs are identified to address this issue:

- Speciated N-containing (NO, NO_2, N_2O) and PM emissions from in-use on-road, non-road, and other fuel combustion (e.g., residential);
- Determine NO/NO_2 emission ratios and NH_3 emission factors for different combustion sources;
- Improve non-road locomotive, marine, and aircraft emissions;
- Determine extended idling emissions and locations, fleet composition, and defeat device presence of trucks;
- Determine deterioration factors for any fuel combustion sources.

Emission Issue 3: Urban Biogenic Emissions

In urban areas, biogenic Volatile Organic Compounds (VOC) emissions usually don’t dominate over anthropogenic sources, but urban vegetation can be a major source of VOCs and a significant contributor to ozone and secondary organic aerosol formation. Urban biogenic emissions are very uncertain in emission inventories due to the lack of appropriate detail in urban land cover classifications and emission factors. Biogenic VOCs, such as isoprene and monoterpenes, are very reactive and emitted by urban vegetation within cities, where NO_x from combustion is available for ozone formation, or they can be transported from vegetation surrounding the urban areas. In some cities, such as New York City, biogenic VOCs can be the main VOCs related to ozone formation. In many cities, efforts are underway to increase the urban vegetation to reduce the urban heat island effect, and therefore detailed knowledge of the urban biogenic VOC emissions is needed to understand current and future urban ozone formation. The following research needs are identified to improve urban biogenic emissions:

- Update urban speciated biogenic emission inventories;

- Better parameterization of urban specific emission factors related to stress such as drought and forest edge effects;
- Comparison of the emission parameterization of urban vegetation with natural forest or grassland ecosystems;
- Improve land cover classification and biomass density maps by leveraging existing and upcoming VPRM (Vegetation Photosynthesis and Respiration Model) inputs for CO_2 respiration.

Emission Issue 4: Evaluate Emissions from Sources other than Mobile Sources

Mobile source emissions have declined significantly over the past decades and currently are not the largest source of VOC emissions in large cities anymore; emissions from volatile chemical products (VCPs) are the major source of VOCs in densely populated areas. Over the past decade, the declining trend in ozone has slowed down in Los Angeles and other urban areas. To further improve air quality in major urban areas, VOC and NO_x emissions need to be further reduced. The composition of VCP and cooking emissions is vastly different from mobile sources and generally contain many oxygenated VOCs that are often not measured by routine monitoring networks and are not included or incorrectly lumped in chemical mechanisms. The following research needs are identified to evaluate non-road emissions.

- Quantify VCP and cooking emissions;
- Determine VOC speciation and temperature and seasonality dependence of emissions from VCP and cooking;
- VOC and NOx source apportionment of VCP and cooking versus mobile sources in various areas using currently available and future measurements and modeling effort for ozone attribution;
- Understand the future trend in VOC/NOx ratios for VCP and cooking.

Emission Issue 5: PM Emissions: Dust, Tire and Brake Wear

Mobile source PM emissions have reduced significantly and are expected to further decline in the future. Dust and tire & brake wear emissions are not expected to decline because the number of vehicles will continue to increase even if the new vehicles are electric vehicles. Tire & brake wear PM emissions will thus continue into the future and there is concern about the toxicity of those emissions, as they may contain Cr-VI and other toxic substances. The following research needs are identified to improve dust, tire, and brake wear emissions:

- Conduct field studies to measure dust, tire, and brake wear emissions;
- Identify toxicity of tire and brake wear emissions.

Emission Issue 6: Guidelines for Improving Inventories

There is often a lack of communication between emissions inventory developers and inventory validators, so the developers don't get the necessary information, detail, and data from validators for future improvements. Emission inventories, as one of the main inputs for air quality and climate models, are in constant need of updating and improvements to account for trends in emissions, activities, and new technologies. Bottom-up and top-down emission inventories rely on many different data sources such as detailed activity data or sectoral specific emission factors. Some of these data sources are more accurate and up to date than others. Inventory developers need specific validation data from the measurement community to improve specific knowledge gaps in inventories. The following research needs are identified to develop guidelines for improving emissions inventories:

- Quantify uncertainties in inventories and validation methods;
- Improve communications between emission inventory developers and validators;
- Focus on determining sectoral speciation;
- Develop consistent methods for forecasting of activity data;
- Encourage use of telematics and satellite data.

