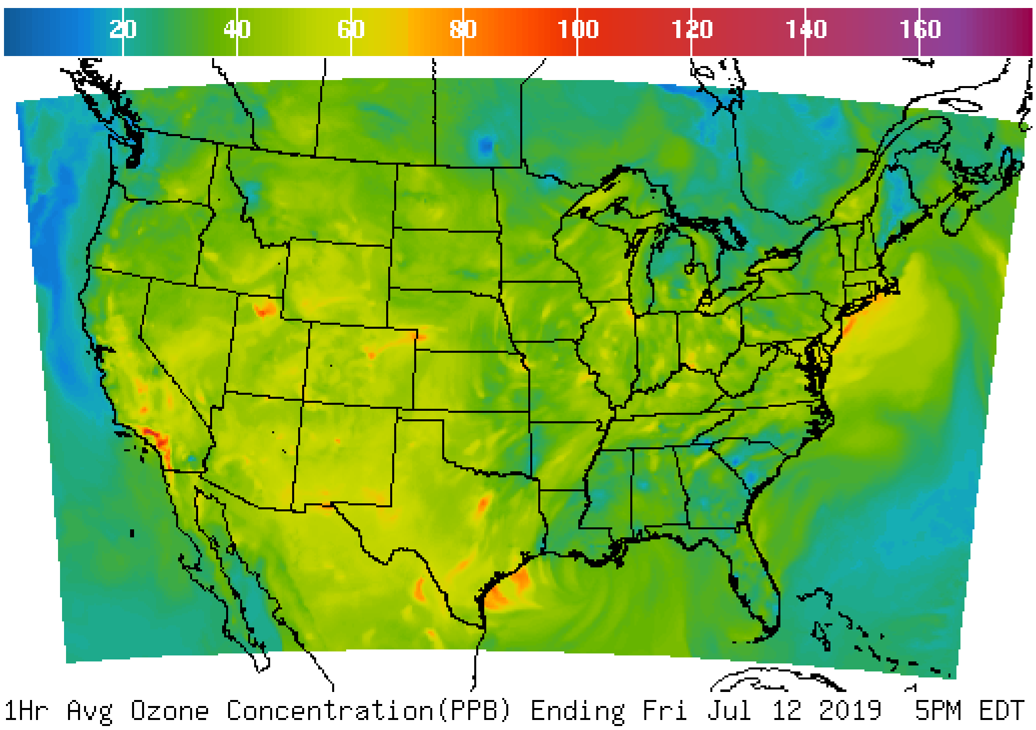
Air Quality 2020 Strategic Directions Workshop Report

Compiled from the November 13, 2021 Meeting



NOAA/NWS/Office of the Science and Technology Integration

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1. Introduction

On November 13 the National Weather Service (NWS) Office of Science Technology and Integration (OSTI) hosted the air quality strategic directions workshop. The main goal of this workshop was to foster community collaboration to improve the global and regional modeling of atmospheric chemistry and air quality. Thirteen top scientists in the fields were invited to share their thoughts and to discuss future modeling priorities in the field and the important gaps to be addressed. Presenters were charged with several questions in three main topics:

1. Current status of your system
   a. What are the primary objectives and forecast priorities of your system?
   b. What are the current capabilities of your system?
   c. What are the main strengths of your system?
2. Operational AQ/AC gaps and deficiencies
   a. What key long-term gaps need to be addressed out to 10 years in order to improve AQ/AC forecasts?
      i. What are the biggest challenges associated with those gaps?
      ii. What strategies are needed to address gaps?
   b. What are the top 3 science improvements needed to improve operational AQ/AC forecast capabilities and what are their expected impacts? (e.g., coupling to other components, data assimilation, temporal scales from hours to seasons, more pollutants/constituents, etc)
   c. Ideas for cost-effective methods
3. Areas needing increase in collaboration
   a. What science improvements/gaps can benefit from enhanced collaboration?
   b. Do we need to improve communication and collaboration among Agencies/Offices/Centers/Labs?
   c. Do we need a unified community chemistry model as a part of the unified forecast system (UFS)?

At the workshop, eleven 15-minute presentations were followed by discussion on six topics whose summary is provided in section 2. Section 3 summarizes the individual's point of view and recommendations from each of the presenters.

2. Summary of main themes discussed at the workshop on improvements and common gaps

The primary result of the workshop is a set of individual findings and recommendations from each of the members, which are provided in Section 3. During the discussion many common themes emerged that were mentioned by two or more members. This section summarizes those common themes.

2.1. **Better initialization and source constraint**:

Improvements in the utilization of satellite and other observational data are recommended which should help with data assimilation (DA) for composition and emissions including the use of multiple wavelengths for aerosol composition and advanced DA methods. Real-time adjustments to emissions (including anthropogenic source-based adjustments are also recommended along with biomass burning emissions (gas emissions, aerosol phase) including future fire behavior (out to S2S - land coupling is key)

2.2. **Improve process modeling**:

The following processes are listed for continued improvements: Chemical mechanisms, including making multiple mechanisms available on the modeling system. Improvements to the meteorological fields aiming at a single forecast for chemistry and meteorology, and better PBL parameterization, cloud resolving, vertical transport, surface fluxes, deposition processes and the diurnal cycle are also listed. The elucidation of stratospheric gas chemistry processes, especially for global S2S prediction is also of importance.

