# 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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## ABSTRACT

The U.S. Weather Research Program convenes expert working groups on a one-time basis to identify critical research needs in various problem areas. The most recent expert working group was charged to “identify and delineate critical meteorological research issues related to the prediction of air quality.” In this context, “prediction” is denoted as “forecasting” and includes the depiction and communication of the present chemical state of the atmosphere, extrapolation or nowcasting, and numerical prediction and chemical evolution on time scales up to several days. Emphasis is on the meteorological aspects of air quality.

The problem of air quality forecasting is different in many ways from the problem of weather forecasting. The latter typically is focused on prediction of severe, adverse weather conditions, while the meteorology of adverse air quality conditions frequently is associated with benign weather. Boundary-layer structure and wind direction are perhaps the two most poorly determined meteorological variables for regional air quality prediction. Meteorological observations are critical to effective air quality prediction, yet meteorological observing systems are designed to support prediction of severe weather and not the subtleties of adverse air quality. Three-dimensional meteorological and chemical observations and advanced data assimilation schemes are essential. In the same way, it is important to develop high-resolution and self-consistent databases for air quality modeling; these databases should include land use, vegetation, terrain elevation, and building morphology information, among others. New work in the area of chemically adaptive grids offers significant promise and should be pursued. The quantification and effective communication of forecast uncertainty are still in their early stages and are very important for decision-makers; this also includes the visualization of air quality and meteorological observations and forecasts. Research is also needed to develop effective metrics for the evaluation and verification of air quality forecasts so users can understand the strengths and weaknesses of various modeling schemes. Lastly, but not of least importance, is the need to consider the societal impacts of air quality forecasts and the needs they impose on researchers to develop effective and useful products.

# 1. Introduction

## 1.1 Scope

The temporal march of weather and the corresponding short-term changes in meteorology are the single largest factor in controlling changes in the magnitude and distribution of air quality conditions. In order to forecast air quality and develop effective emission control and personal protection strategies, it is critical that the meteorological aspects of transport, diffusion, deposition and radiative transfer be effectively characterized and subsequently predicted. This report seeks to identify the important meteorological challenges to air quality forecasting while recognizing the importance of gas and aerosol chemistry and fate (and the influence of meteorology on the chemistry). This report does not, however, seek to identify the important research challenges in atmospheric chemistry. There is strong but not exclusive emphasis on air quality forecasting in the urban zone, recognizing that many of the unmet meteorological research needs apply equally well to regional and rural air quality forecasting.

## 1.2 USWRP and Charge for PDT-11

Over the past six years, the US Weather Research Program has held a series of "Prospectus Development Team" (PDT) meetings to define research issues and opportunities related to the improvement of atmospheric prediction. The general charge given to the PDT-11 Team was to identify and delineate critical meteorological issues related to the prediction of air quality. "Air Quality" refers to the chemical state of the atmosphere including atmospheric 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. "Prediction" 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-β) scale, very short-term forecasting or "nowcasting," and numerical prediction and chemical evolution on time scales up to several days. "High impact" refers to conditions that affect or alter behavior by the general public, government agencies and private sector activities including health and the environment, aviation, surface transportation, electric power, public events, broadcasting, and emergency management.

# 2. Background

Air quality forecasting, compared to weather forecasting, is a young science with roots dating back to the early 1960s. Today, air quality forecasting uses a wide range of techniques to routinely predict ambient concentrations of gaseous pollutants and particulate matter. Air quality forecasting is generally classified into two subgroups based on application: health-alert and emergency-response predictions. Health-alert forecasting focuses on the U.S. Environmental Protection Agency's (EPA) criteria pollutants: ozone ($O_3$), particulate matter ($\leq$10 and $\leq$2.5 $\mu$m in size), nitrogen dioxide ($NO_2$), carbon monoxide (CO), sulfur dioxide ($SO_2$), and lead. Emergency- response forecasting focuses on special situations when chemical, biological, or nuclear materials are emitted into the atmosphere at unplanned times and locations and where the source is either 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. This section addresses: the history and current state of air quality forecasting related to both health-alert and emergency-response prediction in the US; the scope of chemical transport models; and the various uses and the societal benefits of improved air quality forecasts.

## 2.1 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 at municipal air quality agencies began to predict pollution on the local urban scale (e.g. Thuillier and Sandberg 1971). The U.S. Environmental Protection Agency (EPA) was created in July 1970, and established a set of uniform National Ambient Air Quality Standards (NAAQS). As part of the Clean Air Act Amendments of 1970 and 1977, EPA focused on setting air quality standards and controlling pollution at it sources.