Emission Issue 7: Truck Emission Inventory Improvement

Trucks are the main source of urban NO_x emissions and are expected to continue to remain so in the near future, even with passenger vehicles becoming electrified. The VOC/NO_x ratios that determine NO_x-sensitive versus NO_x-limited regimes significantly depend on accurate NO_x emissions from trucks. However, there are still many uncertainties about the location, emission factors, fleet composition, and activity data for truck emissions. The following research needs are identified to improve truck emissions inventory:

- High resolution data and telemetry for truck emissions;
- Determine extended idling emissions, fleet composition, and defeat device presence;
- Develop location-specific truck emissions;
- Quantify benefits of heavy-duty inspection and maintenance.

3.2. Meteorology

Table 3.2 shows the top research issues identified under the meteorology theme. Here are more details on each of those issues and specific research needs that were identified during the workshop to address each of the issues.

Meteorology Issue 1: Consistent Implementation of Planetary Boundary Layer (PBL) Processes in Air Quality and Meteorological Models

The issue is to ensure that PBL processes for chemical species are treated consistently with meteorological scalers. Some AQMs employ PBL schemes that differ from the meteorological model, which can produce unintended errors in the AQ simulation. In meteorological models, PBL processes are constrained by continuous implicit feedback between wind and temperature profiles and turbulent parameters. However, in AQMs the turbulent parameters are either diagnosed from the state variables (e.g., temperature, specific humidity, winds) or input directly from the meteorological model. Without a similar constraint like the meteorological models in the CTM, the transport of chemical species still must be applied identically to the meteorological model. Even when eddy diffusivities are acquired from the meteorological model, there are still inconsistencies if the PBL scheme includes non-local transport such as EDMF schemes or YSU or ACM2. The common practice of testing meteorological/AQM modeling systems with a variety of PBL models (WRF currently has 18 choices) often results in inconsistent chemical and meteorological PBL treatment. The two ways to address this issue are described below including the research needs that were identified:

- In on-line integrated meteorology-chemistry models, the chemical species scalars should be included in the same code responsible for meteorological PBL processes. For coupled models where the meteorological model and the AQM are linked for 2-way synchronized execution but not integrated into single model code, or for off-line models where the AQM is run after the meteorology model, the PBL model in the AQM and the meteorological models should be essentially identical. Research is needed to test the application of such approaches.
- For some PBL models, identical processing of chemical and meteorological traces is simple but for others, such non-local gradient adjustment schemes or higher-order closure (i.e., 2^{rd} order or higher) extension to hundreds of chemical species is more challenging and perhaps impractical. For these models, research is needed to either develop methods to include chemical tracers or assess the error incurred by approximate solutions.
- Deployment of a nation-wide, high vertical resolution, profiling network with hourly frequency for both meteorology and chemical measurements for use in model evaluation.

Meteorology Issue 2: PBL & Atmospheric Surface Layer (ASL) Development and Assimilation Addressing Nocturnal Wind Speed Biases

The issue here is how to reduce persistent high windspeed biases that detrimentally affect AQ modeling. A specific concern here is that meteorological models, upon which air quality models rely, consistently have large wind speed biases at night, along with difficulty in correctly modeling the rise and fall of the PBL. An area of interest that was discussed during the workshop was improving our ability to capture PBL and ASL development, and how to assimilate observational data. Routine measurements of 10-m winds are available from an extensive network of surface meteorology stations across the world. The challenge is to develop new techniques for assimilation of this data in ways that do not distort the PBL dynamics. Assimilation systems that optimize model parameters according to model vs observation wind biases may be feasible strategies. A specific area of research that was identified is as follows:

- Develop ways to adjust the model physics or assimilate observations to reduce biases that detrimentally affect air quality modeling, particularly at night when stagnant winds can lead to high concentrations and in wildland fires.

Meteorology Issue 3: Vertical Profile Measurements of Meteorology, Trace Gases, and Aerosols

Validation of modeling techniques requires observational evaluation. PBL models differ significantly in their simulations of both stable and unstable boundary layers. In daytime conditions when deep convective boundary layers (CBL) often occur, the depth of these layers is critical for determining chemical concentrations in the well-mixed layers. The newly deployed ceilometers network will be valuable for evaluation of PBL depth. At night, when radiational cooling often leads to shallow stable boundary layers (SBL) the intensity of turbulent mixing is a crucial factor for surface level concentrations. At all times, day, and night, modeled vertical profiles of potential temperature, winds, and mixing ratios of water vapor and chemical species need to be evaluated through comparisons to measured profiles. While the NWS radiosonde network provides twice daily profiles of winds, temperature, and humidity at 69 sites in the CONUS, profile measurement that include chemical species such as ozone and that sample more often, including transition times, are not routinely available. Furthermore, wind and scalar gradients are often very steep near the ground during stable conditions such that radiosondes profiles do not have sufficient vertical resolution. The following research need was identified:

- Supplement the NWS radiosonde network and the ceilometer network with a high vertical resolution profiling nation-wide network with hourly frequency for meteorology and chemical measurements to advance PBL model development and evaluation. Measurement systems could include low-level high-resolution radiosondes, tethersondes, kitesondes, drones, aircraft and remote systems such as lidars, ceilometers, sodars, etc.