2.3. **Weather-AQ feedbacks:**

It is recommended to continue improvements of aerosol-radiation-cloud-precipitation interactions and their respective feedbacks including using aerosol-aware radiance data assimilation (DA) techniques. Coupling within ESM of atmosphere, composition, land and ocean (surface-atmosphere exchange) is also important for S2S and strong pollution events.

2.4. **Common evaluation tools:**

The development of common evaluation tools is recommended using routine in-situ, satellite and field mission data sets. These tools should have common protocols, standard metrics, diagnostic quantities, process-based metrics and scale dependence of metrics. Modelers should contribute to field mission design. Testbeds should be expanded.

2.5. Unified modeling and data assimilation platform

A unified modeling approach should be pursued, including modernizing code with modern engineering and flexible, modular design that's easy to update and allows rapid operational implementation if also used in research. Diverse approaches should be pursued during research with a single/streamlined approach for transition to operations. Multiple approaches within a single framework. Questions were raised about Keeping the chemistry as a separate component (online) or embed in physics (inline; subgrid scale transport, deposition, wet scavenging, aqueous chemistry). A common library for chemistry that is implemented in close connection to physics is desirable. Also a unified global to regional modeling structure that uses the same chemistry at global and regional scales.Challenges with high resolution modeling like, gray zone challenges, down to urban scales, high vertical resolution must be tackled.

2.6. Computational efficiency:

The development of machine learning emulators for chemistry in air quality forecasts should be further explored. Forward looking design should be prioritized over patchwork and codes need to be developed utilizing modern software engineering (object oriented, abstract interfaces, factories, flexible data structures, auto testing, code formatter, Dockers). Staffing and computational resources for system development and operations need to be secured. It is also suggested to start exploring exascale computing and the use of the GPUs.

3. Summary of individual presentations

3.1. Ivanka Stajner perspective:

The current air quality/atmospheric composition operational capabilities implemented at the National Oceanic and Atmospheric Administration (NOAA) include global aerosol predictions from the Global Ensemble Forecast System (GEFS)-Aerosol member and regional air quality predictions from the Community Multiscale Air Quality Modeling System (CMAQ), Hybrid Single-Particle Lagrangian Integrated Trajectory model (HYSPLIT), and High-Resolution Rapid Refresh (HRRR).

Future plans for improvements include the following for global predictions: 1) Extend GEFS-Aerosol member prediction from 5 days to Subseasonal to Seasonal (S2S) time scales in the UFS, 2) Focus on improving representation of biomass burning emissions (combine observations, predictions and climatology), and 3) Develop assimilation of AOD data and include and evaluate interactions of aerosols with radiation on S2S time scales. For emissions, include a unified system for NOAA global and regional models based on NASA and Harvard HEMCO and evaluate the potential for data-driven rapid refresh capability for emissions. For regional predictions future plans include: 1) Unification around high resolution Rapid Refresh Forecast System (RRFS) for the short-term weather UFS application, 2) Implement CMAQ online with RRFS for wildfire impacts on air quality (PM2.5 and ozone), 3) Improve the diurnal cycle and plume rise for fire emissions, 4) Improve initialization and assimilation of AOD and NO2 data, 5) Develop a machine learning emulator for chemistry in air quality forecasts, and 6) Coordinate with RRFS development for a smoke tracer including improved diurnal cycle and plume rise for fire emissions and Fire Weather Index (FWI) and evaluate all models using FIREX-AQ data.

The following gaps are identified in the current systems. First, unmet air quality forecasters' requests for high resolution AQ predictions (3km or finer) and extended AQ predictions out to 5 days. Second, there is a need to develop a comprehensive and accurate coupled earth system model for improved operational prediction for AQ and weather applications from hourly to seasonal time scales. Atmospheric composition and AQ need to be predicted accurately and their feedback included in the coupled Unified Forecast System. Finally, staffing and computational resources for system development and operations need to be secured. The identified science improvement needs include: 1) Improving the accuracy of atmospheric composition and AQ predictions focusing on emissions modeling (wildfires and dust, and timely updates of anthropogenic sources), meteorology (e.g. PBL height, cloudiness, vertical transport), and initialization of atmospheric composition concentrations (model state) and emissions using coupled data assimilation (DA), 2) Including feedbacks of atmospheric composition on atmospheric physics and meteorological DA through coupled modeling and DA, and 3) Improving computational efficiency of atmospheric composition DA and prediction. Increased collaboration is desired in building the coupled Unified Forecast System, with shared community atmospheric chemistry components, that NWS uses for operational AQ applications and for operational weather applications from hourly to seasonal time scales. Increased collaboration is desired on all science improvement needs listed above.

3.2. Paul Makar's perspective:

The current operational system of ECCC consists of the Regional Air Quality Deterministic Prediction System (RAQDPS), which uses the Global Environmental Multiscale – Modelling Air-quality and CHemistry (GEM-MACH) model. The model is On-line, but not fully coupled, the chemistry rides within the GEM weather forecast model as a subroutine package, but does not affect the weather. The RAQDPS system is currently being tested at a resolution of 2.5 KM for the western and eastern canada domain.