Air quality forecasting continued its evolution during the 1970s and 1980s, when more air quality agencies forecasted pollution using objective statistical methods that required forecasts of atmospheric conditions as input to predict future pollutant concentrations (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 future-year emissions to achieve NAAQS attainment. 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 early air quality models employed a diagnostic wind field model 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 mesoscale meteorological models have matured, the air quality community has begun coupling real-time prognostic meteorological models with air quality models, keeping separate software for chemistry and meteorology (“offline”, Vaughan et al. 2001; Hogrefe et al. 2001; Jakobs et al. 2001; Mc Henry et al. 2001), or using an integrated approach (“online”, Grell et al. 2000)

In the early and mid-1990s, voluntary emission reduction programs brought about another use for air quality forecasts besides warning the public about unhealthy air. These programs encouraged the public to reduce emission-producing activities on predicted high ozone days, thus seeking to reduce pollution concentrations and avoid NAAQS exceedances. Also in the 1990s, EPA started the AIRNow program (www.epa.gov/airnow) to collect and disseminate real-time ozone and $PM_{2.5}$ data as well as city-specific air quality forecasts. By 2002, the AIRNow program collected real-time air pollution 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 to complex photochemical grid models. EPA also provides education guidance documents on forecasting air quality (U.S. Environmental Protection Agency 1999a).

The scientific and technological advances that helped health-alert forecasting also aided the emergency-response prediction of consequences from accidental or intentional releases of hazardous materials into the atmosphere. Advances in computer technology permitted emergency managers to progress from using tables and graphs to using dynamic interactive models. The early models were Gaussian plume models, which used a single meteorological observation, and evolved to Lagrangian puff and particle models, which used multiple observations and three-dimensional time-varying meteorological fields.

Some of the earliest work in emergency-response prediction started in the Department of Energy’s predecessor agency, the Atomic Energy Commission (AEC). In the 1950s and 1960s, the Environmental Science Services Administration (now the National Oceanic and Atmospheric Administration) Air Resources Laboratory (NOAA-ARL) provided predictions of a stabilized plume trajectory for nuclear testing at the AEC’s Nevada Test Site. Before 1972, many AEC sites implemented site-specific Gaussian-plume dispersion codes driven by just a single wind input. In 1972, the AEC needed real-time estimates of pollutant transport and radioactive diffusion to better respond to nuclear accidents (Knox et al. 1981). This realization led to the Lawrence Livermore Laboratory’s development of 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). Further advances in emergency response modeling capability were influenced by accidents involving significant chemical and radiological releases to the atmosphere. ARAC responded to a number of radiological material release incidents, including the 1979 Three Mile Island (TMI) accident in Pennsylvania (Dickerson et al. 1979), the 1984 Bhopal, India methyl isocyanide spill, and the 1986 Chernobyl radiological accident.

A number of chemical and biological (CB), nuclear and radiological emergency- response modeling capabilities were in place before the terrorist events of September 11, 2001. For example, the CAMEO/ALOHA system was developed by NOAA (1992) to assist local fire departments in assessing the impacts of accidental releases of hazardous chemical. ALOHA is the transport and dispersion model that is part of CAMEO and is based on Gaussian models but accounts for dense gas effects and other specialized effects of a wide range of possible chemicals. In addition, the Hazard Prediction and Assessment Capability (HPAC) modeling system was developed by DTRA (1999) to calculate the effects of releases of biological, chemical, and nuclear agents. SCIPUFF handles the transport and dispersion calculations and is a Lagrangian puff model developed by Sykes et al. (1998).

Since then emphasis on developing urban- and building-scale dispersion capabilities has increased. At the urban scale there are observational and CFD modeling studies aimed at characterizing the initial state and predicting the future state of the flow within street canyons at time scales of minutes and distances up to a few kilometers. Kramer and Porch (1990) and Merilees and Pudykiewics (1990) address the difficulty in predicting the atmosphere for emergency response. They discuss the range of scales of key phenomena from $10^1$ to $10^6$ m. More than 10 years later, improvements have been made in predictions, particularly at the $10^1$ to $10^2$ km scale, and possibly down to a few kilometers using mesoscale prediction models. Much work needs to be done on predictions from the urban (10-km) to building (10-m) scale. Improvement in characterizing initial conditions and forecasting future states of the atmosphere is needed at time and space scales spanning the regional-to-urban scales. Many of the challenges in forecasting at the urban scale were addressed by PDT-10 (Dabberdt et al. 2000).

