

# Meteorological Research Needs for Improved Air Quality Forecasting

Report of the 11th Prospectus Development Team of the U.S. Weather Research Program\*

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While forecasting usually focuses on severe and adverse weather, poor air quality frequently is associated with benign weather and weak synoptic forcing

Since 1994, the U.S. Weather Research Program has held a series of eleven Prospectus Development Team (PDT) meetings to define research issues and opportunities related to improving atmospheric prediction. Our team—PDT-11—was given the charge of identifying critical meteorological issues related to the prediction of air quality (AQ). The march of weather and the corresponding short-term

changes in meteorology are the largest factors in controlling changes in the chemical state of the atmosphere. In the context of our team's charge, "air quality" refers to the chemical state of the atmosphere including constituents that pose a risk to health, those which may alter visibility, and any other aspects of the chemical state of the atmosphere that have a high impact on human activities or the environment. "Pre-

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diction” is taken in a broad context and subsequently referred to as “forecasting.” It includes the depiction and communication of the present chemical state of the atmosphere in the urban zone and on the regional (meso- $\beta$ ) scale, very short-term forecasting or “now-casting,” and numerical prediction and chemical evolution on time scales up to several days. “High impact” refers to conditions that affect or alter behavior by general public, government agency, and private sector activities, including health and the environment, aviation, surface transportation, electric power, public events, broadcasting, and emergency management. We did not, however, seek to identify the important research challenges in atmospheric chemistry. There is also a strong but not exclusive emphasis on the urban zone, recognizing that many of the unmet meteorological research needs apply equally well to regional and rural air quality forecasting.

**BACKGROUND.** Compared to weather forecasting, air quality forecasting is a young science, dating back only to the early 1960s. Air quality forecasts are generally classified into two subgroups: health-alert and emergency-response predictions. Health-alert forecasting focuses on the U.S. Environmental Protection Agency’s (EPA) criteria pollutants, such as ozone, particulate matter, nitrogen dioxide, carbon monoxide, sulfur dioxide, and lead. Emergency-response forecasting focuses on situations where chemical, biological, or nuclear materials are unexpectedly emitted into the atmosphere and where the source is unknown or poorly described.

Forecasting atmospheric conditions is critical for understanding the formation, transformation, diffusion, transport, and removal of these pollutants. Improving atmospheric forecasts to provide improved air quality forecasts suitable for decision makers and the public is a major challenge.

*A brief history of air quality forecasting.* Significant data collection and analysis efforts in the 1950s and 1960s led to a better understanding of air pollution episodes and the atmosphere’s controlling effect on air pollution (Heidorn 1978; Holzworth 1962). During this period, the National Weather Service (NWS; then called the Weather Bureau) issued regional advisories of air pollution potential over the eastern United States (Niemeyer 1960; Boettger 1961), and municipal air quality agencies began to predict pollution on the local urban scale (e.g., Thuillier and Sandberg 1971). The EPA, created in 1970, established a set of uniform National Ambient Air Quality Standards (NAAQS). As part of the Clean Air Act Amendments of 1970 and

1977, the EPA focused on setting air quality standards and controlling pollution at its sources.

During the 1970s and 1980s, air quality agencies forecasted pollution using objective statistical methods that required forecasts of atmospheric conditions as input (Aron and Aron 1978; Aron 1980; McCutchan and Schroeder 1973; Zeldin and Thomas 1975). In the 1980s, State Implementation Plans (SIP) became a regulatory method to control air pollution at its sources by demonstrating how states would reduce emissions to meet the NAAQS. Numerical Eulerian grid models were used to develop SIPs by simulating historical air pollution episodes and demonstrating the effect of future-year emissions reductions. These models employed diagnostic wind-field models to interpolate available meteorological observations to a three-dimensional grid (Collett and Oduyemi 1997). By the 1980s it became possible to replace the diagnostic wind models used with prognostic models (Chang et al. 1987). As prognostic real-time mesoscale meteorological models have matured, the air quality community has begun coupling such models with air quality models, either by keeping separate (“offline”) software for chemistry and meteorology (Vaughan et al. 2002; Hogrefe et al. 2001; Jakobs et al. 2001; McHenry et al. 2001), or using an integrated (“online”) approach (Grell et al. 2000)

In the early and mid-1990s, voluntary emission-reduction programs brought about a new use for air quality forecasts—encouraging the public to reduce emission-producing activities on predicted high ozone days, thus, seeking to avoid exceeding the NAAQS. Also in the 1990s, EPA started the AIRNow program ([www.epa.gov/airnow](http://www.epa.gov/airnow)) to collect and disseminate real-time ozone and 2.5- $\mu\text{m}$ -particulate data, as well as city-specific air quality forecasts. By 2002, the AIRNow program included data from over 85 air quality agencies throughout the United States, as well as ozone forecasts for over 250 cities, which are distributed via the Internet and to commercial weather service providers for their television and newspaper customers. Health-alert forecasts are formulated using a very wide range of techniques, from simple empirical methods first used in the 1960s to advanced statistical models and complex photochemical grid models. The EPA also provides education guidance documents on forecasting air quality (EPA 1999a).

The scientific and technological advances that helped health-alert forecasting also aided emergency-response predictions. As computer technology evolved, emergency managers progressed from using tables and graphs to using Lagrangian puff and par-

title models, which incorporate multiple observations and three-dimensional time-varying meteorological fields.

Some of the earliest work in emergency-response prediction started in the 1950s in the U.S. Department of Energy's predecessor agency, the Atomic Energy Commission (AEC), in connection with above-ground nuclear testing. In 1972, the AEC recognized the need for real-time estimates of transport and diffusion (Knox et al. 1981). To meet this need, the Lawrence Livermore National Laboratory developed the Atmosphere Release Advisory Capability (ARAC), an advanced, three-dimensional modeling system of pollutant dispersion, and improved communications for disseminating predictions to local officials (Dickerson and Orphan 1976; Sherman 1978; Lange 1978). ARAC has since responded to a number of accidents, including radiological releases at the Three Mile Island nuclear power station in Pennsylvania (Dickerson et al. 1979), and at Chernobyl, Ukraine (1986), and the 1984 Bhopal, India, methyl isocyanide release.

A number of chemical, biological, nuclear, and radiological emergency-response modeling capabilities were in place before the terrorist events of 11 September 2001 (hereafter 9/11). For example, the Computer-Aided Management of Emergency Operations (CAMEO)–Areal Locations of Hazardous Atmospheres (ALOHA) gas and chemical modeling system was developed in 1992 by the National Oceanic and Atmospheric Administration (NOAA) to assist local fire departments in assessing the impacts of accidental releases of hazardous chemicals. The Hazard Prediction and Assessment Capability (HPAC) modeling system was developed by the Defense Threat Reduction Agency (DTRA 1999) to calculate the effects of releases of biological, chemical, and nuclear agents. HPAC uses a Second-Order Closure Integrated Puff (SCIPUFF; Sykes et al. 1998), a Lagrangian puff model, to simulate transport and diffusion.

Since the 9/11 attacks, the emphasis on developing urban- and building-scale dispersion modeling capabilities has increased. Observational and computational fluid dynamics (CFD) modeling studies have been aimed at predicting flows within street canyons at time scales of minutes and at distances up to a few kilometers. Improvements have also been made in predictions at the scale of 10–100 km. However, much work still needs to be done on predictions between these two distance ranges—from the urban (10 km) to the building (10 m) scale. Many of the challenges in forecasting at the urban scale were addressed by PDT-10 (Dabberdt et al. 2000).

*Air chemistry models.* Air chemistry models describe the fate and transport of atmospheric chemical constituents in both the gas and aerosol phases. They now track about 100 chemical species, interacting through mechanisms involving hundreds of chemical reactions. Because of the important role that aerosols play in radiative transfer, weather, and health impacts, most air quality models now include more detailed descriptions of aerosol dynamics and calculate size-resolved aerosol composition, radiances, and photolysis rates interactively with the cloud and aerosol fields. With today's computational power and efficiencies, air chemistry models can simulate pollution distributions in urban air sheds with spatial resolution of a few kilometers, or they can cover the globe with horizontal grid spacing of less than 100 km. These models are able to provide quantitative information on the distributions of many of the atmosphere's key trace gases and aerosols. Air chemistry models have become an essential element in atmospheric chemistry studies, and they also provide science-based input for decision makers locally, nationally, and globally.