The following key long-term gaps out to 10 years are outlined. 1) On-line paradigm: if you haven't already gone there, you must. There are too many advantages, especially for, 2) Higher resolution forecasting: met models are going there, and AQ models will have to follow suit. This becomes prohibitively expensive for off-line. 3) Linking Global and Regional forecasts: Need to follow the weather paradigm of a global forecast providing boundary conditions for a regional forecast. 4) Forest fire forecasts as part of full chemistry forecast (Canada has been doing this for 5 years now, and our aim is to eventually merge the forest fire forecast with the main AQ forecast, we are very close to doing this. 5) Weather / AQ feedback: both NOAA (Georg' Grell's WRF-CHEM group) and ECCC have found significant improvements (>90% confidence) in weather forecasts if feedbacks are included. ECCC has done this with full chemistry, and found PM2.5, O_3, NO_2 forecasts also saw improvements. ECMWF and WMO are moving this way as well. The one-platform, on-line paradigm becomes necessary here. 6) Chemical Data Assimilation: we're seeing payoffs, e.g. stratospheric chemistry in GEM/GEM-MACH, Organic aerosols being applied to acid deposition. Satellite data! 7) Linkages between "climate" chemistry and "air-quality" CO_2 levels affect deposition rates, so we need to include CO_2 emissions and transport. CH_4 as a chemically reactive tracer and the effects of black carbon impacts on weather through feedbacks need to be considered too.

Suggestions on Science Improvements: 1) On-line paradigm should be adopted. 2) Common modelling platforms for different applications should be adopted, to the extent possible. The Canadian approach is to use one platform for development and different forecasts and then merge these back into the main branch, this is Cost effective. 3) Same chemistry (same model would be better, again, if possible) at global and regional scales. 4) Weather / Air-quality feedbacks, the ultimate aim should be a single forecast for both. 5) On-line forest fire emissions modelling. 6) Increase use of satellite-based information for model inputs; NRT emissions, vegetation data, etc. 7) Process improvements “motherhood statement” but don’t forget it, there is lots of “new science” still to reach the forecasting stage, like secondary organic aerosol formation, forest canopy turbulence and shading and particle direct and indirect effects are still being improved.

3.3. Rohit Mathur’s perspective:

The EPA has continued development and scientific improvement of the CMAQ system; documentation & model code can be found at https://www.epa.gov/cmaq. The latest version, CMAQ 5.3 provides updates to the representation of primary and secondary aerosols which have helped reduce PM bias significantly. Ozone bias has also improved significantly by drastically reduced wintertime O_3 underestimation and reduced overestimation in the summer. Manipulation of emission inputs to CMAQ has been made easier by deploying the Detailed Emission Scaling, Isolation, and Diagnostic (DESID) Module; which allow for the scaling of emissions by species, sector and location, which is useful for NRT emission-adjustment and ensemble modeling. It also helps Introducing emissions of new pollutants by scaling to an existing one like CO or total VOCs as well as scaling an emissions source computed inline in CMAQ such as wind-blown dust, biogenic VOCs, etc. Efforts are also underway to improve the representation of wildfire emission quantification, speciation, spatial and temporal variability, and vertical allocation to help better represent their impacts on O_3 and PM2.5. Other areas where there is room for improvement include, reconciling top-down & bottom-up “real-time” emission adjustments using satellite data as well as emerging traffic activity datasets which could potentially be used to modulate emissions in near real-time and account for longer-term emission change trajectory; reducing dry deposition uncertainty and the assimilation of aloft AQ observations to improve next day forecast. Future improvements should also include consistent representation of air pollution process-interactions across scales. For example, linking CMAQ with the Model for Prediction Across Scales (MPAS) should produce seamless mesh refinement to local scales, finer resolution in regions of interest and coarser resolution across the rest of the world to capture interactions with large-scale processes. Establishing a long-term record of air quality, reanalysis would help understand trends and model response; this could be done by archiving of NAQFC output.

3.4. Bryan Duncan's and Christoph Keller's perspective:

The current NASA Global modeling and Assimilation Office (GMAO) air quality forecasting capabilities include, the Goddard Earth Observing System (GEOS) Forward Processing for aerosols using the GOCART model, GEOS-Composition Forecast for trace gases and aerosol using the GEOS-chem model and the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) for aerosols using the gocart model for reanalysis of the atmosphere. The objective is to support NASA missions and not necessarily 'optimized' for air quality, but it has the strength of coupled aerosols and weather, global and high-resolution. Current identified gaps and deficiencies in AQ modeling include: 1) Moving to finer spatio-temporal resolutions, which is desired for AQ models; this is hampered by the need for fine spatio-temporal representation of processes and emissions and ultimately computing costs which limit moving to fine resolutions. 2) No direct assimilation of trace gas observations. and 3) Anthropogenic emissions are specified (assume 'business-as-usual').

The proposed top 3 science development priorities are: 1) Better integration of observations including coupled data assimilation of aerosols (AOD) and gas-phase species (CO, O3, NO2, and possibly HCHO), the incorporation (potentially thru assimilation) of additional data sources, e.g. surface observations, could low-cost sensors help? 2) Improved representation of emissions including real-time data to inform anthropogenic emissions (e.g., satellite NO2; CO, NO2 & VOCs from mobility data, etc.) and wildfire emissions. 3) Reduce computational costs, taking advantage of new hardware/software (e.g., GPUs) and incorporate machine learning methods to speed up forecasts (e.g., through chemistry, radiation, transport). Areas that could benefit from increased collaboration include, working toward a multi-model forecasting system, (like CAMS European regional ensemble)? Share forecasts for ensemble predictions and Enhance existing interagency exchange of advances in numerical modeling and related methods (e.g., machine learning applications). We also need ensure complementary (i.e., not competing/repeating) goals of the various AQ model systems, e.g. GEOS-composition forecast focuses on global (not US) atmospheric composition and provides boundary conditions, including natural sources of pollutants like lightning for EPA and NOAA AQ models. More clearly identify where NASA GMAO can support the national AQ modelling needs. Attention should also be given to the Communication of forecasts to diverse stakeholders and public, who are typically not familiar with AQI or concentrations, for instance. How should we reach a wider audience? How do we handle assimilation and emission estimates of trace gases and aerosol data from geostationary satellites? NASA GSFC/GMAO also plans short-term reanalysis for two field campaigns (CAMP2EX, FIREX-AQ) that will assimilate aerosol data from geostationary satellites.