Meteorology Issue 4: Spatial Observations of Chemical Surface Fluxes

Dry deposition and bi-directional surface fluxes of gaseous and aerosol species are some of the most uncertain components of air quality models. Currently, there are very few measurements available for comparison with models and that too for very few species, mostly ozone, and only at a few special field experiment sites for limited durations. In addition, there are no standard measurement protocols or sets of measured parameters. Thus, comparisons to models are difficult and uncertain. The following research needs were identified:

- Routine network measurements of dry deposition and bi-directional fluxes of chemical species would greatly advance model development and evaluation;
- Co-locate chemical flux measurements with surface sensible and latent heat fluxes and CO_2 fluxes. One way to achieve this would be to add chemical fluxes to existing networks such as FLUXNET.

Meteorology Issue 5: Better Representation/Verification/Assimilation of Clouds and Lightning

Clouds have multiple effects on air quality including aqueous chemistry, wet scavenging, convective transport, and sun shading. Sun shading affects temperature and PBL growth rand educes photochemistry, which affects pollutant concentrations. NWP models typically simulate clouds in two ways: resolved scale condensation and microphysics and subgrid convective cloud using specialized parametrizations. Assimilating cloud related information from satellites, radar, and lightning detection networks have been shown to improve meteorological and air quality simulation. The following research need was identified:

- Further development, evaluation, and operationalizing current assimilation techniques using data from satellites, radar, and lightning networks.

3.3. Chemistry

Table 3.3 shows the top research issues identified under the chemistry theme. Here are more details on each of those issues and specific research needs that were identified during the workshop to address each of the issues.

Chemistry Issue 1: Chemistry of Today and Tomorrow

Organic aerosol (OA) is a major contributor to particulate matter (PM), and OA challenges scientific understanding by having complex molecular composition and numerous, diverse sources. This research topic emphasizes that challenges faced today in understanding OA will become even greater as organic emissions to the atmosphere respond to changing technologies, energy carriers (fuels), and other factors. Continued emphasis on reducing detrimental effects caused by PM pollution can be expected to lead to policies that further lower emissions and change the chemical environment of the atmosphere. Current understanding of OA is shaped by laboratory experiments that use chambers to produce OA under controlled conditions (temperature, humidity, pre-existing aerosol, NOx, etc.). However, chamber data that are most widely used to underpin air quality models are not adequately reflective of environmental conditions and sources. The following research needs for more relevant data were identified:

- Laboratory experiments over a wider range of conditions that improve overlap with current and future atmospheric conditions;
- Identify methods to best extrapolate from chamber conditions to the atmosphere, i.e., models;
- Further expand coverage of OA precursor emissions from traditional internal combustion engines to new fuels, volatile chemical products (VCPs), cooking, asphalt, biomass burning, and more-diverse biogenic volatile organic compounds (VOCs).

Chemistry Issue 2: OA (SOA) Temperature Dependence

This research need statement shares motivation with "Chemistry of Today and Tomorrow" while emphasizing that temperature strongly influences atmospheric OA concentrations and thus provides powerful opportunities to evaluate and improve our understanding of atmospheric OA. Observations in Los Angeles and around the nation show that summertime PM2.5 increases with temperature. In some locations this has been because of increased electricity generation by coal burning and associated higher SO2 emissions when it is warm. However, as NOx and SO2 emissions decrease, the residual temperature dependence of aerosol is driven by SOA. Understanding this temperature dependence and evaluating options for controlling PM2.5 on the hottest days are aspects of aerosol chemistry that test our understanding of process and mechanisms in ways that are different from examination of average concentrations. The following research needs were identified:

- Conduct experimental studies that characterize OA temperature dependence for relevant precursors;
- Conduct ambient measurements that characterize temperature dependence of SOA together with temperature dependence of precursor emissions;
- Compare observed OA temperature dependence against AQMs.