Although meteorological and chemical processes are strongly coupled, until recently the chemical processes in air quality modeling systems were usually treated offline of the meteorological model [as in the Community Multiscale Air Quality (CMAQ) model; Byun and Ching 1999], whose output provided the transport function. This type of system is usually termed a Chemical Transport Model (CTM). In the newer online approach there is no CTM; the chemical processes are part of the meteorological model. This has a number of potential advantages for air quality forecasting, such as better characterization of the time-resolved dispersion of air pollutants.

The Weather Research and Forecast (WRF) model is well suited to become the cornerstone for a next-generation air quality prediction system. This model, currently under development ([www.mmm.ucar.edu/wrf/users/document.html](http://www.mmm.ucar.edu/wrf/users/document.html)), is nonhydrostatic, with several dynamic cores, as well as many choices for physical parameterizations to represent processes that cannot be resolved by the model. This allows the model to be applicable on many different scales. A first version of an online WRF-based air quality prediction system (WRFAQ) for ozone prediction already exists ([www.wrf-model.org/WG11](http://www.wrf-model.org/WG11)); the chemical modules are based on the online coupled Pennsylvania State University (PSU)–National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5)–chemistry (Chem) model (Grell et al. 2000). The official future release of this model (planned for 2005) will include many additional

**TABLE 1. User needs for air quality forecasts.**

Sector	Group or organization	Forecast products						Forecast period		
		Regional daily maximum	Local or city predictions	Air quality index (AQI)	Forecast uncertainty	Visibility predictions	Human exposure	Short range (0-48 h)	Mid-range (48-168 h)	Seasonal predictions
Public	Sensitive groups	✓	✓	✓			✓	✓		
	General public	✓	✓	✓			✓	✓		
	Outdoor workers/recreation	✓	✓	✓			✓	✓		
Decision makers	Air quality agencies									
	- Episodic or special sampling		✓		✓	✓		✓		
	- Emission-reduction programs	✓	✓	✓				✓		
	- Health/air awareness	✓	✓	✓			✓	✓		
	Emergency response	✓	✓		✓		✓	✓		
	Industry (e.g., power)	✓	✓		✓		✓	✓	✓	
	Aviation	✓			✓	✓		✓		
	Transportation		✓			✓		✓		
	Health care	✓	✓	✓			✓	✓		
	Environment	✓	✓	✓	✓	✓	✓	✓	✓	
Forecast and park service	✓	✓		✓	✓		✓	✓		
Media	Television weathercasters	✓	✓	✓		✓	✓	✓		
	Internet content providers	✓	✓	✓		✓	✓	✓		
	Newspapers	✓	✓	✓		✓	✓	✓		
Researchers	Air quality scientist	✓	✓	✓		✓	✓	✓	✓	
	Air quality regulators	✓	✓	✓	✓	✓	✓	✓	✓	
	Field measurement studies	✓			✓	✓	✓	✓	✓	

chemical modules from other air quality prediction systems and a choice of offline coupling.

**Users and societal benefits.** There are three main classes of users of air quality information and forecasts: the public, decision makers, and researchers. Table 1 provides a matrix of the different types of users and their needs for air quality forecasts. The public, via the broadcast media, is the largest user group. This group requires air quality forecasts that are clear, easily understood, and consistent. The EPA has developed several standardized methods to easily communicate pollution information to the public. The Air Quality Index (AQI), formally the Pollutant Standards Index (PSI), provides a standardized scale from 0 to 500 for all criteria pollutants (EPA 1999b), as shown in Table 2.

**THE NEED FOR IMPROVED PHYSICAL UNDERSTANDING.** *Planetary boundary layer.* **CHARACTERISTICS.** Much of our deliberations focused on the structure of the planetary boundary layer and associated measurement and modeling limitations and challenges. The planetary boundary layer (PBL) is the lowest layer of the troposphere. Its lower boundary is in contact with the earth's surface, and it is usually capped aloft by a statically stable layer of varying intensity. The PBL depth (i.e., the height of the base of the capping inversion) varies in time and space, but typically ranges up to several kilometers in clear-sky daytime conditions over land. The PBL is not always well defined, as in the presence of frontal boundaries, deep convection, or multiple low-level inversions.

The so-called mixed layer is an important feature of the PBL. It is a turbulent layer that results from strong winds, wind shear, or free convection. Buoyantly generated mixed layers, caused by heating at the earth's surface or radiative cooling at the tops of cloud or fog layers, are usually statically unstable. Mixed layers may be in contact with the earth's surface, and their vertical extent then defines the atmospheric mixing depth. But at other times, particularly at night, mixed layers can occur aloft. The classic surface-based mixed layer (see Fig. 1) evolves in several phases over the course of a typical fair-weather day over land.

The dynamic nature of the PBL (Stull 1988) influences the concentration and residence time of pollutants in the atmosphere and, hence, air quality. Our ability to accurately predict air quality is limited by a lack of knowledge of the physical influences on PBL structure (including the way it changes over different types of land cover and throughout the day and

## BENEFITS OF IMPROVING AIR QUALITY FORECASTS

**PUBLIC HEALTH.** Accurate time- and location-specific health alerts can help the public reduce acute exposure when high pollution levels are expected. Routine daily forecasts enable the public to make healthier choices (e.g., exercising only on low-pollution days).

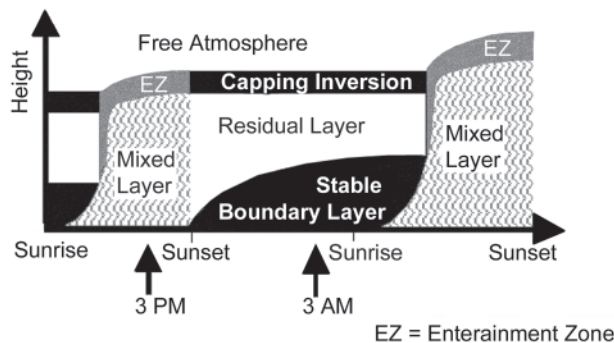
**PLANNING.** Air quality forecasts allow organizations to plan business or activities more effectively. For example, the U.S. Forest Service needs these forecasts to ensure that its planned tenfold increase in prescribed burning will not cause violations of the NAAQS. Forecasts can be used by the government and industry to reduce emissions on predicted high-pollution days, thus, avoiding the high cost of continuous emission controls.

**EMERGENCY RESPONSE AND RISK MANAGEMENT.** Effective emergency-response forecasting helps organizations better understand and manage the consequences of accidental or intentional releases of hazardous material into the atmosphere. With that information, they can reduce exposure, both by effective responses (e.g., sheltering in place, evacuating) and by planning remedial actions.

**FORENSICS.** When hazardous materials are released into the atmosphere, the type and quantity of substance released are usually not known. This requires not only measurements, but also accurate dispersion modeling of plume concentrations and ground deposition.

**WILDFIRES AND SMOKE.** Improved prediction of weather and air quality can assist air quality agencies in planning controlled burns, as well as aiding firefighters in setting up command posts, managing or fighting fires, and protecting themselves from exposure to smoke. Additionally, the public benefits from evacuation guidance and protective measures.

year), which itself is partly the result of the current sparsity of routine observations. It is essential that a high-resolution, nationwide observing network be established to monitor the diurnal variation of the height and structure of the PBL and the mixed layer. Further, enhancing our capability to numerically model boundary layer structure will require comprehensive observational studies—both intensive short-term programs and extended long-term monitoring. These observations need to be linked to corresponding observations of air quality and chemistry.



**FIG. 1. Schematic of mixed-layer evolution (Stull 2000).**

**IMPORTANCE IN AIR QUALITY MODELING.** The mixed-layer depth,  $z_p$ , of the PBL is particularly important for air quality forecasts because it imposes a limit to vertical dispersion and is a fundamental scaling length for characterizing the neutral and convective boundary layer. The strength of the capping inversion at  $z_p$ , the presence of clouds, and the rate of growth (or destruction) of the inversion strongly determine the vertical transport or dispersion of pollutants both into and out of the PBL. The magnitudes of these transports are not well known but are important for many problems such as regional photochemical and particulate matter (PM) models.