3.5. Jerome Fast's perspective

The Department of Energy's (DOE) Office of Biological and Environmental Research (OBER) funds research on chemistry and aerosols relevant to climate across multiple spatial and temporal scales to improve fundamental understanding and model representation of processes associated with the aerosol lifecycle (e.g. absorbing aerosols, SOA, biogeochemistry) and aerosol-radiation-cloud-precipitation interactions (feedback effects), and develop computationally efficient algorithms for next generation climate models that are moving towards global cloud-system resolving (Δx = 3 km) scales. Priority science improvements for AQ Forecasting include. 1) Urban Scales: The ability to predict pollutants over neighborhood scales. 2) Diurnal Cycle: Improving predictions of not only peak concentrations important for human health, but better representation of minimum concentrations and diurnal variability of pollutants of interest. 3) Data Assimilation: Constraining initial conditions of a forecast by integrating chemical and aerosol data into model predictions. 4) Coupling: Include full coupling between meteorology and chemistry for physical and numerical consistency and representing feedback effects which can be important for large perturbations such as smoke and dust. A fully-coupled AQ model is a conceptually simpler system to maintain than separate offline models.

The primary long-term gaps and challenges, related to chemistry and aerosols are: 1) Anthropogenic Emissions: It is important to update emission rates due to changing human activities that vary from year to year, such as accounting for the impact of COVID-19 pandemic. 2) Biomass Burning: While much progress has been made to include near-real time information, predicting future fire behavior is still challenging. 3) Secondary Aerosols: There are still significant uncertainties in chemical mechanisms that affect aerosols, particularly SOA and aqueous chemistry; therefore, a path forward is needed to adopt updates to formation and removal processes in AQ models as science advances. 4) Chemical Complexity and Realism: There are always tradeoffs between accuracy, physical complexity, and computational efficiency that need to be accounted for. For example, ozone and particulate forecasts may be reasonable, even if the underlying mechanisms/parameterizations are known to have uncertainties. 5) Ensemble

Forecasts: While ensembles are performed for meteorological forecasts, ensemble chemical forecasts that encompass a range of uncertain parameters could provide a valuable probabilistic approach to AQ forecasting. 6) Software/Hardware: As computer hardware and software architectures change over time, it is important to consider how long legacy codes should be maintained or whether an effort is needed to modernize code. 7) Data Assimilation: Data assimilation of chemistry and aerosol largely confined to the surface where most routine measurements are made. Are there adverse effects of not assimilating data aloft? While assimilation of satellite AOD is now routine, how that AOD is distributed to aerosol components still causes problems and better techniques are needed.

The long-term gaps and challenges related to coupling are: 1) Gray Zone: the treatments of PBL and convection at subgrid scales will still be an issue even when meteorological models go to km scales. If Large Eddy Simulation (LES) models are employed for urban scales, the behavior of chemical mechanisms at those scales is largely unknown. 2) Clouds: There is currently a lack of consistency in the treatment of convective transport, aqueous chemistry, aerosol-radiation-cloud-precipitation interactions in both explicit and parameterized clouds. 3) Radiation: It is not clear at what scales will 3-D radiation become significant, not only for meteorology (and secondary effects on chemistry) but for photolysis. 4) Urban Forecasting: Urban canopy / urbanization datasets will need to be updated regularly, similar to anthropogenic emissions.

3 main points:

- AQ forecast development activities should target those related to improving the treatment of urban spatial scales, diurnal temporal scales, data assimilation of trace gases and aerosols, and coupling chemistry with meteorology in a consistent manner.
- The primary science gaps and challenges related to chemistry and aerosols include updating anthropogenic emissions in a timely manner, developing methods to account for fire behavior predictions in real time, and continuing to improve the representation of SOA, aqueous chemistry, and organic-inorganic interactions based on new findings.
- In terms of computational resources needed for AQ forecasts, a strategy is needed that permits increased complexity and realism in models, includes ensemble predictions targeting key AQ parameters, and provides a path forward to modernize codes for new hardware infrastructure.

3.6. Edward J. Hyer's perspective

The Naval Research Laboratory provides aerosol predictions to support prediction of environmental operating conditions including visibility and sensor performance for Navy operations. The Navy Aerosol Analysis and Prediction System (NAAPS) was developed to accurately forecast visibility reducing events. It was the first operational global aerosol forecast model with 144-hour forecasts 4x/day of dust, smoke, sea salt, anthropogenic and biogenic fine mode aerosols, it relies on a wide array of satellite data. A global model provides initial and boundary conditions for regional models as requested per domain. Regional domains can run with flexible configurations (for instance, dust-only) to balance accuracy with computational demands.

