INTEGRATED METEOROLOGY AND CHEMISTRY MODELING
Evaluation and Research Needs

by Jonathan Pleim, Rohit Mathur, S. T. Rao, Jerome Fast, and Alexander Baklanov

Over the past decade several online integrated atmospheric chemical transport and meteorology modeling systems with varying levels of interactions among different atmospheric processes have been developed. A variety of approaches to meteorology–chemistry integration with different process-level algorithms for chemical feedback effects have been implemented in these systems. There have been many reasons cited for coupling meteorology and air quality into an integrated modeling system, including the following:

1) improved numerical weather prediction by including the effects of aerosols and gases on radiation and cloud microphysics as well as improving satellite retrievals and data assimilation for NWP operations by providing more accurate profiles of aerosols and radiatively active gases;
2) regional climate–chemistry modeling, including direct and indirect radiative forcing from short-lived climate forcers (SLCF);
3) improved air quality modeling due to closer coupling of dynamical and chemical processes and the inclusion of aerosol and gas feedback effects on radiation/photolysis, clouds, air temperature, and planetary boundary layer (PBL) processes, and further on air chemistry and chemical composition; and
4) realistic assessment of the efficacy of various emission control policies in improving ambient air quality under real-world conditions.

The benefits of online integrated models over sequential meteorology and chemical transport (offline) modeling, however, have not yet been well characterized from both a scientific point of view as well as from a policy perspective. The first

WORKSHOP ON INTEGRATED METEOROLOGY AND CHEMISTRY MODELING

What: Forty scientists from government, academia, and the private sector in the United States, Canada, and Europe discussed issues among different applications of integrated meteorology and chemistry modeling, such as numerical weather prediction, air quality modeling, and climate modeling.
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AFFILIATIONS: Pleim and Mathur—Environmental Protection Agency, Research Triangle Park, North Carolina; Rao—North Carolina State University, Raleigh, North Carolina; Fast—Pacific Northwest National Laboratory, Richland, Washington; Baklanov—Danish Meteorological Institute, Lyngbyvej, Denmark
CORRESPONDING AUTHOR: Jonathan Pleim, U.S. Environmental Protection Agency, E243-03, Research Triangle Park, NC 27711
E-mail: pleim.jon@epa.gov

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workshop analyzing initial experiences in integrated meteorology–chemistry (met–chem) modeling was organized in Copenhagen, Denmark, more than five years ago, in 2007 (Baklanov et al. 2011). Since that time great progress has been made in this new modeling approach, which now needs to be reviewed and integrated. A thorough weighing of the advantages of online versus offline systems for various applications would help clarify the usefulness of integrated modeling systems for policy analysis and identify future research needs. There is also a clear need for comprehensive evaluation of these systems, including process-level model intercomparisons and validation.

With the objectives of understanding the current state of the science, identifying the gaps in the model process representation and capabilities, and setting priorities for model development and evaluation research, a Workshop on Integrated Meteorology and Chemistry Modeling was convened by the U.S. Environmental Protection Agency (USEPA) with support from the U.S. Department of Energy (USDOE) and the European Framework for Online Integrated Air Quality and Meteorology Modeling [EuMetChem; European Cooperation in Science and Technology (COST) ES1004]. The goal of this workshop was to bring together key scientists from North America and Europe who are involved in the development and evaluation of regional-scale coupled met–chem models to i) discuss strategies for assessing and demonstrating the benefits of integrated modeling, ii) identify scientific gaps (structural, algorithmic, and processes) in current regional-scale integrated atmospheric models, iii) identify and develop new approaches for key missing processes, iv) develop approaches for systematic evaluations of key process algorithms that represent the coupling and feedbacks between atmospheric chemistry and meteorology using observations from different field campaigns, and v) assess the role of these models to guide air pollution and climate policy.

There were 40 scientists from government laboratories, academia, and the private sector from the United States, Canada, and Europe who participated in discussions of these issues, bringing together perspectives of different applications of integrated models in *numerical weather prediction*, *air quality modeling*, and *climate modeling*. Three invited talks given by leading scientists focused on these three application areas. After six brief additional talks by workshop participants on related topics, the afternoon was spent in three facilitated group discussions on 1) process gaps in integrated met–chem models, 2) observations needs and evaluation of integrated met–chem models, and 3) policy relevance and impacts on air quality, climate, and forecasting.