The collapse of  $z_i$  in the late afternoon is not satisfactorily understood, although preliminary studies (Ching et al. 1981; Hanna and Chang 1992) indicate that the turbulence first dies away at the top of the PBL. The problem is compounded because in most

areas,  $z_i$  is not easily estimated for a significant fraction of the time when there is no well-defined capping inversion. Instead there may be multiple weak inversions. This situation needs to be better resolved in air quality models.

At night  $z_i$  can be very small (a few meters with nearly calm winds and clear skies), yet many air quality modeling systems arbitrarily impose a minimum  $z_i$  of 100 or 200 m to avoid problems with constrained vertical mixing. Also, observing systems, such as some radar wind profilers, report  $z_i$  as the lowest-range measurement (60–100 m for UHF profilers). The challenge is to measure both the lowest portions of the nocturnal PBL and the upper reaches of the capping stable layer with sufficient height resolution and temporal continuity. These demanding sampling requirements can be resolved with multisensor systems that use both UHF profilers to address the long-range challenge of measuring the top of the PBL and optical or acoustic profilers to sample the very lowest nocturnal layers. Also, emerging multifrequency UHF profiler technology (Palmer et al. 1999) offers significant promise to provide height resolution that is an order of magnitude better than current single-frequency systems.

In urban areas, studies show that  $z_i$  is enhanced by about 20% during the day due to thermal inputs. Similarly, urban  $z_i$  values may not collapse at night due to thermal inputs and mechanical mixing by building obstacles (e.g., Ludwig and Dabberdt 1973). Research efforts are needed to better estimate  $z_i$  for input to urban air quality models. These should also include

**TABLE 2. AQI values, categories, and pollutant concentration thresholds for the criteria pollutants. Source: EPA (1999b).**

AQI	AQI category	O <sub>3</sub> (ppb) 8 h <sup>a</sup>	O <sub>3</sub> (ppb) 1 h	PM <sub>2.5</sub> (μg m <sup>-3</sup> )	PM <sub>10</sub> (μg m <sup>-3</sup> )	CO (ppm)	SO <sub>2</sub> (ppm)	NO <sub>2</sub> (ppm)
0–50	Good	0–64	—	0.0–15.4	0–54	0.0–4.4	0.000–0.034	( <sup>b</sup> )
51–100	Moderate	65–84	—	15.5–40.4	55–154	4.5–9.4	0.035–0.144	( <sup>b</sup> )
101–150	Unhealthy for sensitive groups	085–104	125–164	40.5–65.4	155–254	9.5–12.4	0.145–0.224	( <sup>b</sup> )
151–200	Unhealthy	105–124	165–204	65.5–150.4	255–354	12.5–15.4	0.225–0.304	( <sup>b</sup> )
201–300	Very unhealthy	125–374	205–404	150.5–250.4	355–424	15.5–30.4	0.305–0.604	0.65–1.24
301–400	Hazardous	( <sup>c</sup> )	405–504	250.5–350.4	425–504	30.5–40.4	0.605–0.804	1.25–1.64
401–500	Hazardous	( <sup>c</sup> )	505–604	350.5–500.4	505–604	40.5–50.4	0.805–1.004	1.65–2.04

<sup>a</sup> Areas are generally required to report the AQI based on 8-h ozone values. However, there are a small number of areas where an AQI based on 1-h ozone values would be more precautionary. In these cases, in addition to calculating the 8-h ozone index value, the 1-h ozone index value may be calculated and the maximum of the two values is reported.

<sup>b</sup> NO<sub>2</sub> has no short-term NAAQS and can generate an AQI only above a value of 200.

<sup>c</sup> When 8-h O<sub>3</sub> concentrations exceed 374 ppb, AQI values of 301 or higher must be calculated with 1-h O<sub>3</sub> concentrations.

estimates of  $z_i$  uncertainties, which are presently estimated to be about  $\pm 30\%$  during the day and  $\pm 100\%$  at night, and account for the not-infrequent situation where there is no  $z_i$  but just a gradual approach to the free troposphere.

Contemporary air quality models use standard boundary layer theories to estimate wind, temperature, and turbulence profiles in stable conditions. There are several problems with this approach that are not well recognized by many users:

- 1) The standard PBL theories strictly apply to what can be classified as weakly stable boundary layers. As winds drop and skies clear, many areas experience moderate to strongly stable conditions. In these cases, the standard theories may apply only to the lowest 5 m or so.
- 2) Standard models do not include an important deep layer of the atmosphere, in which pollution plumes are often found, above the shallow (5–50 m) stable boundary layer. At night, the region from about 50 to 1000 m can have several alternating layers of strong and weak (or even neutral) stability. Elevated plumes (e.g., power-plant plumes) may mix vertically through a weakly stable layer, but they may or may not be able to mix through adjacent strongly stable layers. Current EPA regulatory models [e.g., Industrial Source Complex (ISC) 3; see EPA 1995] simulate these layers as a single deep layer with constant temperature gradient. The newly proposed AERMOD model (developed by the AMS/EPA Regulatory Model Improvement Committee; Cimorelli et al. 1998; Paine et al. 1998) will account for layers if they are observed. Mesoscale models currently do not have adequate vertical resolution to adequately resolve shallow elevated stable layers.
- 3) During the night, and at heights above  $z_i$  during the day, there can be several shallow inversion layers with mixing layers interspersed. These can play a large role in vertical transport, yet are nearly impossible to forecast.
- 4) Stable boundary layers (SBLs) are known to be intermittent, with periods of low turbulence interrupted by turbulent bursts. Richardson number theory should be applied to help explain these bursts.
- 5) As the rural SBL approaches the city, it is eroded by urban-induced thermal inputs and mechanical mixing.

The above-boundary layer issues are being partially addressed by meteorological programs such as

the 1999 Cooperative Atmosphere–Surface Exchange Study (CASES-99; Poulos et al. 2002) and the Vertical Transport and Mixing Experiment (VTMX; Doran et al. 2002). The results of these studies need to be transferred to air quality models. However, there is still a strong need to observe and parameterize winds and turbulence above the surface-based SBL. Remote sensing devices are needed to measure vertical profiles of winds, turbulence, and temperature in key locations.

**MEASUREMENT CHALLENGES.** The vertical structure and height of the PBL can be determined (directly or remotely) from vertical profiles of temperature, moisture, aerosols, turbulence, and other properties. However, there are difficulties in observing  $z_i$ ; it is often ambiguous, and the various in situ and remote sounders have different sampling limitations. Measuring both the lowest portions of the nocturnal PBL and the upper reaches of the capping stable layer with sufficient height resolution and temporal continuity for AQ forecasting is a significant challenge.

Currently, there is no nationwide network that routinely monitors the diurnal variation of the height and structure of the PBL. The most comprehensive system for PBL measurements is the NWS upper-air rawinsonde observation (RAOB) network, which provides twice-daily in situ soundings of winds, pressure, temperature, and humidity. But the RAOB network is sparse for air quality purposes (in 1999 there were 100 stations in the United States with an average separation of 315 km), and it reports only mandatory and significant levels in near-real time, although high-resolution data are available in archive mode. Boundary layer UHF wind profilers better meet the PBL monitoring requirements, but there are still only about 85 operational systems in North America. Soundings of winds, pressure, and temperature from commercial aircraft (during takeoff and landing) are a valuable source of profile data in and near the urban boundary layer (Moninger et al. 2003), but the resolution is poor.

A number of different approaches exist to determine mixing height. It is important to emphasize that the methods are closely connected to the instruments that are used (Gryning and Batchvarova 2001). Seibert et al. (2000) discuss measurement platforms and their relative merits for determining mixing height. The lack of a single method has led to ambiguities when mixing heights determined from different theoretical models and measuring platforms are compared (Gryning and Batchvarova 2001).

Recently, there have been intensive campaigns to investigate the PBL under specific meteorological

conditions, for example, the summertime ESCOMPTE/CLU campaign in Marseilles, France (Cros et al. 2002), and the urban tracer meteorological field campaign (URBAN 2000) VTMX stable boundary layer study in Salt Lake City, Utah (Allwine et al. 2002; Doran et al. 2002). The extensive data collection by these and other such campaigns will allow a number of issues to be addressed. However, in both of the examples cited here the urban setting is in complex terrain. PBL behavior under a wider variety of meteorological conditions with continuous data collection remains to be addressed.