The near-term NRL Directions for Forecast Improvement include:

1) Composition: evaluate expanded tracer sets. We are interested in whether forecast skill can be improved by adding tracers to improve simulation of aerosol composition, especially absorption. This is motivated by desire to improve visibility solutions at wavelengths outside the visible, into the UV and IR.

2) Expanding observations for aerosol DA. A large number of innovative satellite retrievals are now mature enough to consider for operational testing; the most promising of these are multi-sensor retrievals that obtain quantities previously unavailable. We are examining how to extend and update our data assimilation capability to benefit from these new data sources.

3) Coupling between aerosols and NWP. We are pursuing multiple aspects of aerosol-NWP coupling, including aerosol-aware radiance DA, aerosol-radiation coupling and Joint NWP/Aerosol DA. Aerosol forcing vs NWP uncertainty only matters where/when it matters, so any implementation must balance accuracy vs computational cost. For aerosol-aware DA and IR-specific applications, can we do better than dust “bulk optical properties" (OPAC #5)?

4) Downscaling global to regional. Limited-area models can benefit from the global data assimilation to improve their initial and boundary conditions, but there are several obstacles to obtaining a good result. For example global model terrain isn't just smoother, it's lower. This will cause trouble with aerosols in the PBL; Can we do something smarter than “interpolate and stretch/compress” the profile from the global model to match the limited-area model profile? Model predictions will always be smoother in space and time than obs, but this can be improved with more detailed initialization. New GEO sensors can provide that detail; consistent products from a LEO/GEO constellation (NOAA Enterprise Algorithms) bring this much closer to reality.

None of our development efforts are self-contained, all are collaborative and our current efforts do not nearly cover all of the areas where aerosol forecasts can be improved. NRL is continually seeking collaboration and partnership from agencies and universities to build scientific understanding and improve our operational systems.

3.7. Gabriele Pfister's perspective

The National Center for Atmospheric Research (NCAR) Atmospheric Chemistry Observations and Modeling Laboratory (ACOM) is dedicated to the development and support of community atmospheric chemistry models in order to support the scientific community but also to meet the needs of decision makers. To be successful in this effort, atmospheric chemistry models need to couple with other Earth system components, cover scales from urban/local to regional to global, extend from the surface to the top of the atmosphere, predict on time scales from hours to decades, connect atmospheric composition with weather and climate and be efficient to be used in operational (and semi-operational) applications. Future modeling systems need to change spatial scales in a consistent manner, resolve multiple spatial scales consistently within a single simulation, couple model components that represent different earth system processes and easily mix and match model components for specific applications. The MUltiScale Infrastructure for Chemistry and Aerosol (MUSICA) initiative is a new community model-independent infrastructure, which will enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion. It couples to other earth system component models (land, ocean, sea ice, etc.) and follows a whole atmosphere framework enabling simulations spanning the entire range of the atmosphere from the surface to the thermosphere. MUSICA will facilitate the use of a variety of chemistry schemes, physics parameterizations and atmospheric models in a flexible modular way. The identified key future needs, in terms of science, include the need to reduce uncertainties in emissions and deposition processes, improved urban representation (online urban models, plume rise), simplification of chemical and aerosol schemes while preserving complexity and multi-scale representation, and improvements in meteorology (clouds, boundary layer). In terms of Infrastructure which is essential to enable scientific advancements, we need improvements on data assimilation for improving initial conditions and emissions (prepare for GEO AQ era), but key questions remain such as:What is the appropriate method? How to adjust species not observed? We also need near-real time processing of anthropogenic emissions from local to global; link online emission models to near-real time activity data (ability to adjust to sudden events); a flexible, modular "model-independent" design ("one for all") chemistry and aerosol interface with common emission tools and evaluation framework and adaptable data assimilation tools. It is also important to note that vertical refinement needs to go along with horizontal refinement. Community engagement/collaborations should start at design work - CCPP is a start. Forward looking design should be prioritized over patchwork and codes need to be developed utilizing modern software engineering (object oriented, abstract interfaces, factories, flexible data structures, auto testing, code formatter, Dockers).

3 main points:

- Development of unified modeling systems is crucial for advancing science
- Future systems need to be modular, flexible and adaptable and prepare for exascale computing
- Priority need to be placed on cross-organizational collaborations for infrastructure design and development

3.8. Vaishali Naik's perspective

NOAA Geophysical Fluid Dynamic Laboratory (GFDL) has developed different models for atmospheric predictions at different scales, among them SHIELD for subseasonal to seasonal (S2S) predictions, SPEAR for seasonal to decadal predictions, CM4 for decades to centuries climate processes and Earth System Model 4 (ESM4) for decades to centuries climate composition. GFDL-ESM4 is a seamless atmospheric chemistry component with 121 tracers including 18 aerosol and 58 gas phase prognostic tracers, five prognostic ideal tracers, and 40 diagnostic chemical tracers and include 248 reactions, including 43 photolysis reactions, 190 gas-phase kinetic reactions and 15 heterogeneous reactions.

The Science improvements needed for better prediction of AQ include, 1) Advances in the fundamental understanding of chemical, physical and biological processes that influence AQ needed to enhance predictive capability. 2) Reducing uncertainties in emissions from known sources and poorly constrained chemicals including, spatial and temporal resolution and real-time emissions. 3) Enhance comprehensiveness by representing interactions between land, ocean and atmosphere in a fully coupled sense. 4) Systematic and thorough evaluation of the parameterizations implemented for representing different processes that characterize AQ, including chemical mechanisms, interactive emissions, deposition and cross-component coupling.