The first invited speaker, Jerome Fast of the Pacific Northwest National Laboratory, provided perspectives on the use of integrating met–chem modeling for air quality applications and assessments. Fast stressed the need for consistent modeling techniques for meteorology and chemistry in coupled systems as well as process evaluation by employing modeling testbeds that facilitate comparisons to field campaign data (e.g., Fast et al. 2011). The advantages for online coupled models for air quality applications include the following (see Zhang 2008; Grell and Baklanov 2011):

- high temporal coupling (data exchange frequency > once per hour) for high spatial resolution modeling to resolve high-frequency meteorological dynamics (e.g., wind speed and directional changes, PBL height variations, cloud formation, and rainfall) that have important effects on chemical transport, transformation, and removal;
- more realistic representation of concurrent chemical and physical processes through consistent dynamical, physical, and numerical modeling;
- coupling that allows the simulation of chemical effects on meteorology, such as aerosol scattering and absorption of radiation; aerosol effects on cloud microphysics through cloud condensation nuclei (CCN) activation; and dynamic treatment of radiatively active gases, such as O_3, N_2O, and CH_4, which are important for longwave radiative transfer calculations; and
- more realistic modeling of meteorologically dependent emissions, such as windblown dust, biogenic emissions, and sea salt.

The main disadvantage of online modeling is the increased computational cost particularly for multiple emission scenario experiments used by policy makers where constant meteorological forcing is applied for quantifying the impacts of emission perturbations. However, it should be noted that meteorological forcing does not remain constant in the real world.

Fast stressed that the engineering aspects of coupling meteorology and air quality are mature, but many inconsistencies and numerical issues still remain. Further research on aerosol feedback effects are needed, particularly for the representation of aerosol–cloud interaction. Evaluation of coupled systems requires additional observational data to validate feedback processes that focus on the optical and cloud microphysical effects of aerosols. While coupled models have the potential to improve the fidelity of air quality modeling, such improvements have been difficult to demonstrate with routinely available measurements because of the confounding uncertainties in meteorology, physics, and emissions. The impacts of radiative feedback effects are likely to be of secondary importance for air quality applications, except for extreme pollution cases.

The second invited talk was presented by Johannes Flemming of the European Centre for Medium-Range Weather Forecasts (ECMWF), who provided perspectives on the use of integrated met–chem modeling for operational weather forecasting. While it was acknowledged that many of the benefits of integrated met–chem modeling for numerical weather prediction (NWP) are similar to those for air quality or climate application (such as including chemical feedbacks on radiation and clouds), it has been difficult to demonstrate significantly improved statistical forecast skill attributable to the incorporation of these effects into the operational models, although improved aerosol climatology has reduced temperature errors in 1–10-day forecasts. The principal motivation for operational centers (e.g., ECMWF) has been to add chemical data assimilation to NWP data assimilation systems to improve assimilation of satellite radiances and 4D variational data assimilation (4DVAR) using aerosol optical depths (AOD) and trace gas observations. Flemming also noted that diagnostics of atmospheric chemistry processes related to transport and lightning can help improve NWP modeling.

Mark Z. Jacobson of Stanford University presented the third invited talk titled "Pushing the Envelope with Numerical Modeling." Jacobson has developed comprehensive atmospheric modeling systems, including integrated meteorology and chemistry processes on spatial scales ranging from global to urban. The Gas, Aerosol, Transport, Radiation, General Circulation, and Mesoscale Meteorology Model (GATOR–GCMM) developed by his group includes one of the most detailed treatments of explicit cloud and aerosol microphysics and radiation interactions among current modeling systems. While the impacts of black carbon (BC) on the absorption of clear-sky radiation and on cloud droplet number and size are well acknowledged, its effect on cloud properties varies depending on whether it exists within cloud water or between cloud droplets; inclusion of these effects were shown to increase column-integrated heating rates in midlevel clouds by 2.8 times that of BC in clear sky and 2.4 times that of interstitial BC (Jacobson 2012). Absorption by BC inclusion speeds up cloud dissipation, allowing more sunlight to reach the surface in a positive feedback. The combined effects of indirect aerosol forcing, cloud absorption, and semidirect effects can lead to a "boomerang effect," where clouds increase with aerosol loading up to a point (AOD ~ 0.4) and then decrease with further increase in the aerosol burden (Ten Hoeve et al. 2011). BC enhancements of radiation absorption are closely related to relative humidity and are greatest in areas of high humidity and clouds. Jacobson also spoke about advances in near-explicit gas and aqueous chemistry in 3D models, subgrid evolution of aircraft exhaust, and implementing the treatment of wind turbines into a 3D global/regional model.