Chemistry Issue 3: Gas-Phase Mechanism Evaluation

Gas-phase reactions are central to understanding atmospheric oxidants, PM, and many toxic air contaminants. Compared to other portions of air pollution chemistry, the gas-phase chemical mechanisms are a mature field with an established core understanding that is extensively tested and evaluated. Nevertheless, new information emerges, and established knowledge is refined, creating an ongoing need for mechanism maintenance and evaluation to provide confidence that air quality management strategies are well-grounded. For example, chemical mechanisms for biogenic VOCs (isoprene and terpenes) have evolved substantially in recent years. Oxidants are very sensitive to reactions that deplete NO_x, e.g., formation of nitric acid or peroxyacyl nitrate (PAN), such that even small rate constant refinements are important. There is uncertainty in the atmospheric fate of organic nitrates (ONs) produced when NOx is oxidized which influences the extent to which the nitrogen is recycled back to NOx over multi-day timescales that are relevant to long range transport and background ozone. The following research needs were identified:

- Conduct gas-phase mechanism evaluation that considers the speciation (chemical composition) of HO_x and NO_y, the amount of NOx recycled from NO_y, sensitivity of ozone production to VOC/NO_x ratio, and other factors. The evaluation should consider the influence of temperature such as winter/summer differences and climate change. Evaluations should exploit the full range of available data including laboratory chamber studies, field studies in the ambient environment, and experimental studies that perturb ambient air (e.g., by adding NO_x) and measure response.
- Investigate how uncertainties in mechanism parameters (reaction rate constants and stoichiometric coefficients) influence overall mechanism uncertainty and even develop alternate mechanism realizations (e.g., “hot” and “cold” versions of the same mechanism structure) that support “ensemble” applications of air quality models. A well-known example of ensemble modeling is when hurricane forecasts present the forward path as an envelope rather than a single trajectory.

Chemistry Issue 4: NH_3 – SOA Interaction

Both observations and laboratory experiments suggest that Ammonia (NH_3) can modulate secondary organic aerosol formation, but pathways for representing this are not well understood or represented in air quality models. Future research efforts should focus on the following:

- Conduct laboratory experiments at atmospherically relevant concentration levels;
- Develop observational constraints to guide development of parameterizations for atmospheric models and their evaluation;
- Develop mechanistic representations for inclusion in AQ models.

Chemistry Issue 5: Halogen Activation (Sources)

Atmospheric halogens (Cl, Br, I) contribute to VOC oxidation, influence the fate of NOx, create new particles (nucleation), and perturb oxidants (ozone, peroxides, HO_x radicals) with implications for background ozone, ozone production and atmospheric lifetime of VOCs and methane. Impacts relevant to ozone nonattainment include ozone depletion by halogens in the marine boundary layer affecting background ozone, and enhanced ozone production in urban/industrial areas when nitryl chloride ($ClNO_2$) forms overnight and is photolyzed the next day to release Cl-atoms. VOC degradation by halogens, mainly Cl, shortens the atmospheric lifetime of methane and VOCs including toxic air contaminants. Characterizing halogen sources remains challenging both in terms of emission estimates and chemical processes. Sea salt is an important reservoir of Cl and Br but chemical interactions are necessary to "activate" them to the gas-phase. Ocean surface waters emit iodine compounds due to biological activity and chemical reactions in sea water initiated by ozone deposition. Halocarbon (e.g., HCFC, halon) degradation is another atmospheric source of halogens. AQ models increasingly include halogens in their chemical mechanisms but their ability to describe the impacts of halogens frequently is limited by errors in the halogen sources. For example, nitryl chloride concentrations measured at inland locations (e.g., Boulder, CO) are not reproduced by models based on known source terms suggesting that models systematically understate the role of chlorine in continental atmospheres. Br activation from sea salt is difficult to get right in part because widely used aerosol composition models include Cl but omit Br. The following research need was identified to address the halogen chemistry:

- Continued ambient measurements, complemented laboratory experiments, and model development to better characterize halogens sources and their influence on air quality.

Chemistry Issue 6: Urban Sulfate Production

Several mechanistic pathways that oxidize SO_2 to SO_4^{2-} are well-known including gas-phase reaction with OH radical and aqueous-phase reactions with peroxides, ozone, and molecular oxygen catalyzed by transition metals. However, limited measurements in cold (sub-freezing temperatures), dark (low to absent photochemistry), and polluted regions (e.g., Fairbanks, AK; China) reveal relatively high particulate SO_4^{2-} levels, the origin of which are not explained by the known pathways. Following research needs were identified to address knowledge gaps in understanding of atmospheric chemical pathways occurring in these extreme atmospheric conditions:

- Expanded ambient measurements of S(IV) and S(VI);
- Chamber studies of S(IV)→S(VI) conversion at relevant conditions;
- Improve the understanding of the influence of aerosol pH and thermodynamics;
- Leverage data from planned and future field studies such as the Alaskan Layered Pollution and Chemical Analysis (ALPACA).