3.9. Georg Grell's perspective

The Global System Laboratory (GSL) of the Earth System Research Laboratory (ESRL) conducts world-class applied research and directed development resulting in technology transfer of environmental data, models, products, and services that enhance environmental understanding with the outcome of supporting commerce, supporting NWS in protecting life and property, and promoting a scientifically literate public. Chemistry transport models are usually run offline, online or inline. We should be moving away from the offline setting and adopt online or inline coupling. To further advance coupling we need to start merging more with the physics and use sub-grid scale tracer transport for some turbulent transport schemes including deposition, sub-grid scale tracer transport for some convective parameterizations and wet-scavenging and aqueous phase chemistry for some sub-grid and grid-scale approaches. Chemistry modules can be extremely complex, but with proper coding standards can be moved without "too much" effort into other modeling systems; for example the WRF-Chem Chem_driver is now used inline in GEFS-aerosol, RAP-Smoke, and HRRR-Smoke.

The optimal future as we see it: make involvement of community easy and interesting for users. We are using CCPP for physics, let's use CCPP for at least most of the chemical modules. Lower level routines should be independent of CCPP and/or NUOPC. An example of an advantage is that the plume rise in CCPP will work for GEFS-aerosols, HRRR-Smoke, and CMAQ if it is used in the physics module, there is no need to reimplement into a complex chemical component. Routines that adhere to CCPP can already be moved to other modeling systems using shared libraries of lower level routines that are independent of coupling or models as much as possible. Let's make sure we have physics that can handle the atmospheric composition variables. I consider a community approach extremely important. In UFS, leave room for some complexity (only having GOCART will not catch too many interested scientists) and computer code should be "easy" to work with, this would be true if lower level routines are clean. Preparative work on RRFS Physics is underway. Both GF convective parameterization and most importantly MYNN/EDMF approach is now fully coupled with an indefinite number of tracers. This is being tested in RAPv5 which is being run in real-time with gas-phase and aerosol chemistry (reduced mechanism) at GSL including COVID-19 emissions and biomass burning emissions included. All tracer transports and wet scavenging are in RRFS physics. Biomass burning impacts on ozone chemistry is included in producing air quality forecasts. Aerosol impacts are included on radiation as well as on photolysis and different approaches are being looked at as it does not make sense to have the same approach. CMAQ (WF1) can use much more realistic approaches like aerosol module specific lookup tables and full online Mie calculations.

What is needed now and in the future for global and regional AQ forecasting at NWS/EMC. In the Next few years, for regional: Is the complexity in CMAQ really necessary, knowing the uncertainty in other parts of the modeling system. If so, can we simplify somewhere? Better physics coupling for microphysics, maybe also for other aspects of physics parameterizations. For global: We need global gas-phase chemistry that includes some knowledge about the stratosphere. Better physics coupling for microphysics but definitely also for other aspects of physics parameterizations. Solid evaluation of existing atmospheric composition interaction approaches (radiation, microphysics, convection) from medium range to S2S is also necessary. In the long term for the Regional we need to have something in RRFS that is much much simpler than CMAQ that can run on an hourly cycle, but will have more choices for physics coupling for microphysics. For the global, global storm-scale earth prediction capability, including aerosols/chemistry and coupled data assimilation. Regional and global Improvements through Machine Learning (ML) techniques, exascale computing start using the GPU and better parallelizations.

3.10. Gregory Frost's perspective

The NOAA Chemical Sciences Laboratory (CSL) performs air quality (AQ) and atmospheric chemistry (AC) modeling research on emissions, chemical reactions, physical processes, and their impacts on atmospheric composition. We use chemical-transport models for our field mission planning, forecasting, and analysis of observations. We develop emission inventories, produce model-ready emissions input, and evaluate emissions approaches through observational comparisons. We assess and improve chemical mechanisms using observational comparisons, and we develop and evaluate planetary boundary layer parameterizations. We use AQ/AC models as a transfer standard to compare in-situ measurements with remote-sensing observations and to evaluate Unified Forecast System (UFS) components under development.

The main strengths of CSL's approach to AQ/AC modeling are:

- Flexibility, in our ability to use different approaches to chemistry, emissions, initial and boundary conditions, domain, and resolution;
- Rapid response, in our ability to update emissions in response to regulatory and societal changes, and to improve chemical mechanisms using findings from field studies;
- Leveraging strong NOAA Lab/Line Office collaborations: CSL works closely with GSL on WRF-Chem, HRRR-Smoke, and RAP-Chem development, and with GSL, Air Resources Laboratory (ARL), NCEP's Environmental Modeling Center (EMC), and with NESDIS STAR on UFS development;
- Community involvement: the large WRF-Chem user community produces continuous improvements to model algorithms;
- Evaluation capability, through CSL's easy access to field observations and close interactions with field and satellite instrument teams;
- The freedom to innovate, explore new ideas, make mistakes, and improve.

