Meteorological Processes Affecting Air Quality – Research and Model Development Needs

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BACKGROUND

Meteorology modeling is an important component for air quality modeling systems that defines the physical and dynamical environment for atmospheric chemistry. The meteorology models used for air quality applications are based on numerical weather prediction (NWP) models that were developed over the past several decades primarily for forecasting the weather. While many of the same characteristics and processes are important for both weather forecasting and for air quality modeling, there are particular meteorological conditions, such as stagnant high pressure systems and convergence zones associated with occluded fronts, that are especially conducive to air pollution episodes but are of lesser interest to weather forecasters¹. Furthermore, there is general recognition that many of the greatest uncertainties in air quality modeling systems stem from uncertainties in the dynamical and thermodynamic processes simulated by meteorological models².

There are many meteorological processes affecting air quality. Radiation and cloud cover have direct effects on photolysis rates for photochemistry and are the primary input to the surface energy budget. Surface heating drives the sensible and latent heat fluxes that influence nearsurface air temperature and humidity and drive the diurnal evolution of the planetary boundary layer (PBL) which controls the mixing depth for air pollutant dispersion. The three dimensional wind fields are responsible for advection of trace gases and aerosols. Even small errors in wind speed and direction can results in large displacements of urban and industrial pollutant plumes. In addition to their interactions with radiation, clouds also contribute to aqueous chemistry processes, wet scavenging and deposition, and aerosol processing. Meteorology also controls surface fluxes of important chemicals, both upward from the surface as emissions of biogenic volatile organic compounds from vegetation and windblown dust and pollen and to the surface as dry deposition. Some chemicals, such as ammonia and mercury, are now being modeled as bi-directional fluxes where they emit or deposit according to the concentration gradient across the air-surface interface. All of these surface processes are strongly influenced by near-surface atmospheric turbulence which is controlled by static stability, wind shear, and surface roughness³. Vegetation also has important influences on surface exchange processes both by

direct uptake and/or emissions of pollutants and by contributing to evaporative moisture fluxes through transpiration.

Meteorological Processes Affecting Air Quality: What are the Gaps?

Inaccurate model representation of any of the processes mentioned above can lead to errors in air quality modeling results. Thus, it is worthwhile to identify some of the most serious gaps in the ability of meteorological models to adequately represent these processes. Because clouds directly affect so many chemical and physical processes, errors in cloud extent and characteristics propagate to errors in chemical concentrations and depositions. Model analysis studies using synoptic typing have constantly shown much poorer performance for types characterized by cloudiness⁴. Also, a common problem for air quality modelers, particularly forecasters, is whether or not afternoon shallow convection occurs, which can significantly reduce peak afternoon concentrations of ozone and other oxidants but increase heterogeneous cloud oxidation of important aerosol precursors. Observations of the radiative, oxidative, and turbulent mixing characteristics of shallow cumulus, and their proper treatment within regional transport models, are therefore key gaps in air quality modeling.

Surface level concentrations are very sensitive to the timing of morning and evening transitions in surface fluxes and PBL mixing which coincide with high emissions during morning and evening rush hours. Hence, accurate modeling of these transitions, which is closely related to land surface processes, is essential for accurate diurnal concentration simulations. Since the highest emission rates are in more developed areas, surface parameterizations that account for the characteristics of urban and suburban developments can improve surface fluxes, near surface stability, and PBL mixing during these critical transition periods. Considerations such as the heat capacity of built and impervious surfaces, reduced effective albedo due to radiation trapping in street canyons, and high roughness lengths of building canopies can be important for modeling pollutant dispersion at high to medium grid resolutions (1-12 km). While urban schemes have been added to meteorology models such as the Weather Research and Forecasting (WRF) model⁵, they are limited to the grid cells that are predominantly urban land use and are therefore applied mainly to high-resolution urban modeling studies⁶. Thus, the effects of development should be routinely incorporated in meteorology and air quality models applied at regional, mesoscale and local scales.

Other gaps include: stable boundary layer (SBL) and nocturnal low level jets which control long range transport⁷; Accurate vegetation distribution, type, and phenology, which are needed for surface fluxes of heat, moisture, and chemistry in all seasons; and chemical fog and cloud deposition in complex terrain (occult deposition). Also, models have difficulty representing

flow separation and isolation of stable cold pools, which trap pollutants for extended periods leading to high concentrations. Such cold pool pollution events are common in the western US predominantly in the winter⁸.

RECOMMENDATIONS

The gaps identified and the recommendations for further research and development outlined in this paper were distilled from the discussions at the workshop on Future Air Quality Model Development Needs and the two invited presentations on Meteorological Processes Affecting Air Quality. While these recommendations are not exhaustive, they are the product of focused discussions by a group of air quality and meteorology modelers with considerable experience and knowledge.