3.4. Regional and Local Air Quality Modeling

Table 3.4 shows the top research issues identified under the regional and local air quality modeling theme. Here are more details on each of those issues and specific research needs that were identified during the workshop to address each of the issues.

Modeling Issue 1: Multi-component Satellite / Ground Data Assimilation

There is no perfect method to measure or predict air pollution concentrations across broad regions, but the merging of satellite measurements, ground-based measurements, and model predictions seems to take advantage of the strengths of multiple techniques. This approach has traditionally focused on $PM_{2.5}$ mass and NO_2 but expanding capabilities of both satellites and low-cost ground sensors will soon yield multi-component $PM_{2.5}$ measurements. New methods are needed to take advantage of this data.

Air pollution control programs over the past 5 decades have improved air quality across the US by reducing emissions from the largest and most common sources. Remaining pockets of air pollution reflect regional problems exacerbated by local sources and local meteorology. As concentrations have been reduced, the accuracy of our methods to quantify remaining pollution levels must improve. Data assimilation methods is one way to improve predictions of various components of air pollution to identify health impacts, quantify source contributions, and design targeted control programs to further improve public health. The following research needs were identified to address this issue:

- Data science methods that combine measurement data into continuous fields while still respecting conservation of mass, and chemical kinetic/thermodynamic principles;
- "Big data" to test new methods for data integration;
- Intercomparison studies to identify the most promising methods.

Modeling Issue 2: Coupling + Feedbacks between Air Pollution and Meteorology

The highest air pollution exposure events in the western US are now almost exclusively driven by wildfires. The greatest impacts occur when wildfire plumes are trapped near the surface, but this process is dynamic and complex. Chemical transport models struggle to predict concentrations on the scales needed to represent this behavior, and yet our analysis of future pollution events in a warming world with increased wildfires depends on this ability. To make matters worse, the frequency and severity of wildfires across the western US has increased in recent years due to the impacts of climate-influenced drought. The scientific consensus is that future conditions will be even more challenging, leading to more wildfire impacts on air quality. The public health implications will depend strongly on the dissipation patterns of smoke downwind of the wildfire. Data assimilation methods used to improve exposure estimates in historical fires cannot be used in the future. We need to improve the fundamental abilities of coupled meteorology-air pollution models to predict fire plume behavior, and to understand the limits of our ability to predict chaotic fire behavior during individual events. The following research needs were identified to address this issue:

- New coupled algorithms within weather models that are computationally efficient;

- Multiscale models with adaptive grids or meshless techniques.

Modeling Issue 3: Characterization of Global Scale Processes that Act as Boundary Conditions for Cities

As emissions in the US continue to decline, "background" concentrations account for an increasing fraction of the urban air pollution. At the same time, epidemiological studies continue to detect public health effects at lower concentrations, pointing to reduced thresholds for ambient air quality standards. Understanding the trends in future concentrations for background pollutants will be critical in planning attainment strategies. Previous studies suggest background concentrations for ozone in the U.S. range between 30 – 60 ppb depending on the location, which accounts for a large fraction of the National Ambient Air Quality Standard (NAAQS) for ozone. Emissions control programs focus on limiting local O_3 production to 10-40 ppb depending on the level of this background concentration. Planning for future compliance with the O_3 NAAQS requires the ability to reliably predict future concentrations of background O_3. Similar issues exist for the 5 µg m^{-3} $PM_{2.5}$ standard set by the World Health Organization Background concentrations of $PM_{2.5}$ in California are currently estimated to be 3-5 µg m^{-3}. The following research need was identified to address this issue:

- Global scale models that use the same chemical mechanisms as regional scale models;
- Global scale models that can reproduce historical trends in background concentrations, identify critical sources/mechanisms, and project those into the future.

Modeling Issue 4: Machine Learning + Explainable Artificial Intelligence (AI)

Machine learning / artificial intelligence methods are proliferating rapidly in all areas of data science, including within the field of air pollution and population exposure. Many of these methods are "black boxes" that predict outcomes using variables that cannot be subjected to quality control checks that confirm physically plausible ranges for important physical / chemical parameters.

"Explainable Artificial Intelligence" is a field that seeks to formulate machine learning models using parameters with real-world significance (variables that have physical, chemical, etc. meaning). Such models can be independently verified against measured values to build confidence in the model formulation. The capabilities and limitations of verified models are better understood, and situations in which these models can be extrapolated outside the range of their training data can be more easily predicted. Explainable AI has the potential to improve the predictive ability of air quality models while at the same time maintaining strong linkages to our fundamental understanding of atmospheric processes. The following research needs were identified in this area:

- Complete list for algorithms to replace AQM processes and to bias correct AQM results;
- Explain machine learning and AI algorithms results with atmospheric physics and chemistry.