CSL believes that the most important long-term gap in improving operational AQ/AC models is smoothing the path for Research-to-Operations (R2O) transitions. This gap can be addressed by evolving the UFS into a modeling system that serves the needs of *both* Research and Operations. These advancements would enable the UFS to continuously improve its model components through research collaborations between NOAA Labs and Line Offices and with the broader non-NOAA community, similar to the experiences of WRF-Chem and other community modeling systems. A truly community-based UFS would allow for a diversity of approaches for chemistry, emissions, physics, and other model components. Another UFS advancement that should be considered is the ability to carry out standardized evaluations using non-routine observations, including measurements from targeted field studies. A modern UFS AQ/AC model would allow for more timely updates to emissions inputs and chemical modules. Most importantly, the UFS must provide researchers freedom to do new science that will eventually become the next R2O transition.

The top 3 science improvements needed to improve operational AQ/AC forecast capabilities and their expected impacts are as follows:

1. Emissions: operationalize rapid updates to anthropogenic emissions, explore different approaches to improve biomass burning emissions, and

investigate biogenic and wildfire emissions and their feedbacks in a changing climate;
2. Chemical mechanisms: provide a diversity of mechanisms in forecasting systems; and
3. Chemical data assimilation (CDA): evaluate CDA methods using in-situ observations.

These improvements could be realized in the next 5-10 years by leveraging and expanding existing partnerships between NOAA Labs, Line Offices, and with Federal and academic partners. The following cross agency collaborations are already happening, but could be further strengthened:

- Rapid emissions updates: CSL + ARL, OAR + NESDIS + NWS, NOAA + NASA + EPA;
- Biomass burning emissions: OAR + NESDIS + NWS, NOAA + NASA + USFS;
- Biogenic and wildfire emissions: NOAA + NASA + EPA + USFS;
- Diversifying mechanisms: NOAA + NCAR + EPA;
- CDA methods: UFS R2O and HSUP2 Projects + UFS Application Teams + UFS Working Groups, NOAA + NASA + JCSDA.

A unified community chemistry model should be included as part of the UFS. Examples of successful community chemistry models that the UFS could emulate include NOAA and NCAR's WRF-Chem, the U.S. EPA's CMAQ, NASA's GEOS-Chem, and NCAR's MUSICA.

3 main points:

- CSL uses air quality/atmospheric chemistry (AQ/AC) models for research that improves the understanding of chemistry, emissions and physical processes, knowledge that CSL transitions to NOAA's operational prediction systems.
- The main strengths of CSL's approach to AQ/AC modeling are flexibility, an ability to rapidly respond to changes, the highly collaborative nature of our work, our model evaluations relying on a variety of observations, and our freedom to innovate.
- From CSL's perspective, evolving the Unified Forecast System to truly serve the needs of both Research and Operations will ultimately smooth the path for Research-to-Operations transitions.

3.11. Rick Saylor's perspective

The Air Resources Laboratory (ARL) is developing the NOAA Emissions and eXchange Unified System (NEXUS) to provide a community emissions processing system for UFS atmospheric composition models (both global and regional). Operational AQ/AC gaps and deficiencies are: 1) There is a vital need for a near-real-time emissions processing system that can provide emissions that are more up-to-date and better represent today's economic and meteorological conditions. Some progress has been made in this area, but a dedicated effort and funding to achieve this goal is needed. 2) Wildfire predictive science: Current wildfire emissions are based on satellite data of fire location and intensity from several hours ago. Research is needed to predict where fires will be in 24-48 hours so that smoke emissions can be better represented. Improved characterization of emissions as a function of fuel type and fire intensity is needed as it is a more accurate representation of plume injection heights and enhanced understanding of in-plume chemistry and SOA formation. 3) Enhanced representation of surface-atmosphere exchange processes and canopy effects, including canopy radiative, chemical and deposition processes are needed. Parameterizations for deposition and biogenic emissions were developed many decades ago and have not been substantially changed in models since that time. As horizontal and vertical resolutions continue to increase, parameterizations that were developed for use in models with 80-120 km grid cells may not be adequate for much finer resolutions. 4) A unified global/regional AQ/AC forecast system should be developed. BCs are becoming more important as U. S. air quality improves; a real-time global system to provide the best BCs (gaseous species as well as smoke and dust) for the regional modeling system is needed. 5) The transported species numerical bottleneck needs to be worked on as emulated machine learning chemistry can only provide so much computational speedup. This is a difficult problem but potentially could be attacked via several pathways: custom compute hardware; numerical innovations; machine learning emulation, Lagrangian parcel transport (for a global model). 6) Nested high-resolution domains, for example the I-95 corridor/NE U.S., California or others, could be developed and used to provide high-resolution forecasts in high-pollution areas rather than creating a 3-km CONUS forecast system that provides the same resolution over high and low pollution regions. 7) Exploratory research should be undertaken to evaluate the feasibility of AQ forecast ensembles. Reduced chemistry models or machine learning assisted forecast models could be developed and tested using perturbed emissions, alternate boundary layer parameterizations, wildfire injection heights, as well as meteorological ensemble members to drive the AQ ensembles and produce ozone and PM2.5 forecasts with inherent uncertainty estimates. 6) Improved vertical resolution in models is needed, especially near the surface as there is much more observed structure than can be simulated with current resolutions. This would improve the transport of smoke and dust plumes and provide better representation of near-surface boundary-layer processes.