After several short talks by workshop participants, the rest of the workshop was devoted to discussions in three themes: 1) process gaps in integrated met–chem modeling, 2) observational needs and evaluation of integrated met–chem models, and 3) policy relevance and impacts on air quality, climate, and forecasting applications. The focus of the process discussion was on interacting meteorological and chemical processes and feedbacks. There was consensus that the importance of feedbacks as well as the techniques used to model them depend greatly on spatial and temporal scales and the purpose of application. A prime example is aerosol interactions with warm and mixed-phase microphysics in convective clouds. Global-scale models cannot resolve these processes so their effects are represented by statistical approaches. Improved modeling techniques for cloud–aerosol–radiation processes and interactions across all scales were identified as a key gap in need of further research. Studies involving cloud-resolving models with explicit integration of cloud dynamics, cloud and aerosol microphysics, and chemical processes are needed for advancing our understanding and development of improved parameterizations. Modeled water vapor biases are a related and old-but-persistent issue that may be improved by better surface flux and PBL modeling techniques. Improvements in model representation of scavenging and wet removal of gases and aerosols were also identified as an important modeling gap. Increasing attention on urban environments and the importance of feedback effects on urban climate was also discussed. It was recognized that the perturbed climate in urban areas (i.e., urban heat island) may be exacerbated or mitigated by the radiation and cloud effects of air pollutants. Since gas and aerosol concentrations and population densities are the greatest in developed areas, impacts on human health and welfare are most acute in these locations. Thus, coupled met–chem modeling with urban parameterizations was identified as a new important research area.

The evaluation discussion focused on the challenges of designing and implementing meaningful experiments, field studies, and observation programs that target aerosol feedback processes and parameters. There was consensus that the community must strive to test and intercompare modeling techniques for representation of direct and indirect aerosol effects, both to understand their importance across spatial and temporal scales and to assess their accuracy. Closure studies, testbeds [e.g., the aerosol testbed described by Fast et al. (2011)], and the use of emerging in situ and remote measurements of cloud–aerosol interactions (aerosol and cloud droplet size distributions) were identified as possible means to further explore in this regard. Additionally, experiments that include single particle measurements of aerosols to discern mixing state and optical properties are needed to understand and develop effective models of aerosol direct effects. Since aerosol size distributions are important for both direct and indirect effects, the evaluation of modal versus sectional representations along with numbers of modes and sections should also be performed. Improved modeling techniques for nucleation and scavenging were also identified as high priorities. Observational datasets that can help characterize the mixing state of airborne aerosols in different environments and those that can be used to assess the representativeness of internal, external, and core–shell models as well as the evolution of mixing state changes with particle aging are needed to design, evaluate, and further evolve model paradigms.

The final part of the discussion focused on the policy relevance of integrated met–chem modeling for air quality, NWP, and climate applications. The climate modeling community already considers feedbacks from gases and aerosols on radiative forcing and CCN effects on clouds and precipitation to be essential processes to include in climate modeling systems. The effects of these processes on the shorter time scales relevant to air quality applications are, however, subtle. Modeling studies have shown significant aerosol feedback effects on simulated ambient concentrations in areas of high aerosol loading, such as during outbreaks of wildfires or in severely polluted areas (e.g., Asian urban regions). Since air quality regulations mainly focus on extreme values of pollutant concentrations (e.g., fourth highest ozone concentration, 99th percentile for particulate matter), the practice of using constant meteorology to drive offline air quality models to evaluate emission control scenarios could be especially prone to error from the neglect of aerosol–cloud–radiation interactions and needs to be assessed. Coupled systems are important for modeling at urban scales where frequent data exchange between meteorological and chemical components are needed. In addition, higher aerosol concentrations in urban areas can affect urban heat islands and perturb precipitation patterns. Aerosol effects on precipitation are especially challenging to model across various scales. While uncertainties are large, modeling studies suggest that the effects of aerosol concentrations and composition on cloud and precipitation processes could be very significant. If future studies support these findings, accurate modeling of clouds and precipitation might be the most compelling reason for implementing integrated meteorology and chemistry modeling for NWP and air quality in addition to climate applications.

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