Modeling Issue 5: Quantifying Uncertainty for Ensembles

Ensemble air quality predictions can quantify the uncertainty in AQM predictions. Independent models applied by knowledgeable researchers can produce a range of outcomes that define the distribution of possible pollutant concentrations. Understanding this uncertainty is important when using AQMs to design emissions control programs, estimate exposure concentrations, etc.

AQMs are based on equations describing emissions, transport, chemical reaction, deposition, etc. Some of these processes are described at the fundamental level while others are highly parameterized. Uncertainties in model parameters and model formulations can lead to errors in the predicted concentrations. Intercomparisons between models can quantify the uncertainty in the model predictions and help to identify key parameters/processes that contribute to this uncertainty.

The basic research needs identified in this area include:

- Multimodel (and multi-inputs to single or multiple models) applications to assess how uncertainties propagate to air quality model results;
- Application of inverse and adjoint multi-model applications to quantify the uncertainties in such applications (e.g., inverse/adjoint modeling to provide top-down emissions estimates), and their dependency on *a priori* inputs and models;
- Fundamental research on how to use models that are not independently developed in ensemble modeling, and how their use relates to model evaluation;
- Developing guidance for the use of ensemble models in regulatory policy analysis;
- Ensemble analysis of the role of background and anthropogenic formation on pollutant concentrations.

Modeling Issue 6: Decision Support Tools for Non-Technical Persons

Most of the top decision-makers in state and federal agencies are not working hands-on with cutting-edge modeling techniques. These decision-makers need tools to explore the air quality implications for a range of policy decisions that require an understanding of how future air quality will respond to changes in emissions.

Numerous projects in recent years have focused on the development of simplified models that can quickly predict air quality under a wide range of policies. The accuracy and limitations of these models must be better understood before they can be used to make major policy decisions.

The basic research needs identified in this area include:

- Develop tools to integrate multiple aspects to be considered in decision making;
- Public outreach for the availability and potential of such tools;
- Cross comparisons between simplified and full AQMs;
- Identification of promising methods for simplified AQMs.

4. SUMMARY

The 2022 AQRN workshop's objective was to brainstorm on future air quality research issues and anticipate future air quality research needs for use by the research community. Over 60 participants representing different stakeholder groups attended the two-day workshop where invited speakers first presented background information and research needs on different themes (emissions, meteorology, chemistry, and regional and local air quality modeling) of the workshop. This was followed by breakout sessions and prioritization exercises in those sessions as well as a plenary session to identify the top research issues and needs for different themes. The list of air quality research issues and research needs identified as part of the 2022 AQRN workshop can serve as a guide to research organizations when prioritizing their own research activities and facilitating collaborations to leverage limited resources. This can also serve as a guide to researchers who are looking to collaborate with others on these high priority topics. Many research projects could address multiple issues simultaneously.

Acknowledgements

Authors would like to acknowledge funding support from Coordinating Research Council and California Air Resources Board to sponsor the 2022 AQRN workshop, as well as the organizing committee, presenters, and other participants of this workshop for their contribution.

Appendix A

The original CRC Air Quality Research Needs workshop was held in February 2016 at Georgia Institute of Technology. The proceedings of the meeting were published in *EM* in July, 2021 (link). Table A.1 summarizes the top research needs identified by the attendees, and Table A.2 lists CRC research projects related to these priority areas that were funded.

Table A.1: 2016 AQRN Workshop Top 11 Results

No.	Subject	Topic
1	Improved Spatial and Temporal Allocation of Emissions	MOVES & Regional
2	Enhance the Use of Measurements to Evaluate Emission Inventories and Models	MOVES
3	Understand the Influence of NOx on SOA/PM Formation and Ozone	Secondary Pollutants
4	Undertake Air Quality and Emission Trend Analysis	Regional
5	Characterize Emissions and Composition of Secondary Pollutant Precursors from Gasoline and Diesel Nonroad Sources	Secondary Pollutants
6	Improve Big (and Small) Data for Nonroad Activity	MOVES
7	Address Transfer Line and Chamber Wall Losses	Secondary Pollutants
8	Assess the Role of Water on SOA	Secondary Pollutants
9	Improve Future Emissions Inventory Projections	MOVES
10	Condensation Rules for Chemical Mechanisms	Regional
11	Fires: Wild and Prescribed	Regional