Collaboration across OAR labs has improved significantly and collaboration across agencies is a worthy goal, but requirements and applications are different for each agency (forecasting vs. regulatory vs. mission support vs. pure science). Incentives (i.e., funding) are needed to promote inter-agency collaboration. Unified models are a good thing, but there is also value in having a diversity of models, for example RADM vs. ADOM vs. STEM, Climate models (more than 40 different models in CMIP6) and different chemical mechanisms like RACM vs. SAPRC vs. CB mechanisms.

3 main points:

- A near-real-time emissions processing system that can provide emissions that are more up-to-date and better represent current economic and meteorological conditions.
- Improved wildfire predictive science, including forecast fire behavior, emission characterization, plume injection heights, and plume chemistry and SOA formation.
- Updated representation of surface-atmosphere exchange processes and canopy effects, including canopy radiative, emission, chemical and deposition processes.

Appendix A. Acronyms list

AC: Atmospheric Composition
ACOM: Atmospheric Chemistry Observations and Modeling Laboratory
ADOM: Acid Deposition and Oxidant Model
AOD: Aerosol Optical Depth
AQ : Air Quality
AQI: Air Quality Index
ARL: Air Resources Laboratory
BC: Boundary Conditions
CAMS: Copernicus Atmosphere Monitoring Service
CAMP2EX: Cloud, Aerosol and Monsoon Processes Philippines Experiment
CB: Carbon Bond
CCPP: Common Community Physics Package
CDA: Chemical Data Assimilation
CH_4: methane
CM4: Climate Model 4
CMAQ: Community Multiscale Air Quality Modeling System
CMIP6: Coupled Model Intercomparison Project Phase 6
CSL: Chemical Science Laboratory
CO: Carbon monoxide
CO_2: Carbon dioxide
CONUS: Continental United States
DA: Data assimilation
DESID: Detailed Emission Scaling, Isolation, and Diagnostic
DOE: Department Of Energy
ECCC: Environment and Climate Change Canada
ECMWF: European Centre for Medium-Range Weather Forecasts
EDMF:Eddy Diffusivity-Mass Flux
EMC: Environmental modeling Center
EPA: Environmental Protection Agency
ESM: Earth System model
ESRL: Earth System Research Lab
FIREX-AQ: Fire Influence on Regional to Global Environments and Air Quality
FWI: Fire Weather Index
GEFS: Global Ensemble Forecast System
GEO: Geosynchronous Equatorial Orbit
GEOS: Goddard Earth Observing System
GEM: Global Environmental Multiscale
GFDL: Geophysical Fluid Dynamic Laboratory
GMAO: Global modeling and Assimilation Office

GOCART: GOddard Chemistry Aerosol Radiation and Transport
GPU: Graphics Processing Unit
GSL: Global System laboratory
HCHO: Formaldehyde
HEMCO: Harmonized Emissions Component
HRRR: High-Resolution Rapid Refresh
HYSPLIT: Hybrid Single-Particle Lagrangian Integrated Trajectory model
HSUP: Hurricane Supplemental
IR: Infra Red
JCSDA: Joint Center for Satellite Data Assimilation
LES: Large Eddy Simulation
LEO: Low Earth Orbit
MACH: Modelling Air-quality and CHemistry
MERRA-2: Modern-Era Retrospective analysis for Research and Applications
MUSICA: MUltiScale Infrastructure for Chemistry and Aerosol
MYNN: Mellor–Yamada–Nakanishi–Niino
NAAPS: Navy Aerosol Analysis and Prediction System
NASA: National Aeronautics and Space Administration
NCAR: National Center for Atmospheric Research
NESDIS: National Environmental Satellite, Data, and Information Service
NEXUS: NOAA Emissions and eXchange Unified System
NOAA: National Oceanic and Atmospheric Administration
NO_2: Nitrogen dioxide
NRL: Naval Research Laboratory
NWP: Numerical Weather Prediction
NWS: National Weather Service
O_3 : Ozone
OAR: Oceanic and Atmospheric Research
OBER: Office of Biological and Environmental Research
OPAC: Optical Properties of Aerosols and Clouds
OSTI: Office of Science and Technology Integration
PBL: Planetary Boundary layer
PM 2.5: Particulate Matter 2.5
PNNL: Pacific Northwest National Laboratory
MPAS: Model for Prediction Across Scales
NAQFC: National Air Quality Forecast Capability
NRT: Near Real Time
NUOPC:National Unified Operational Prediction Capability
RAQDPS: Regional Air Quality Deterministic Prediction System
RAP: RAPid refresh

RADM: Regional Acid Deposition Model
RACM: Regional Atmospheric Chemistry Mechanism
RRFS: Rapid Refresh Forecast System
SAPRC: Statewide Air Pollution Research Center
SHIELD: System for High-resolution prediction on Earth-to-Local Domains
S2S: subseasonal to seasonal
SPEAR: Seamless system for Prediction and EArth System Research
SOA: Secondary Organic Aerosol
STAR: Satellite Applications and Research
STEM: Sulfur Transport Eulerian Model
UFS: Unified Forecast System
US: United States
UV: Ultra Violet
VOC: Volatile Organic Compounds
WMO: World Meteorological Organization
WRF-CHEM: Weather Research and Forecast - CHEMistry

Appendix B. Workshop presentations

Ivanka Stajner (link)
Paul Makar (link)
Bryan Duncan and Christoph Keller (link)
Jerome Fast (link)
Edward J. Hyer (link)
Gabriele Pfister (link)
Vaishali Naik (link)
Georg Grell (link)
Gregory Frost (link)
Rick Saylor (link)