Managing Air Quality in a Changing Climate

*Where Do We Stand and Where Are We Headed?*

This article provides a brief review of history, current status, major challenges, and future prospects of 3D regional air quality models.
Background

Air quality refers to the chemical state of the atmosphere at a given time and place. Like weather, air quality affects everyone. Air pollutants include gaseous and particulate species that may lead to adverse health effects, such as eye irritation, premature death, and cancer. In addition, these pollutants can cause visibility impairment, acid deposition, climate change, water quality deterioration, and eco-environmental system damages. Changes in future energy/fuel use and emission control programs will change emissions, which will change future air quality.

Weather refers to short-term (minutes to months) changes in meteorological variables, such as temperature, humidity, wind, precipitation, and cloudiness in the atmosphere. Climate refers to the long-term pattern (typically over 30 years) of weather, such as averages of temperature, precipitation, and sunshine in a particular region. While short-term air quality is affected by meteorology, long-term air quality is affected by climate. For example, changes in temperature will affect the formation rates of ozone (O₃) and fine particulate matter (PM₂.₅), in both short- and long-term. Conversely, changes in the concentrations of climate-relevant species (see Table 1), such as greenhouse gases (GHGs) and PM₂.₅ will affect the Earth’s radiative budget; PM₂.₅ can also affect cloud formation through aerosol direct, semi-direct, and indirect effects. Extreme climate change may significantly impact air quality and human health through compounding effects. An example is the co-occurrence of drought, heat wave, and wildfires leading to persistent extreme hot/dry conditions under stagnation, which, in turn, cause extreme air pollution episodes with non-linear increase in adverse human health effects.

As outlined in the 2015 A&WMA Critical Review by Fiore et al.,¹ air pollution and climate change are two major environmental problems occurring at various spatial scales from local to global scales. The complex feedback mechanisms between them pose unprecedented challenges for the mitigation of air pollution and adverse climate change. Despite a historic separation of the research communities for tackling the two issues, their interplays through various feedback mechanisms are receiving increasing attentions by both research and regulatory communities. This is because the understanding of those complex feedback mechanisms requires coordinated, multidisciplinary research efforts; and the emission control strategies aiming at reducing air pollution may exacerbate adverse climate change (e.g., reduction of sulfate improves air quality but may enhance local warming). Integrated mitigation strategies are thus required to effectively address both issues. Three-dimensional (3D) air quality models (AQMs) provide a powerful tool to simulate air pollutants and their health and climatic impacts, and to assess the co-benefits and tradeoffs of air quality control, human health improvement, and climate change mitigation. Such information is invaluable to the development and evaluation of the win-win, holistic emission control strategies for both pressing issues.

History

3D AQMs have evolved into five generations since 1970s, with roughly one generation per decade, reflecting the advancements in scientific understanding and numerical and computational technologies. Reviews of some AQMs can be found elsewhere.²-⁷ The first generation AQMs (e.g., the Sulfur Transport Eulerian Model, version 1 [STEM I]⁹) were developed in early 1970s. Those models treated transport, emissions, and very simple chemistry with a few to ~30 reactions among only a few transported species. The second generation AQMs (e.g., the Regional Acid Deposition Model [RADM]¹⁰) expanded the chemistry to simulate 50–100 gas-phase reactions and 10–40 aqueous-phase reactions among 30–60 transported species. They treated bulk or internally-mixed aerosols, and parameterized dry deposition. Some treat resolved/convective cloud, cloud scavenging, and wet deposition processes.

Unlike the first- and second-generation AQMs that focused on a single pollutant/pollution problem, the third-generation AQMs (e.g., the Community Multiscale Air Quality [CMAQ] modeling system¹¹,¹²) were designed to address multipollutants and/or pollution problems by including more comprehensive chemistry (typically 100–300 gas-phase reactions and 20–100 aqueous-phase reactions) and aerosol and cloud microphysics. While the

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first-generation models used analyzed meteorological fields, the second- and most of third-generation models used offline calculated meteorological fields that cannot simulate the feedbacks of chemistry to meteorology. A few third-generation models, such as GATOR-MMTD\textsuperscript{13-15} and MCCM\textsuperscript{16} included coupled meteorology and chemistry.