**LAND SURFACE FEATURES.** The evolution and vertical mixing of the daytime boundary layer is largely forced by surface heating. The portion of surface net radiation that becomes latent heat is determined by soil evaporation, vegetative evapotranspiration, and evaporation from wet surfaces. Mesoscale meteorological models often include land surface models (LSMs) that explicitly include these processes along with prognostic simulation of soil moisture in several layers (e.g., Chen and Dudhia 2001a; Xiu and Pleim 2001). The addition of an LSM greatly enhances the realism of modeled PBL processes (Pleim et al. 2001; Xiu and Pleim 2001; Chen and Dudhia 2001b). Pleim and Byun (2001) showed that including an LSM and an associated dry deposition model also significantly improved air quality model results, such as ozone concentration.

Modeling the soil moisture is one of the main reasons for including an LSM in an AQ modeling system. Without realistic soil moisture fields, especially at root depth, LSMs generally add more error than skill to an air quality forecast. One approach to this problem is to run offline LSMs, often referred to as Land Data Assimilation Systems (LDASs), that continuously assimilate observed precipitation and other observed meteorological fields. Soil moisture fields from an uncoupled LDAS can be used to initialize soil moisture for mesoscale forecasts. Other approaches are to use atmospheric observations, such as surface air temperature and humidity, to “correct” the soil moisture (e.g., Bouttier et al. 1993; Giard and Bazile 2000) or to use satellite observations of skin temperature tendencies (Dabberdt and Davis 1978; McNider et al. 1994; McNider et al. 1998).

Stomatal and canopy conductance is another key area of research and model development. A new generation of improved stomatal models is based directly on calculations of photosynthesis rates (e.g., Berry and Farquhar 1978; Collatz et al. 1991). Models based on plant physiology add new requirements to vegetation databases. The type of photosynthetic biochemical

system, either C3 or C4, is critical information that is not readily available from most current databases, because land-use categories are usually too broad to distinguish species.

Another important LSM ingredient is the description of seasonal variations of vegetation. Some models use climatologies of seasonal leaf-out and leaf-fall by day of the year and latitude. Others estimate leaf-out and leaf-fall according to model parameters, such as deep soil temperature. Crop models that describe growth according to environmental conditions are also used in some models. More direct information of vegetative state can be derived from satellite data [e.g., Normalized Difference Vegetation Index (NDVI)]. Difficulties include cloud interference and uncertainties in relating spectral data to vegetative parameters.

All surface-atmosphere exchange processes involved in a combined meteorology and photochemistry model system should be closely coupled to ensure maximum consistency and interactivity. For example, dry deposition can easily be coupled to an LSM using common stomatal and aerodynamic resistances (Pleim et al. 2001). In this way, not only are the land-use data consistent between meteorology and chemistry components, but the dry deposition computations benefit from explicit soil moisture modeling in the LSM. A third component that should be similarly coupled is the biogenic emissions model. Unfortunately, the vegetation data required for estimation of biogenic emissions are considerably more detailed. Thus, advances in surface-air exchange modeling largely depend on obtaining more sophisticated, high-resolution land-use and vegetation data.

Surface (with subsurface) schemes need to be evaluated in conjunction with PBL estimates. In the urban environment, in particular, the need for air quality forecasts is great, but relatively little attention has been devoted to evaluating surface schemes. Recently a number of schemes have been developed that take into account various aspects of the complexity of the urban surface (e.g., Dabberdt and Davis 1978; Grimmond and Oke 2002; Hanna and Chang 1992, 1993; Best 1998; Guilloteau 2000; Masson 2000; Martilli 2001; Grimmond and Oke 2002). All available urban surface schemes must be evaluated across a wide variety of conditions.

**Urban meteorology.** Urban air quality models, such as the EPA’s (1995) ISC3 model with urban land use, the EPA’s new urban algorithm in AERMOD (see Cimorelli et al. 1998; Paine et al. 1998), the Atmospheric Dispersion Modeling System (ADMS;

Carruthers et al. 1998), or the Urban Dispersion Model (UDM) suggested by Hall et al. (2001), need to account for the reduced wind speeds, enhanced turbulence, and altered stability that are typical of urban areas. The primary need, as in air quality models applied to rural areas, is to prescribe representative values of wind speed, turbulent energy components, and Lagrangian time scales within and just above the urban canopy. This is particularly difficult in urban areas because of the nonhomogeneity of the surface.

Urban air quality modelers consider four regimes of distance scales. The small-scale (< 100 m) regime deals with emissions released in street canyons, where the plume grows until it is constrained laterally by the buildings (e.g., Dabberdt and Hoydysh 1991). This scale may also require modeling of exchanges with the air inside buildings (Spengler et al. 2000). The block-scale or neighborhood-scale (100–1000 m) regime deals with plumes that grow laterally to encompass several buildings and may grow vertically to the top of the buildings. Here it is important to account for the wind and turbulence within the urban canopy, but also to account for the effects of the buildings themselves, for example, the heat from their walls in the daytime (Grimmond et al. 1991; Arnfield and Grimmond 1998; Grimmond and Oke 1999), or the way plume material stalls in their wakes (e.g., Dabberdt et al. 1994). The heating effects on building walls can also be important during the day (Grimmond et al. 1991; Arnfield and Grimmond 1998; Grimmond and Oke 1999). The third regime is the intermediate scale (1–10 km), where the pollutant plumes cover several blocks and most of the plume is above the buildings. In this case the urban area can be treated as an underlying roughness surface and it is important to specify the roughness length, displacement height, and friction velocity, in addition to the sensible heat flux and turbulence using standard boundary layer formulas. The fourth spatial regime is the urban region (10–100 km), encompassing a city's central business district, suburbs, and rural surroundings, where lateral inhomogeneities in land-use types must be considered. The key technical problem for all four regimes is the specification of vertical wind, turbulence, and temperature profiles, both below and above the urban canopy.

**Clouds and cloud processes.** Clouds are critical in understanding and predicting air quality, yet they remain one of the largest sources of uncertainties in air quality modeling. Clouds impact air quality in four areas: 1) the PBL, 2) photochemistry, 3) surface char-

acteristics, and 4) pollutant transport. The magnitude of their impact depends on their depth, breadth, lifetime, and microphysical characteristics. A further complication is that the effects of anthropogenic constituents on the cloud (e.g., aerosols that act as cloud condensation nuclei or alter the thermodynamics of clouds) are nonlinear, and as of yet are not well understood. Numerous modeling studies have shown that cloud processes have potentially large effects on local, regional, and global distributions of sulfate aerosols, ozone, peroxides, and other key photochemical species (e.g., see Chameides and Davis 1982, 1983; Chameides 1984; Jacob 1986; Walcek and Taylor 1986; Hegg et al. 1986; Chaumerliac et al. 1987; Lelieveld and Crutzen 1990, 1991; Liang and Jacob 1997; Matthijsen et al. 1997; Walcek et al. 1997; Barth et al. 2002).

Clouds affect chemical concentrations through a variety of dynamical, radiative, microphysical, and chemical processes. Entrainment and detrainment of air masses, especially venting of the PBL, can lead to vertical and lateral redistribution of chemical constituents with potentially large effects on the direction and magnitude of eventual outflow. Clouds also redistribute solar radiation, causing strong but complex alterations in the photochemical actinic fluxes not only within the cloud, but also above, below, and in the surrounding air. Actinic fluxes within cloud droplets and in the near field of ice crystals may also be of some importance (especially near cloud top) but are very poorly understood.

Cloud microphysical processes are influenced by chemical composition, and in turn they affect the exchanges of pollutants (gases and aerosols) with liquid or ice phases. The multiphase chemistry that follows is complex and not fully understood, but it may be of considerable importance to the transformations and ultimate fate of pollutants upon rain out or reevaporation. Also, production of nitrogen oxides by lightning remains poorly characterized but may also be important to photochemistry, especially in the presence of hydrocarbons (Tuck 1976; Borucki and Chameides 1984; Liaw et al. 1990; Price and Rind 1994; Ridley et al. 1996; Crawford et al. 2000; Tie et al. 2001).

On balance, clouds are thought to usually decrease the level of atmospheric constituents that are considered to have adverse effects on the environment, for example, ozone, nitrogen oxides, hydrocarbons, and particles. Because there has been little research in this area, however, that assumption is speculative. At the same time, cloud processes can have adverse impacts on the environment and human health as, for ex-

ample, in the case of acid rain and wash-out of radionuclides.