Table A.2: CRC-Funded Projects Since 2016 Using AQRN Results in Prioritization

CRC No.	Project Title	AQRN Top 11 Subject
A-129	Observation-based Quantification of Background Contributions to Maximum US Ozone Concentrations	4
A-128	Quantifying the Effects of VOC/NOx Chemistry on Tropospheric Ozone Production	3, 10
A-126	Analysis of Impact of COVID-19 on Emissions and Air Quality in Southern California	1, 4
A-125	The rising importance of non-combustion emissions in urban atmospheres	1, 2
A-124	Evaluation of Ozone Patterns and trends in 8 major US metropolitan areas	4, 11
A-123	Uncertainty in ozone changes from control strategy implementation	4, 9
A-121-2	Biogenic vs Anthropogenic VOC Analysis During Peak Ozone Events in the SoCAB	1, 2
A-121	Direct Measurement of Ozone Sensitivity to NOx and VOC in the South Coast Basin	2, 3
A-120	Empirical Analysis of Historical Air Quality and Emissions Information to Develop Observationally-based Models of Ozone-VOC-NOx relationships in Southern California and the Comparison to Air Quality Models	3, 4
A-119	Improving Modeling Techniques and Data Availability for Source Characterization	1, 6, 9

A-118	Role of meteorology, emissions, and smoke on Ozone in the South Coast Air basins	4, 11
A-115	Developing Improved Vehicle Population Inputs for 2017 National Emissions Inventory (NEI)	1, 9
A-114	Characterizing Primary Organic Aerosol Partitioning from In-Use Motor Vehicle Emissions	5
A-113	Influence of NOx on SOA and Ozone Formation – Chamber Study	3
A-112	Relative Reduction Factors Using Anthropogenic Ozone Increments	1, 4, 9

CRC project reports are posted at https://crcao.org/published-reports-full/

Appendix B

In 2018, CRC and the Engine Manufacturers Association convened the Southern California Ozone Research Symposium (SCORES) to bring together leading experts to review and discuss the capabilities and limitations of air quality models to simulate air quality trends as observed in the past years in southern California. The symposium results were published in the December, 2018 issue of *EM*. Several CRC research projects have been funded that address the top needs, as listed in Table B.1.

Table B.1: 2018 Southern California Ozone Research Symposium; Top 5 Research Needs
NOTE: These do not need to be Southern CA specific projects.

No.	Subject	CRC Projects
1.01	Observational response of ozone to changes in NOx and VOC More experimental data are needed to characterize the real-world relationships between NOx and VOC transformation to ozone. Examples of experimental approaches are projects such as in-situ, dual-chamber observations and experimentation at several ground sites, and aircraft surveys to understand spatial patterns. Some aircraft data are available that could be analyzed further, such as data from the California Air Resources Board's CalNex program. New flight monitoring precursor concentration information is needed to measure and analyze the current ozone air quality regime.	A-121, A-121-2
1.02	Short, medium and long-term relationships and evaluation of ozone with meteorology More accurate characterization of the meteorological parameters is needed to better capture their influence on air quality variability over daily to decadal time-scales. Errors in meteorological fields used to drive air pollution models can influence the model's ability to accurately estimate air quality trends, thus affecting researchers' ability to make accurate inferences on plausible factors dictating discrepancies between model and observed trends. For instance, systematic low bias in early morning surface wind speeds could artificially overestimate model NOx, which may over- attribute errors in mobile emissions. Similarly biases in temperature, radiation, ventilation, and air-surface exchange can influence biases in predicted air pollutant concentrations. These relationships must be characterized more accurately over short, medium, and long-time scales, so that more robust inferences on model-predicted changes in air quality can be made.	A-118, A-124
1.03	Mobile Source Emissions Research is needed to identify data gaps to accurately characterize variability in heavy-duty vehicle (HDV) emissions and how to temporally and spatially allocate these emissions. Data is needed to understand how HDVs equipped with selective catalytic reduction deteriorate based on maintenance intervals. Satellite trend data could be used for gathering the emissions information. NOTE: This is not intended to be a Real World Emissions Project.	A-125,
1.04	Biogenic Vegetation Improved characterization of the Southern California coastal area biogenic vegetation coverage is needed particularly because it is urban and changing. The drought and flood cycles create changes in vegetation type and amount of area	

	covered. Research is also needed to determine how the biogenic vegetation chemical speciation has changed.	
1.05	Dynamical Model Evaluation (in Southern California) Chemical transport models (CTM) are used to assess control effectiveness and demonstrate future attainment. Required levels of emission control are pushing models toward chemical regimes where the CTMs have not been robustly evaluated. Multi-decadal periods witnessing significant technological and emission changes could be analyzed to determine the trends in the ozone decline, plateau, and uptick. Trends in precursor species and other secondary pollutants should be analyzed along with trends in background ozone and long-range transport contributions. Efforts should be devoted towards developing historical emission inventories that consistently represent the changes in emissions of various precursor species over the multi-decadal period based on changing activity data and speciation profiles reflective of control technologies and fuel formulation changes.	A-120