In addition to much more comprehensive chemistry, aerosol, and cloud treatments, the fourth-generation AQMs (e.g., GATOR-GCMOM\textsuperscript{17,18} and the Weather Research and Forecasting model with Chemistry [WRF/Chem]\textsuperscript{19}) have two distinct features. First, they use online-calculated meteorological fields from advanced meteorological models (e.g., the WRF model) that allows the simulation of all important feedbacks between chemistry and meteorology/climate.\textsuperscript{19-23} Second, some are downscaled by a urban- and/or local-scale models, such as a human exposure model to simulate the health effect of pollutants\textsuperscript{24,25} or an urban traffic model to simulate air pollution at a freeway or neighborhood scale.\textsuperscript{26}

Since the early 2010s, fifth-generation AQMs have emerged. Their major feature is the use of one model framework across scales with unstructured variable resolution mesh, which allows smoothly-varying mesh transitions and, thus, overcomes possible abrupt transitions that may occur when using traditional one- and two-way grid-nesting techniques. Scale-aware physical parameterizations are being developed to provide seamless simulations from global to local scales. The fifth generation models are designed to simulate the interactions of small-scale phenomena (e.g., clouds, small hydrologic basins, and small estuaries) with large-scale phenomena (e.g., planetary atmospheric waves and earth–ocean circulations). An example of the fifth generation model is the Model for Prediction Across Scales for Atmosphere (MPAS-atmosphere) (MPAS-A) released by the U.S. NCAR in 2013.\textsuperscript{27}

## Current Status

Significant progress has been made since the 1970s in scientific understanding, and model development, application, and evaluation of AQMs. Oxidant and sulfur chemistry are well understood. The topics that are less understood include heterogeneous chemistry, aqueous-phase chemistry of organics, and the relative contribution of different PM components to health effects. The topics that are least understood include PM\textsubscript{2.5} and its climatic effects, in particular, the formation of secondary organic aerosol (SOA), the role of mixing states of aerosols (i.e., internal vs. external mixtures), and the direct and indirect radiative effects of aerosol. There have been numerous applications of AQMs worldwide at various grid resolutions from 1 km to 120 km; many of them focused on severe air pollution episodes such as regional hazes in China;\textsuperscript{28,29} and some focused on long-range transport of pollutants;\textsuperscript{30,31} and real-time air quality forecasting.\textsuperscript{32,33} Most model applications use offline-coupled AQMs over various airsheds; applications of online-coupled AQMs have been increased rapidly.

There have been increasing surface and satellites databases in the United States and beyond. Among them, the notable field campaigns include the California Research at the 2010 Nexus of Air Quality and Climate Change (CalNex) that focused on the nexus of air quality and climate change over California;\textsuperscript{34} and the 2013 Southern Oxidant and Aerosol Study (SOAS) (http://soas2013.rutgers.edu/) that aimed at better understanding...
understanding of biosphere–atmosphere interactions in the southeastern United States. However, there remains a lack of high-resolution data (e.g., hourly) for size-resolved PM$_{2.5}$ mass/number, and composition, wet and dry deposition fluxes, long-term and clean background data, and data from aerosol or cloud closure experiments.

There are increasing numbers of systematic evaluations of multiple models from multiple participants over a common testbed/episode using common emissions and other inputs. One such an example is the Air Quality Model Evaluation International Initiative (AQMEII) initiated by European Commission, the U.S. Environmental Protection Agency (EPA), and Environment Canada in 2012, which represents the up-to-date comprehensive assessment of capabilities of current generation AQMs in reproducing observations over Europe (EU) and North America (NA). Phase 1 of AQMEII (AQMEII1) focused on the evaluation of regional scale, offline-coupled AQMs,\textsuperscript{35,36} while phase 2 (AQMEII2) focused on the evaluation of online-coupled meteorology-air quality models.\textsuperscript{37} The ongoing phase 3 (AQMEII3) evaluates global and regional modeling systems driven by consistent emissions over EU and NA. Many modeling groups from EU and NA have participated in the three phases of AQMEII.

While most AQMs show good performance for O$_3$ with normalized mean biases (NMBs) of 10–20% and acceptable to marginally acceptable performance for PM$_{2.5}$ mass concentrations with NMBs <30–50%, they perform relatively poor for nitrate and organic PM, radiative properties, and PM number and size distributions with NMBs of 50% or higher. The worst performance lies in cloud variables, such as cloud droplet number concentrations and cloud optical depths that depend strongly on the model treatments of aerosol-cloud interactions. Most evaluations were performed for mass concentrations and fewer for other properties (e.g., wet/dry deposition, visibility,
PM number/size, radiative properties). While most evaluations were operational performance evaluation that calculates statistics, other higher levels of evaluations, including diagnostic, mechanistic, and probabilistic evaluations are increasing.

**Major Challenges and Future Outlook**

Despite significant progress in the past several decades, some limitations and deficiencies remain in accurately simulating air quality and its interactions with climate. First, most models do not contain accurate representations of several key processes or properties, such as the formation and hygroscopic properties of SOA, new particle formation, mixing states of aerosol, and aerosol-cloud interactions. Second, despite the use of an increasingly fine grid resolution, current AQMs cannot explicitly capture the fine-scale structure that characterizes climatic changes (e.g., clouds, Table 2. Major scientific and policy-relevant questions for O3 and PM2.5 pollution control in a changing climate.