As discussed earlier, air quality is highly sensitive to the structure of the PBL. Clouds will significantly alter this structure and increase the difficulty of accurately characterizing and forecasting the state of the boundary layer. The degree to which clouds alter the PBL will depend upon the forcing mechanisms that form the clouds, for example, frontal passage, wave propagation, or convection. These same forcing mechanisms are also important factors in the evolution of the PBL in the absence of clouds. Clouds alter the energy balance of the PBL by changing the vertical profiles of temperature and humidity, and the radiative properties of clouds modify the radiant energy that heats the air and surface.

Photochemistry is sensitive to the flux of ultraviolet (UV) radiation. Clouds scatter or absorb this radiation depending on their albedo. Thin clouds may actually increase photochemical reactions as a result of multiple scattering, but more often will decrease the net radiation through extinction, with a resulting decrease in photochemistry. The degree of extinction depends not only on the optical depth of the clouds and the fraction of the clouds that they cover, but also on their altitude and geometry with respect to the solar zenith angle. Even higher clouds like cirrus may eventually need to be taken into account for accurate AQ forecasts.

Precipitation from cloud systems changes the characteristics of surfaces by increasing soil moisture, changing the surface temperature, and altering the albedo. The modifications of the surface characteristics result in subsequent changes in the structure of the PBL as surface energy fluxes are altered, as well.

Clouds transport aerosols from the PBL, both vertically and horizontally. Removal of aerosols by scavenging occurs when cloud systems precipitate. Nucleation scavenging is thought to be more common than is, droplets form on aerosols and then grow to precipitation size by condensation, deposition, coalescence, or aggregation. Some aerosols, however, are also removed by collision and collection with hydrometeors. The detailed physics of these two processes are still under investigation. Aerosols and some gaseous species are removed by deep convection that produces strong updrafts. The depth of such clouds may vary from less than 1 to more than 10 km. Clouds may transport aerosols horizontally if these clouds form in one region and then advect to another.

Air quality forecasting in the presence of clouds is difficult because of the multiple, nonlinear ways in which clouds interact with other parameters that af-

fect traditional AQ. Forecasting the effects of intense releases of chemical, biological, or nuclear materials in the presence of clouds is equally or perhaps more difficult. Present understanding of these interactions is limited. And whereas there is a very good understanding of the theoretical aspects of cloud microphysics, cloud models are limited in their ability to adequately predict the formation and evolution of clouds with respect to the time of initiation, their horizontal and vertical extent, probability and magnitude of precipitation, and their lifetime.

An accurate prediction of cloud characteristics requires accurate information about the structure of the PBL, local convergence zones, cloud condensation nuclei (CCN) supersaturation spectra, and regional meteorology, for example, frontal systems, and larger-scale winds. Much of this information is missing or sparse in regions where AQ forecasts will be made.

There are a number of research needs that involve both theoretical and observational process studies to improve our understanding of the physics behind cloud processes in polluted areas and their impact on local AQ.

- 1) Models are needed to evaluate the sensitivity of PBL structure, surface characteristics, photochemistry, aerosol evolution, and cloud formation on the time scales important to AQ forecasts.
- 2) Field programs are needed to study cloud formation and microphysics in large urban areas. The data from these projects would be used to refine the models recommended above.
- 3) New approaches for parameterization of convection and cloud microphysics should be tested and developed. One example would be parameterization schemes that are based on ensemble techniques or on a combination of ensemble and data assimilation techniques (Grell and Devenyi 2002).

### **NEED FOR IMPROVED CAPABILITIES FOR ESTIMATING UNCERTAINTY AND PREDICTABILITY AND FOR EVALUATING MODELS.**

*Modeling.* Current model evaluation and uncertainty assessment tools are inadequate to support quantitative AQ forecasting and, thus, require improvement and augmentation. Ongoing community efforts using, for example, the Community Multiscale Air Quality Model (Models-3/CMAQ, designed as a long-term air quality planning tool) and WRF should be incorporated as fully as possible in the effort to accelerate the development of an operational air quality forecasting model. As with the WRF model, the meteorology and chemistry communities

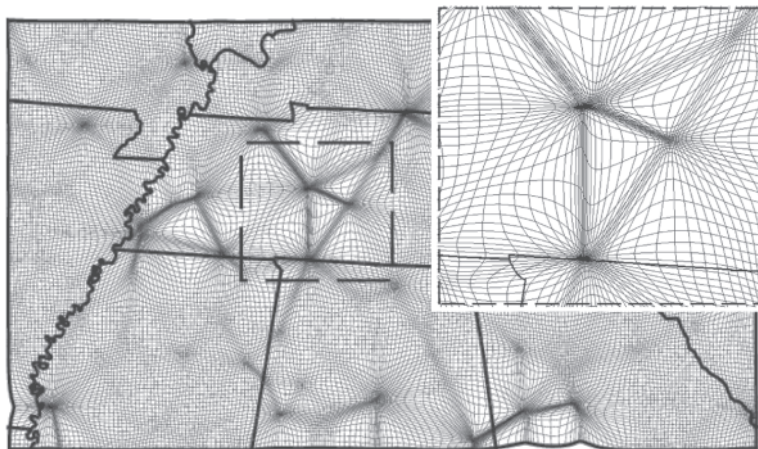
should collaborate in developing such a model, which should include a four-dimensional data assimilation capability and extensions to facilitate data assimilation research. Furthermore, a common predictive modeling platform should be developed to allow different parameterizations to be evaluated in an “all other things being equal” manner. Through this platform, researchers’ contributions could be integrated into the common operational model more effectively—sometimes directly—and efficiently. A data archiving/mining facility attached to the platform would facilitate sharing available data, which is particularly important for data assimilation research.

**Adaptive grids.** The diverse aspects of air quality forecasting necessitate a multiscale model. Grid nesting is the numerical technology facilitating multiscale modeling in the above-mentioned community models. Adaptive grids, an alternative technology, may offer new potential. Numerical difficulties associated with nested grid interfaces can be surmounted by a continuous grid using refinement or enrichment techniques. By the use of dynamic adaptive grids, computational resources can be allocated more wisely to the resolution of scales needed for a better forecast. This way, the gaps between local and mesoscale and between meso- and global scales can be bridged more efficiently. In an online meteorology–chemistry model, such as the WRF model, adaptive grids may help to resolve important dynamic and chemical features needed for a more accurate forecast.

The adaptive grid–refinement algorithm of Srivastava et al. (2000) offers many of the features mentioned above. In this algorithm, the nodes of a structured grid are repositioned continuously to minimize the grid resolution errors. The grid scales are refined automatically by a weight function that assumes large values in regions where the errors have the potential to grow. Because the number of nodes is constant, refinement in one region is accompanied by coarsening in other regions. This results in the optimal use of computational resources. In addition, it yields a continuous multiscale grid where the scales change gradually; hence, grid interface problems seen in nested grids are avoided. The adapted grid can be mapped onto a uniform grid in the computational space using

a coordinate transformation. Once this is done, existing numerical methods developed for current uniform grid models can be used for the solution. The adaptive grid algorithm has been applied to problems with increasing complexity and relevance to air quality modeling. Starting with pure advection tests (Srivastava et al. 2000), it was then applied to reactive flows (Srivastava et al. 2001a) and to the simulation of a power-plant plume (Srivastava et al. 2001b). In all of these applications, the adaptive grid solution was very accurate. To achieve the same level of accuracy with the fixed, uniform grid required significantly more computational resources. Finally, the algorithm was incorporated in a comprehensive air quality model and an ozone episode was simulated. A snapshot of the adapting grid from that simulation is shown in Fig. 2.

An alternative approach to grid refinement is grid enrichment (Tomlin et al. 1997). In this approach an unstructured grid is used. Cells are added as they are needed and are removed when their returns diminish. These two alternatives should be compared, and their advantages and disadvantages for air quality modeling should be identified. Currently, the meteorological data needed to drive the adaptive grid air quality model are interpolated from a fixed, uniform grid meteorological model. The ideal solution would be to run the meteorological and air quality models in parallel and on the same grid that is adapting to a



**FIG. 2.** Snapshot of the dynamic grid in a simulation of an ozone episode in the Tennessee valley (Odman et al. 2002). The grid is adapting to NO concentrations; this leads to clustering around urban and power-plant plumes as shown in the insert. Grid lengths vary by two orders of magnitude between the largest and smallest cells. The O<sub>3</sub> mixing ratios predicted by the adaptive grid model were much closer to observations than the fixed grid, even when the latter used 4 times as many grid nodes. This was due to superior resolution of the urban and point source plumes in the adaptive grid simulation.

mix of dynamic and chemical state variables in which resolution errors may be large. The adaptation criteria that are needed for more accurate air quality forecasts could be developed and evaluated by comparing their individual improvements over fixed, uniform grid forecasts.