Appendix C

2022 AQRN WORKSHOP ORGANIZING COMMITTEE

- Sandy Winkler (co-chair), Ford
- Chris Rabideau (co-chair), Chevron
- Naresh Kumar (workshop facilitator), DRI
- Tim French, EMA
- Tyler Fox, US EPA
- Mike Kleeman, UC Davis
- Toshi Kuwayama, California Air Resources Board
- Sang-Mi Lee, South Coast Air Quality Management District
- Rohit Mathur, US EPA

WORKSHOP AGENDA

November 8, 2022

8:30 am – 8:40 am	Welcome	CRC
8:40 am – 8:55 am	Introduction to the Workshop	Naresh Kumar, DRI
8:55 am – 9:00 am	Emissions Session Introduction	Janssen/Warneke
9:00 am – 9:20 am	Emissions Research Needs: A Mobile Source Perspective	Megan Beardsley, EPA
9:20 am – 9:40 am	Established and Emerging Priorities of Mobile Source Emission Inventories in California	David Quiros, CARB
9:40 am – 10:00 am	Improve Understanding of Emission Trends through Air Quality Monitoring and Modeling from Local to Regional Scales	Ling Jin, LBL
10:00 am – 10:05 am	Meteorology Session Introduction	Russell/Pleim
10:05 am – 10:25 am	Challenges in Modeling Land-Atmosphere Coupling, Boundary Layer, and Urban-Scale Processes for Air Quality	Jerome Fast, PNNL
10:25 am – 10:40 am	Break	
10:40 am – 11:00 am	Research Needs for Modeling Meteorology and Air Quality in Mountainous Regions	Heather Holmes, U. of Utah
11:00 am – 11:20 am	Meteorological Modeling Challenges Affecting Air Quality Simulations	Arastoo Biazar, U. of Alabama
11:20 am – 11:25 am	Chemistry Session Introduction	Mathur/Yarwood
11:25 am – 11:45 am	Temperature, Ozone and Aerosols: An Observational Perspective on Urban Chemistry Today and in an Electrified Future	Ron Cohen, UC Berkeley
11:45 am – 12:05 pm	The current State of SOA Modeling and the Path to Representing SOA Formation Given Changing Sources and	Kelley Barsanti, NCAR

	Chemical Conditions	
12:05 pm – 1:00 pm	Lunch	
1:00 pm – 1:20 pm	Anthropogenic Amplification on Production of Biogenic Secondary Organic Aerosols	Jingqiu Mao, U. of Alaska
1:20 pm – 1:25 pm	AQ Modeling Session Introduction	Kleeman/Lee
1:25 pm – 1:45 pm	New Approaches and Applications for Air Quality Modeling, including Integration of Satellite Data	Ted Russell, GA Tech
1:45 pm – 2:05 pm	Anthropogenic and Biogenic Contributions to Ozone Formation in California	Mike Kleeman, UC David
2:05 pm – 2:25 pm	Hemispheric to Global Scale Modeling Research Needs	Barron Henderson, EPA
2:25 pm – 2:40 pm	Brainstorming Orientation	Naresh Kumar, DRI
2:40 pm – 3:00 pm	Break	
3:00 pm – 4:00 pm	Plenary Brainstorming to identify and discuss big picture issues	All
4:00 pm – 5:00 pm	Breakout Brainstorming sessions For specific research needs	All
6:00 pm – 8:00pm	Networking event	

<u>November 9, 2022</u>

8:00 am – 9:00 am	Continue breakout brainstorming sessions	All
9:00 am – 9:30 am	Flipchart balloting to identify top 10 needs	All
9:30 am – 10:00 am	Break / Prepare talking points for breakout reports	
10:00 am – 12:00 pm	Breakout reports with discussion (30 min per session)	
	Report from Emissions Breakout	Janssen/Warneke
	Report from Meteorology Breakout	Russell/Pleim
	Report from Chemistry Breakout	Mathur/Yarwood
	Report from AQ Modeling Breakout	Kleeman/Li
12:00 pm – 12:45 pm	Lunch	
12:45 pm – 1:30 pm	Final discussion and flipchart balloting to identify top 10 overall needs	All
1:30 pm – 1:45 pm	Discuss results	All
1:45 pm – 2:00 pm	Next steps and Closing	Naresh Kumar, DRI
2:00 pm – 3:00 pm	Optional UC Davis tours	