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<tr>
<th>KEY TOPICS</th>
<th>KEY QUESTIONS</th>
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<tr>
<td>Sensitivity of O3 and PM2.5 formation to precursor emissions</td>
<td>To what degree should NOx and VOCs emissions be reduced to control O3 and PM2.5 pollution? Does PM2.5 pollution control require controlling of emissions of additional precursors (SO2, NH3)?</td>
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<td>Are emission control strategies effective for both O3 and PM2.5?</td>
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<td>How can we improve controls on dispersed primary emissions of PM2.5 (which are a large source of exposure to billions of people in developing countries)?</td>
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<td>How much O3 and PM2.5 can be formed from biogenic VOCs?</td>
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<td>To what extent can biogenic SOA be controlled via controlling anthropogenic emissions?</td>
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<td>Source apportionment and governing processes of O3 and PM2.5</td>
<td>What source category contributes the most to the O3 and PM pollution?</td>
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<td>What role does regional/intercontinental transport play in urban/local pollution control?</td>
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<td>How much reductions in CH4 emissions can further reduce ambient O3 pollution through reducing global tropospheric O3?</td>
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<td>What are the most influential modifiable factors that govern the regional heterogeneity of air pollutants in various regions on a variety of temporal and spatial scales in a changing world?</td>
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<td>Air quality–climate interactions</td>
<td>What are the important feedback mechanisms between chemistry and climate? How can we accurately represent these feedbacks in 3D models?</td>
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<td>How can the direct, semi-direct, and indirect aerosol effects be accurately quantified?</td>
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<td>What is the relative importance of the climatic impacts of pollutants from anthropogenic and natural sources? What are the relative contributions of each pollutant to climate forcing?</td>
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<td>What are the main uncertainties associated with anthropogenic climate change predictions and how can they be reduced?</td>
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<td>What are the compounding extreme climate events that will lead to extreme air pollution episodes?</td>
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<td>Win-win emission control strategies for controlling air pollution, adverse human health effects, and adverse climate change</td>
<td>Do emission control strategies of certain species co-benefit air quality control, human health improvement, and climate change mitigation?</td>
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<td>How useful would the controlling of near-term climate pollutants (e.g., CH4 and black carbon) be to supplement the CO2 control strategies?</td>
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<td>Is sulfate injection into stratosphere a plausible way to combat global warming?</td>
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<td>How can we convince both developing and developed countries to reduce their emissions for air quality and climate change mitigation and develop an agreement acceptable to all parties involved?</td>
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precipitation, mesoscale circulation, sub-grid convective system) due to limitations in relevant parameterizations/algorithms. Third, most models have limited capabilities in reproducing observed temporal/spatial variations of health-related pollutants. Finally, there remain large uncertainties in the air quality/climate model formulations, inputs, analysis methods, and measurement data used for model validation.

These deficiencies led to the largest uncertainties in current estimates of direct and indirect effects of aerosols on climate. Accurately simulating those feedbacks requires fully-coupled models and presents significant challenges in both scientific understanding and computational demand. While both offline and online coupled meteorology/climate–air quality models are actively used, online coupled models represent the direction of next-generation AQMs, they are increasingly used for simulations in support of policy-making, real-time forecasting, long-term climate simulations, and earth system modeling. Other major challenges are to quantify the uncertainties associated with major processes and parameters, represent complexity of the coupled climate–air quality systems within the current computational constraint, and integrate observations into models to improve the models’ capabilities.

In combating the two major challenges, a number of important issues must be addressed by the scientific and policy communities. These issues include the sensitivity of $O_3$ and PM formation to precursor emissions, their source apportionment and governing processes, major air quality–climate interactions, and the development of win-win integrated emission control strategies that co-benefit air quality, human health, and climate change mitigation. Table 2 summarizes major scientific and policy-relevant questions for each issue. For example, the most important public

References

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The most important public health policy question in both developing and developed countries is how to improve controls on dispersed primary emissions of PM$_{2.5}$.

Conclusion

Air pollution due to high concentrations of climate-relevant pollutants continues to be a pervasive problem worldwide and thus a central focus of current air quality management and climate mitigation efforts for many countries. 3D air quality models provide an invaluable tool to reproduce past pollution episodes and forecast future air quality. Fully-coupled climate/meteorology–air quality models have the capabilities of simulating climate/meteorology–air quality interactions and predicting future extreme climate and pollution events, and their correlations; they thus represent the future direction of the next-generation models. A key to the management of air quality in a changing climate is the development of win-win emission control strategies that co-benefit air pollution control and climate change mitigation. 

38. Seaman, N.L. Meteorological modeling for air-quality assessments; Atmos. Environ. 2000, 34, 2231-2259.