*Improved verification and evaluation metrics.* Because of the limited supply of appropriate datasets, there are severe practical limits on assessing model performance by comparing predictions with observed data. Therefore, model evaluation should be a multistep process that includes 1) a scientific peer review; 2) diagnostic and performance evaluations with data obtained in trial locations and, if possible, in the same circumstances as the model's intended applications; and 3) supportive analyses (modeling system verification, sensitivity, and uncertainty analyses). Completing each of these components requires that specific model goals and evaluation objectives be defined.

In air quality forecasting, uncertainties in the model's initial state, emission and deposition rates, and boundary values, to name only a few variables, must be considered. Feedbacks between the meteorological and air quality components—which have mostly been studied as separate systems—are also critical to improved AQ forecasting. What is the relationship between mixing depth heights and near-surface concentrations? What is the role of ambient aerosols in influencing the surface energy budgets or altering the moisture fields via cloud interactions? How do these feedbacks impact weather and AQ forecasts? Sensitivity analysis studies are needed to quantify these feedbacks, which in turn can help prioritize future research efforts.

There are several approaches to this effort, including ensemble studies, direct sensitivity analysis, and adjoints. Navon (1988) describes a mathematical framework of the adjoint parameter estimation, identifiability, and regularization issues with applications to meteorology and oceanography. The adjoint technique is an efficient approach to identify sensitive regions, where uncertainty in the model parameters can lead to large errors in the model forecast, and to explore important feedback processes.

We use the term “verification” to mean ascertaining, in as objective a manner as possible, how well a meteorological and air quality modeling system is performing the tasks for which it was designed. Models are envisioned as “cartoons of reality,” because they simulate only a portion of the natural variability. Their “tasks” are limited by the assumptions made in the construction of the model and the physical processes

that are characterized. Differences between what is predicted and what is observed result from a combination of errors in model formulation (which can lead to systematic biases), propagation of measurement and input uncertainties (which can be amplified due to nonlinear effects), and the fact that nature contains more variability than do the models.

Venkatram (1988) provides a convenient framework for describing how observations and predictions differ. However, this employs the concept of ensembles, which in reality are imperfectly known. Ideally, one would compare the observed and predicted ensemble averages in order to objectively characterize any systematic bias in the model's predictions. Some success in doing that has been obtained in sorting observations into pseudoensembles for evaluation of short-range dispersion models (American Society for Testing and Materials 2001), but much work remains to be done.

Because uncertainties propagate forward in a prediction model, it is helpful to assess performance in a “front to back” sequence. For instance, the performance of the air quality model is dictated, to a certain extent, by any uncertainties in the characterization of the meteorology. The transport and dispersion of the emissions is based on the stated meteorological conditions. Often, a portion of the emission inventory is based on the representation of the meteorological conditions. Certain chemical processes are strongly influenced by the presence of and dynamics within clouds.

We conclude that standardized “physics based” evaluation metrics are needed. It is important to realize that the frequency distributions of the observations and predictions are inherently different. Thus, simple skill scores have limited use, and then only if one realizes that seemingly correct predictions can be easily achieved through a combination of offsetting errors. More sophisticated metrics that diagnose the characterization of the physical processes are required. Physics-based metrics would allow objective statistical tests to be made of whether differences in different models' results should be deemed significant. From such statistical comparisons, “measures of success” can then be developed.

Uncertainty in model predictions arises from the use of input that does not meet the assumptions upon which the modeling is based. For instance, a grid model expects specification of volume average values for, say, ambient temperature or wind information for each cell in the simulation, but it may receive instead values extrapolated from point measurements. These differences between what the model expects and what

it receives cause model predictions to deviate from an estimate of the ensemble average for the conditions that actually exist.

Modern AQ models are systems of models, and standard methods for characterizing model uncertainty have yet to be agreed upon or adopted (Irwin et al. 2001). Most available examples involve the use of Monte Carlo sampling (Irwin et al. 1987; Hanna et al. 1998, 2001; Dabberdt and Miller 2000). In this technique, replicate samples are drawn from distributions that characterize the uncertainties in selected input values and model parameters, and each sample is used to develop an estimate of the deviations from the predicted ensemble average, from which a distribution can be developed for characterizing the nature of these deviations (based on results from all of the samples).

Several promising new ensemble techniques have been developed to represent the uncertainties in weather predictions (e.g., to estimate the uncertainty in predicted wind direction or boundary layer mixing). Ensemble predictions can quantify uncertainty information caused by errors in the deterministic model prediction, which occur because the equations do not capture all atmospheric processes. There are limits to the availability and accuracy of observations, and the models cannot resolve atmospheric processes and features below their gridpoint size.

To account for these problems, a series of model forecasts can be run where the initial conditions and/or model physics or numerics are perturbed to account for the variability (Sivillo et al. 1997). In principle, ensemble prediction systems (EPSs) provide ranges of scenarios that may occur, as well as help to identify the most likely result. Research indicates that an ensemble composed of different models will likely offer better results than an EPS from one model (Toth 2001). Several operational EPSs and their output are currently available (see Tracton and Kalnay 1993, for short-range ensembles; Toth 2001, for medium-range ensembles).

Ideally the EPS will produce significant differences in solutions whose forecast distribution matches the actual frequency of occurrence. NOAA/NWS uses a method called “breeding” to perturb the initial conditions for both the global model ensembles and the short-range ensemble forecast systems. This method allows a limited number of ensemble members to account for most of the forecast variability caused by uncertainties in initial conditions. Rerunning a model with different physics packages (Wandishin et al. 2001) will increase the ensemble diversity and provide a better estimation of model uncertainty.

For air quality applications, Dabberdt and Miller (2000) reviewed the current status of ensemble dispersion modeling and presented the results in which uncertainties with a uniform distribution were assigned to various meteorological and dispersion parameters. Draxler (2003) developed an ensemble dispersion prediction system by perturbing the initial meteorological conditions. When enough ensemble members were run, 41%–47% of the variability was captured when compared to observations. Recently, Scheele and Siegmund (2001) coupled members of a meteorological model prediction system with a trajectory model to estimate forecast error and found that higher-resolution meteorological ensemble outputs were needed to capture complex boundary layer processes. Warner et al. (2002) developed a higher-resolution short-range meteorological model ensemble system to drive a series of air quality simulations. Atmospheric dispersion probability density functions were computed at each model grid point. The encouraging results suggest that these probabilistic approaches may be of value in quantifying the effects of uncertainties in a dynamic model ensemble on dispersion model predictions of atmospheric transport and dispersion.

As the resolution is reduced from regional to urban, and then to neighborhood-scale or less, it becomes increasingly difficult to deterministically characterize the variability seen in nature. This imposes a limit, which is seen to be process-dependent, below which variability will best be characterized by its statistical properties. As an example, Irwin and Smith (1984) warned that disagreement between the indicated wind direction and the actual direction of the path of a plume from an isolated point source is a major cause for disagreement between model predictions and observations. Plumes from such sources typically expand at an angle of approximately  $10^\circ$  as they proceed downwind, and seldom is this angle larger than  $20^\circ$ . With such narrow plumes, even a  $2^\circ$  error in estimating the plume transport direction can cause very large disagreement between predicted and observed surface concentration values. Weil et al. (1992) analyzed nine periods from the Electric Power Research Institute’s Kincaid experiments, where each period was about 4 h long. They concluded that for short travel times (where the growth rate of the plume’s width is nearly linear with travel time), the uncertainty in the plume transport direction is of the order of a quarter of the plume’s total width. Farther downwind, where the growth rate of the plume’s width is less rapid, the uncertainty in the plume transport direction is even larger. The uncertainty in char-

acterizing the position of the plume as a function of downwind distance is seen to be large relative to the width of the dispersing plume. Large differences between observed and predicted concentration values will occur, even if the plume dispersion is well characterized. Thus, plume transport uncertainties limit our ability to deterministically characterize the time series of concentration values that will be experienced at any one location.

