Integrated Meteorology and Chemistry Modeling: Evaluation and Research Needs

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Workshop on Integrated Meteorology and Chemistry Modeling

What: Forty scientists from government laboratories, academia, and the private sector from the USA, Canada, and Europe participated in discussion of issues related to integrated meteorology and chemistry modeling from the perspectives of different applications such as numerical weather prediction, air quality modeling, and climate modeling.

When: October 18, 2012

Where: Chapel Hill, NC

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:

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 gasses
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 PBL processes, and further on air chemistry and chemical composition
4. Realistic assessment of the efficacy of various emission control policies in improving ambient air quality under real-world conditions.

The benefits of on-line integrated models over sequential meteorology and chemical transport (off-line) 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 analyzing initial experiences in integrated meteorology-chemistry (met-chem) modeling was organized in Copenhagen 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 advantages of on-line vs. off-line 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 inter-comparisons and validation.

With the objectives of understanding the current state-of-the-science, identifying the gaps in model process representation and capabilities, and setting priorities for model development and evaluation research, a workshop on Integrated Meteorology and Chemistry Modeling was convened on October 18, 2012 in Chapel Hill, NC by the US Environmental Protection Agency (USEPA) with support from the US Department of Energy (USDOE) and the European Framework for Online Integrated Air Quality and Meteorology Modelling (COST ES1004 EuMetChem). The goal of this workshop was to bring together key scientists from North America and Europe that 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, 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.

Forty scientists from government laboratories, academia, and the private sector from the USA, Canada, and Europe 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 in air quality, climate, and forecasting.

The first invited speaker, Jerome Fast of Pacific Northwest National Laboratories provided perspectives on the use of Integrating met-chem modeling for Air Quality applications and assessments. Dr. Fast stressed the need for consistent modeling techniques for meteorology and chemistry in coupled systems as well as process evaluation by employing modeling test-beds that facilitate comparisons to field campaign data (e.g. Fast et al 2011). The advantages for online coupled models for air quality applications include (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 allows the simulation of chemical effects on meteorology such as aerosol scattering and absorption of radiation, aerosol effects on cloud microphysics through CCN activation, and dynamic treatment of radiatively active gasses such as O_3, N_2O, and CH_4 that are important for long wave radiative transfer calculations;
- More realistic modeling of meteorologically-dependent emissions, such as wind-blown dust, biogenic emissions, and sea-salt.

The main disadvantage of on-line 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.

Dr. 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 representation of aerosol-cloud interaction. Evaluation of coupled systems requires additional observational data to validate feedback processes that focus on 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 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 Center 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 incorporation of these effects in 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 4-D variational assimilation (4DVAR) using AOD and trace gas observations. Dr. 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". Dr. Jacobson has developed comprehensive atmospheric modeling systems including integrated meteorology and chemistry processes on spatial scales ranging from global to urban. The GATOR-GCMM (gas, aerosol, transport, radiation, general circulation, and mesoscale meteorology) model developed by his group includes one of the most detailed treatments of explicit cloud and aerosol microphysics and radiation interactions amongst current modeling system. While the impacts of black carbon (BC) on absorption of clear sky radiation and on cloud droplet number and size are well-acknowledged, its effect on cloud properties vary 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 mid-level clouds by 2.8 times that of BC in clear sky and 2.4 times that of interstitial BC (Jacobson, 2012). Absorption by BC inclusions speeds up cloud dissipation, allowing more sunlight to reach 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 aerosol burden (Ten Hoeve et al., 2011). BC enhancements of radiation absorption are closely related to relative humidity and greatest in areas of high humidity and clouds. Dr. Jacobson also spoke about advances in near-explicit gas and aqueous chemistry in 3-D models, subgrid evolution of aircraft exhaust, and implementing the treatment of wind turbines into a 3-D 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, (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 feedback as well as the techniques used to model them depend greatly on spatial and temporal scales and 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 old but persistent issue which 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 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 inter-compare modeling techniques for representation of direct and indirect aerosol effects both to understand their importance across spatial and temporal scales as well as to assess their accuracy. Closure studies, testbeds (e.g. the aerosol testbed described by Fast et al., 2011), 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, 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 data sets 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 and 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 meteorology and chemistry modeling for air quality, NWP, and climate applications. The climate modeling community already considers feedbacks from gasses 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., 4^{th} highest ozone concentration, 99^{th} percentile for PM) the practice of using constant meteorology to drive off-line 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 island 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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References

Baklanov, A., A. Mahura, R. Sokhi (Eds.), 2011: Integrated systems of meso-meteorological and chemical transport models, Springer, 242 p., DOI 10.1007/978-3-642-13980-2

Grell, G., and A. Baklanov, 2011: Integrating modeling for forecasting weather and air quality: A call for fully-coupled approaches, Atmos. Environ., 45, 6845-6851.

Fast, Jerome D., William I. Gustafson, Elaine G. Chapman, Richard C. Easter, Jeremy P. Rishel, Rahul A. Zaveri, Georg A. Grell, Mary C. Barth, 2011: The Aerosol Modeling Testbed: A Community Tool to Objectively Evaluate Aerosol Process Modules. Bull. Amer. Meteor. Soc., 92, 343–360. doi:http://dx.doi.org/10.1175/2010BAMS2868.1

Jacobson, M. Z. (2012), Investigating cloud absorption effects: Global absorption properties of black carbon, tar balls, and soil dust in clouds and aerosols, J. Geophys. Res., 117, D06205, doi:10.1029/2011JD017218.

Ten Hoeve, J. E., L. A. Remer, and M. Z. Jacobson, 2011: Microphysical and radiative effects of aerosols on warm clouds during the Amazon biomass burning season as observed by MODIS: impacts of water vapor and land cover. Atmos. Chem. Phys., 11, 3021-3026.

Zhang, Y., 2008: Online coupled meteorology and chemistry models: history, current status, and outlook, Atmos. Chem. Phys., 8, 2895-2932.