- I. Improve data assimilation, including new data sources for wind, temperature, water vapor, clouds, and chemistry: Meteorological modeling for air pollution applications has long relied on four-dimensional data assimilation (FDDA) for retrospective simulations for research and regulatory planning and assessment. A variety of techniques, such as grid analysis nudging, spectral nudging, and observation nudging are available in meteorological modeling systems like the Weather Research and Forecasting (WRF) model. A well designed FDDA strategy incorporating a variety of measurement data and using techniques most appropriate for the scale and objectives of the modeling study can maintain the accuracy of the simulation over unlimited durations⁹. However, recent studies have shown that grid analysis nudging in the lowest model layers, even when limited to only wind nudging, results in greater errors throughout the PBL than restricting FDDA to layers above the PBL 10. A critical need is to augment the twice-daily radiosonde observations with spatially denser and more frequent vertical profile data from radar wind profilers, VAD (Velocity Azimuth Display) profiles from the NWS Doppler radar network, and commercial aircraft measurements (ACARS). Additional observations of clouds, moisture, and surface temperature can be derived from satellite retrievals and used for FDDA. Assimilation of chemical data from satellites, aircraft, and surface networks also needs to be developed.
- II. Improve model physics for PBL, shallow convective clouds, land surface models (LSM)/surface fluxes, deep convection, and precipitation: Since certain aspects of physical processes in meteorological models are more important for air quality applications than for weather forecasting, the needed improvements are likely to come from the air quality modeling community. For example, while PBL processes are important to weather forecast modeling (WFM), the diurnal evolution of turbulent mixing and PBL depth are much more important for chemical transport modeling (CTM). In particular, the rate of morning PBL growth controls entrainment from aloft and influences the photochemical regime. Similarly,

shallow convective clouds are more important for CTM than WFM because they influence photolysis, PBL venting, and aqueous chemistry. Land surface modeling in meteorology and air quality models should be harmonized and further developed to represent heat fluxes (latent and sensible heat fluxes) and chemical fluxes (dry deposition, bi-directional exchange, and biogenic emissions) with maximum consistency using common datasets (e.g., land-use and vegetation indexes) and common parameterizations.

- III. Improve modeling of removal processes: Wet and dry removal processes are the predominant atmospheric loss terms for aerosols, and important gas-phase species that are soluble, highly oxidized, or otherwise assimilated at the earth's surface. Within mass budget estimates and as a source to many ecosystem model applications, reducing uncertainties in the absolute magnitude and physical representation of wet and dry removal processes is often a critical need. Ammonia is a prime example where the bi-directionality of surface fluxes requires adequate estimation of the deposition terms¹¹. Although a mature physical understanding exists for the processes determining the dry deposition of Particulate Matter (PM) and its constituents, routine regional or continental scale observations do not currently exist, and the set of available observations is limited by the land-use categories sampled and by large variability within the reported measurements¹². By contrast, a reasonable North American surface network exists for wet deposition analysis of a few important PM anions and cations, but current model formulations are unable to account for important laboratory and field observations such as the PM size-dependence of rainwater scavenging coefficients. Physical parameterizations of gas-phase and PM constituent scavenging by snow and rain, and the transformations occurring during hydrometeor evaporation/sublimation are essentially unconstrained due to the lack of observations and measurements. Support for observations, laboratory measurements, and the development of physical parameterizations related to wet and dry deposition are certainly needed, but typically overlooked within the air quality model community.
- IV. Develop better coupled or integrated Meteorological and Chemistry models: Coupled (or inline) meteorological and chemistry models have been available for over a decade and are valuable research tools used to study interactions between the chemistry-aerosol-cloud-radiation-climate systems. The indirect feedback effects of aerosol on cloud properties and precipitation are estimated to be one of the largest unknowns related to anthropogenic climate forcing, and the meteorological impact of extreme aerosol events (e.g., dust outbreaks and forest fires) has been shown to be significant in recent on-line model applications¹³. Thus, continued research into the coupling between aerosols and radiation, aerosol and clouds, and clouds and radiation, deserves resources and support. This should also include the application of advanced computational architectures, modeling frameworks,

and numerical infrastructure in support of these computationally demanding calculations. Aside from aerosol feedback studies, air quality applications are increasingly requiring high spatial and temporal resolution, and often the only means of incorporating the effects of model-resolved turbulence is via tight temporal coupling between transport variables from the meteorology with the aerosol and chemistry constituents. Again, support for large, coupled models with documented numerical integrity that are available to both regulatory and research communities is essential for near- and long-term advancements in air quality modeling.

V. New Direction: Adapt AQ modeling to more flexible grid structures and coordinates: As domestic emissions are reduced and global emissions continue to increase, particularly in Asia, the chemical lateral boundary conditions (LBC) used for limited-area modeling are becoming increasingly important fractions of modeled concentrations and deposition¹⁴. Currently, most modeling studies extract LBCs from global model simulations, which in principle is a distinct advancement over the previous practice of using constant LBCs. However, in practice, inconsistencies in chemical mechanisms and speciation and large discontinuities in grid resolution contribute to significant errors. A promising new direction is the development of global icosahedral chemistry/meteorology models with grid refinement. Such models can represent the spatial continuum from global to local scales with chemical and dynamical consistency and seamless resolution refinement. One challenge of such multiscale modeling, however, is the need to develop "scale-aware" physics, particularly for convective cloud parameterizations.

Conclusions

The recommendations resulting form this workshop have primarily focused on the application of air quality modeling systems, which include meteorology models, for retrospective analysis and decision support for air quality regulators. Modeling systems developed for air quality forecasting have many of the same issues and gaps but also present their own unique challenges. For example, reliance on data assimilation for reducing model error is limited to the initialization stage of forecast model runs. Thus, realistic physics and accurate input data are even more critical for air quality forecast systems¹⁵.

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