As the field of air quality forecasting grows, it will be important to be able to measure the improvement in performance of the models, both for communications to the public and to managers. In addition, it will be important to set criteria for model acceptance for the many new and modified models. Some performance measures are available (e.g., fractional bias, geometric variance, figure of merit), but they are not universally used or accepted. In addition, there are no criteria for model acceptance that are used to distinguish “bad” from “good” models, even though many examples are published of model comparisons with data. The chosen performance measures and criteria for acceptance should be useful for public communications as well as scientific studies. For the public, a simple, easily understood measure is needed.

The best way to address this deficiency is to bring together the people who have worked on this topic as well as regulatory agency representatives. The goals of the workshop would be to present examples of current work on model performance measures and acceptance criteria, suggest a set of agreed-upon interim measures and criteria, and set out a comprehensive plan for developing and testing the interim set and improved consensus model performance measures and acceptance criteria. The plan could include an intercomparison of air quality forecast models.

**Assimilation tools.** Quantitative aspects of model-based atmospheric chemistry analyses and forecasts are hampered by the fact that comprehensive CTMs often lack emissions information, key measurements to impose initial and boundary conditions, or science elements, and the processes are poorly parameterized. For the analysis capabilities of CTMs to improve, they must be better constrained through the use of observational data. The close integration of observational data is recognized as essential in weather/climate analysis, and it is accomplished by a mature experience/infrastructure in data assimilation—the process by which models use measurements to produce an optimal representation of the state of the atmosphere. This is equally desirable in CTMs.

Assimilation techniques fall within the general categories of variational {three-(four)dimensional variational data assimilation [3(4)DVAR]} and Kalman filter-based methods, which have been developed in the framework of optimal estimation theory. The variational data assimilation approach seeks to minimize a cost functional that measures the distance from measurements and the “background” estimate of the true state. In the 3DVAR method the observations are processed sequentially in time. The 4DVAR generalizes this method by considering observations that are distributed in time. These methods have been successfully applied in meteorology and oceanography (Navon 1998), but they are only just beginning to be used in nonlinear atmospheric chemical models. When chemical transformations and interactions are considered, the complexity of the implementation and the computational cost of the data assimilation are greatly increased.

**Information technology infrastructure.** AQ forecasting is characterized by an immense complexity and large datasets. Users need ready access to model forecasts products, and databases should enable the automatic retrieval of background concentrations and observational data and the construction of application-specific datasets.

**WEB-BASED INTERFACES.** Near-real-time access to remotely sensed and directly measured data is needed for model initialization, as well as for setting some initial and boundary conditions. The infrastructure to support these applications needs to be developed, along with the AQ forecasting system. In particular, interfaces need to be developed for visual data mining of the assimilated fields, where users can request cross sections of the data, zoom in on regions of interest, or follow trajectories (of virtual flights) through the data. Users could also look for sensitivity information and influence function values. These Web-based interfaces, which will enable the sharing of results with remote community members, will rely heavily on high bandwidth and advances in information technologies.

**VISUALIZATION TOOLS.** Visualization tools will play an important role in the realization and utilization of AQ forecasts. The size and complexity of the analysis datasets have greatly increased over the last decade and are expected to continue to grow. Tools are needed that integrate advanced visualization hardware and interactive software to create collaborative virtual environments that allows the user to create, view, navi-

gate, and interact with data, models, and images in an immersive 3D environment, such as that shown in Fig. 3.

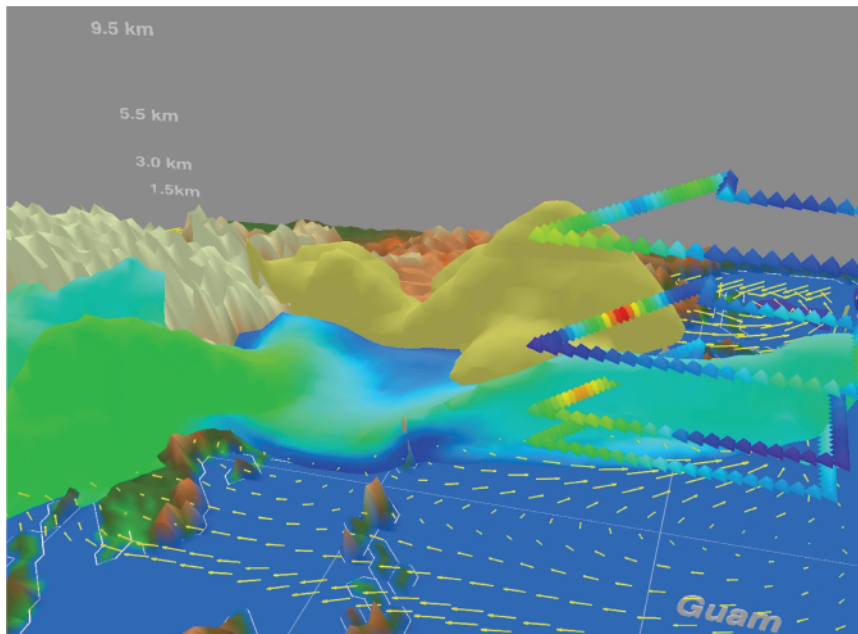
**Observations.** More extensive measurements of meteorological parameters and chemical composition are needed to support data assimilation, AQ forecasting, and AQ forecast model evaluation. Data on winds and turbulence, air temperature, and concentration would be the most valuable; and data on surface energy budgets and fluxes over regionally representative surfaces would also be very useful. Furthermore, increasing demands for air quality information with high temporal and spatial resolution are pushing the need for methodologies that allow air quality forecasts at small

scales (< 5 km). Although meteorological models have advanced to such fine resolutions, knowledge of the physics of surface–atmosphere interactions, needed to specify lower boundary conditions, has not kept pace. This disparity is particularly evident in the spatial coverage and resolution of observations, which often vary both temporally and spatially across the model domain, and in the parameterization of boundary layer processes.

Evaluations of forecasts and forecast models require somewhat different kinds of data, depending on the type and scales of the prediction. Emergency-response models typically require short-range (a few kilometers or less), short-term (a few hours or less) predictions, whereas AQ forecasting is generally longer range and longer term.

For short-range, short-term cases, fairly rapid (1 min or faster) horizontal sampling of airborne material is needed to resolve peak concentrations and any spatial splitting of the plume or puff. Sampling (direct or remote) through the depth of the plume or puff is highly desirable, particularly at several crosswind and along-wind locations. Detailed information on local wind fields, even under light wind conditions, is also required.

For longer-range cases, data with lower spatial and temporal resolution will generally be adequate. These



**FIG. 3. Visualization helps the integration of measured and modeled data (image made using Vgeo software). Shown is measured CO along the airplane's flight path; the brown isosurface represents modeled dust ( $100 \mu\text{g m}^{-3}$ ), and the blue isosurface is CO (150 ppb) shaded by the fraction due to biomass burning (green is more than 50%).**

must include information on horizontal and vertical wind fields; turbulence; vertical temperature structure; concentration measurements (both horizontally and in the vertical), with an averaging time on the order of several minutes to a few hours; topographic, land-use, and vegetation distribution data; and the synoptic situation.

Surface databases need to reflect the temporal scales of surface characteristics, which are generally dynamic and change with season over vegetated areas, or where snow cover is present in winter. In addition, accurate estimates of emissions and improved source characterization are needed to support AQ forecasting and AQ forecast model evaluation. While data assimilation techniques can be deployed to estimate emissions distributions, measurements of chemical constituents are needed to characterize emissions sources and to study transport processes. If the sources are known, measurements of tracer species provide valuable information on transport time scales that is not available from more routine physical state variables. If the sources are not known, species ratios (e.g., trace metals, hydrocarbons) can be used for identification and characterization. However, such measurements are currently made at only a handful of surface sites and are often only of short duration. Indeed, the number of observations available for

**TABLE 3. Summary of the recommendations of PDT-II for addressing the meteorological challenges connected with air quality forecasting.**

Themes	Recommendations
PBL and mixed-layer characterization	<ul style="list-style-type: none"> <li>• Improve estimation of the temporal and spatial variability and uncertainty of the height of the PBL.</li> <li>• Parameterize winds and turbulence above the shallow, surface-based stable layer, and use remote sensing of this deeper layer in key areas.</li> <li>• Use a nationwide observing network to routinely monitor (with high resolution) the diurnal variation of the height and structure of the PBL. Exploit and supplement existing measurement systems.</li> <li>• Enhance numerical modeling of the PBL. Associated meteorological observations must be linked with chemical measurements.</li> </ul>
Land surface characterization	<ul style="list-style-type: none"> <li>• Improve AQ forecast accuracy, vegetation and land-use databases by requiring better plant speciation. Resolution should exceed model grid resolution in order to support subgrid-scale variability in land use.</li> <li>• Improve seasonal and interannual vegetation variations that are important for dry deposition.</li> <li>• Create a more realistic model treatment of spatial and temporal variations in soil moisture. Soil moisture initialization also needs improvement.</li> </ul>
Clouds and cloud processes	<ul style="list-style-type: none"> <li>• Research is needed to determine the fraction of the total removal of aerosols from clouds that is due to nucleation scavenging, and how much is attributable to collisions of aerosols with hydrometeors.</li> <li>• Incorporate clouds more accurately into AQ forecasts, which requires improved models to evaluate the sensitivity of AQ components (PBL structure, surface characteristics, photochemistry, aerosol evolution, and cloud formation) on the appropriate time scales.</li> <li>• Create field programs to study cloud formation and microphysics in large urban areas, over a variety of latitudes, topography, and chemistry.</li> </ul>
Observations and measurements	<ul style="list-style-type: none"> <li>• Determine the level of spatial and temporal resolution needed for each chemical species, and identify areas where chemical measurements are needed, both for research and operations.</li> <li>• Hold regional meetings to integrate activities and generate plans for network expansion as needed. The use of tethered sondes and commercial communication tower facilities should be considered so that chemical (and meteorological) data can be obtained at several heights above the surface.</li> <li>• Generate a protocol for assessment of data quality (e.g., exchange of calibration sources, calibration procedures, and interference and artifact tests) at field measurement sites.</li> <li>• Obtain data at the spatial (horizontal and vertical) and temporal (daytime and nighttime) resolution needed to run and evaluate air quality forecast models used for short-range, short-term and longer-range, longer-term predictions. Preliminary measurements with high spatial and temporal resolution will likely be needed to determine what spatial and temporal resolution is adequate to sample important features.</li> <li>• Develop instruments that observe turbulence, PBL structure, and surface forcing parameters with better detection limits and higher-resolution measurements. They should also measure directly variables that are currently parameterized.</li> </ul>

chemical assimilation is typically several orders of magnitude smaller than the number of variables in the model.

Because the spatial and temporal distributions of the observations play an essential role in the effectiveness of the data assimilation process, a critical question for the future of chemical forecasting is how to

design observational strategies to support these efforts. Data assimilation tools can be effectively used in the design process. While applications to air quality are just beginning, strategies for targeting observations have been considered in numerical weather prediction (Palmer et al. 1998; Langland et al. 1999). As well, sensitivity studies on the observing network

**TABLE 3. Continued.**

Themes	Recommendations
Observations and measurements (continued)	<ul style="list-style-type: none"> <li>• Observe both the lowest portions of the nocturnal PBL and the upper reaches of the capping stable layer with sufficient height resolution and temporal continuity; emerging multifrequency UHF profiler technology should be explored.</li> <li>• Install a network of sites with sufficient density in the horizontal and with towers and/or remote sensing options to obtain vertical data for air quality model evaluation. The network should be operated long enough to allow the study of seasonal and annual variability.</li> </ul>
Modeling	<ul style="list-style-type: none"> <li>• Combine current modeling efforts and products to develop a common operational air quality forecasting model with fully coupled physical and chemical processes.</li> <li>• Create a common predictive modeling platform for parameterization testing, evaluation, and effective integration of research contributions.</li> <li>• Improve ensemble prediction capabilities to provide improved model uncertainty information.</li> <li>• Develop a data archiving and mining facility to facilitate sharing of available data.</li> <li>• Conduct tests to establish the impact of adaptive grids on computational resource allocation and resolution of dynamic and chemical features.</li> <li>• Carry out sensitivity studies, using a variety of approaches, to quantify uncertainties and feedbacks between meteorological and air quality modeling components.</li> <li>• Enhance physical parameterizations in air quality model meteorological preprocessors to include state-of-the-art boundary layer dynamics at appropriate scales and to ensure that all available information is fully utilized. At the same time, existing capabilities need to be retained for operating models, using lower-resolution data.</li> <li>• Hold workshops to address uncertainty quantification, limits of prediction, performance measures, and criteria for model acceptance.</li> <li>• Create evaluation metrics that diagnose the characterization of physical processes and allow objective statistical tests to determine the significance of differences among alternative models.</li> </ul>
Assimilation tools	<ul style="list-style-type: none"> <li>• Integrate observational network and model design to ensure that the scale of representativeness of surface flux data matches the scale of model resolution.</li> <li>• Use data assimilation tools in the design of observational strategies.</li> <li>• Identify and prioritize strategies to ensure that comprehensive CTMs are better constrained.</li> </ul>
IT infrastructure	<ul style="list-style-type: none"> <li>• Develop Web-based interfaces to support automatic retrieval of observational data, construction of application-specific datasets, and ready access to forecast model products. This activity must be conducted in parallel with activities to improve the air quality forecasting system.</li> <li>• Create tools that integrate advanced visualization hardware and interactive software to create collaborative virtual environments that allow users to create, view, navigate, and interact with data, models, and images in an immersive 3D environment.</li> </ul>

in the context of data assimilation (Rabier et al. 1996; Pu et al. 1997) have shown that the impact of data on the analysis estimate is highly determined by the location of the observations relative to dynamically sensitive regions of the atmosphere.

It would be very useful to have a permanent or semipermanent array of sensors so that seasonal or even annual variabilities could be studied. Such a network might usefully include direct sensors deployed in a horizontal array across the region of interest, supplemented by vertical measurements using tow-

ers or remote sensing. With current wireless technologies, it should be possible to recover data in near-real time to a central computer to facilitate data collection, quality control, and archiving. Such rapid collection, followed by prompt checking of the data, makes network maintenance relatively easy, and ensures high overall system reliability and data quality. As well, this sort of data collection could provide the near- to real-time input needed for the meteorological preprocessors of air quality models. Ideally, especially in the case of forecasts of acute events (e.g.,

emergency-response forecasting), preprocessors would be kept regularly running in an “idle” or background mode in case of an unforeseen emergency.

Emergency-response forecasting is likely to be especially important within an urban area, so detailed information on building distributions and geometry, the location of significant local vegetation (e.g., tree rows or hedges) that can steer the local flows, surface and air temperature, and emission characteristics (release mode, release rate, release temperature and momentum, release quantity, and material type) are essential. To test model predictions, it would be very helpful to have vertical profiles of wind and temperature near the source (perhaps from remote sensors), and—especially at night—information on the depth of the local mixing layer and its spatial and temporal variation. Data on larger-scale local wind flows could be very useful in interpreting the results, especially in complex terrain and/or at night, when organized flows may affect the overall transport. These studies would also help to determine the appropriate spatial and temporal resolution of sensors to adequately sample important mesoscale features.

In the near term, operational data processing and telemetry to a central assimilation hub could be employed to take advantage of ongoing measurements at the growing network of flux observation towers that has emerged in recent years (AmeriFlux and FLUXNET with more than 150 stations worldwide; Baldocchi et al. 2001). Typically, these stations, most of which are located in rural areas, are operated year-round by dedicated personnel and follow state-of-the-art data quality assurance and control procedures. The motivation for these networks is the measurement of ground-level CO<sub>2</sub> fluxes over a wide range of natural and managed ecosystems. However, observational programs at the majority of these stations also include continuous direct measurements of energy balance components and momentum flux; profiles of temperature, humidity, and CO<sub>2</sub> concentration; and a host of soil and vegetation parameters.

**RECOMMENDATIONS.** Table 3 explicitly lays out the PDT-11 team’s recommendations for reducing the meteorological challenges connected with air quality forecasting, which are mostly implicit in the earlier parts of this paper. The recommendations are organized according to seven themes pertaining to needs for improved physical understanding, PBL measurements, and modeling. One of the recommendations was to convene a community workshop to evaluate the various research needs and develop a science plan. This workshop was held 29 April–1 May

2003, and the resulting science plan for air quality forecasting will be published in a future issue of *BAMS*.

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