## 2.2 Air chemistry models

Air chemistry models describe the fate and transport of atmospheric chemical constituents both in the gas and aerosol phases. They have advanced to the point where they now track on the order of one hundred 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. Computational power and efficiencies have developed to the point where air chemistry models can simulate pollution distributions in an urban air shed with spatial resolution of a few kilometers, or can cover the entire globe with horizontal grid spacing of less than 100 kilometers (less than 1 degree). When applied in prognostic studies, these models are able to provide quantitative information on the distributions of many of the key trace gases and aerosol constituents in the atmosphere. Air chemistry models have become an essential element in atmospheric chemistry studies, including important applications such as providing science-based input into best alternatives for reducing pollution levels in urban environments, and assessments into how we have altered the chemistry of the global environment.

Although meteorological and chemical processes are strongly coupled, until recently, the chemical processes in air quality modeling systems were usually treated independently of the meteorological model (as in CMAQ; Byun and Ching 1999); i.e., "*offline*"), except that the transport was driven by output from a meteorological model, typically available once or twice per hour. The chemical modeling system is usually termed Chemical Transport Model (CTM). On the other hand, "*online*" coupling between chemistry and meteorology is fairly new. In an "online" approach there is no CTM, since the chemical transport is done as part of the meteorological model. This has a number of potential advantages for air quality forecasting. For example, it will permit much better characterization of the time-resolved dispersion of air pollutants and conversely, it will also allow the model to calculate the effect of particulate matter on the radiation budget or the interaction with Cloud Condensation Nuclei and hence the meteorological forecast.

The Weather Research and Forecast (WRF) model is currently being developed (http://www.mmm.ucar.edu/wrf/users/document.html) in collaboration between many research institutes. WRF is expected to become the workhorse model for the National Weather Service (NWS) by 2005, and is well suited to become the cornerstone for a next generation air quality prediction system. WRF is non-hydrostatic, with several dynamic cores as well as many different 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. The dynamic cores include a highly accurate and fully mass- and scalar-conserving flux form mass coordinate version, which represents a major improvement over commonly used non-hydrostatic models. Similarly conservative approaches have only recently been implemented in the Operational Multiscale Environment Model with Grid Adaptivity (OMEGA, Bacon et al. 2002) as well as the Japanese numerical weather prediction model (Satoh 2002). A fully conservative flux-form treatment of the equations of motion may be especially important for air quality applications. Another core will be NCEP's Non-hydrostatic Mesoscale Model (NMM, Janjic 2001). This version may well be the first operational version of WRF at NCEP. Since all WRF computer code will adhere to the WRF common modeling infrastructure, any improvement in physical and chemical modules will be easily transitioned to whatever core is used in operations, if found advantageous.

A first version of an "online" WRF-based air quality prediction system (WRFAQ) for ozone prediction already exists (http://box.mmm.ucar.edu/wrf/WG11) and is currently being evaluated with data from NOAA's 2002 pilot study. The chemical modules are based on the "online" MM5/chem model (Grell et al. 2000), which was used by NOAA during a pilot study of air pollution forecasting in the summer of 2002. An official future release of this model (WRFAQV1 in 2005) will include many additional modules (especially including the CMAQ modules, a choice of "offline" coupling, but also chemical modules from other air quality prediction systems) in addition to targeted nesting capabilities.

## 2.3 Users and Societal Benefits

Similar to the way in which weather forecasts are used, a variety of people and organizations use air quality forecasts. Also, like weather forecasts, the applications continuously evolve as forecast accuracy and specificity improve. In general there are three 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 of air quality forecasts. The forecasts are used to plan activities to avoid exposure to pollution and/or reduce emission-producing activities. Like weather forecasts for the public, air quality information needs to be clear, easily understood, and consistent. 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, where an AQI of 100 represents unhealthy air quality (U.S. Environmental Protection Agency 1999b) as shown in Table 2.

Improving the accuracy, coverage, and number of pollutants forecasted provides many societal benefits affecting the public, environment, and economy. These benefits fall into several categories:

- Public health. Accurately forecasting pollutant concentrations can help the public avoid or minimize undo exposure by using the forecasts to alter their behavior before unhealthful events occur. Sensitive individuals (e.g., asthmatics) can use this information to reduce or avoid adverse health effects. 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 behavioral changes (e.g., exercising only on low pollution days) to reduce long-term exposure to pollutants and lower chronic exposure to pollution.

- Operational planning. Air quality forecasts facilitate organizations plan business or activities more effectively. The national parks are periodically affected by haze, which, in turn, affects visitors' health and alters the scenic views. The U.S. Forest Service is planning a 10-fold increase in prescribed burning and must demonstrate to regulators that planned burns will not cause violations of the NAAQS thus requiring some form of air quality forecasting. To reduce air pollution at the source, accurate and reliable pollution forecasts may be used by government and industry to conduct intermittent emission reductions on predicted high-pollution days, thus lowering pollution levels and avoiding the high cost of continuous emission controls.

- Emergency response and risk management. Effective emergency-response forecasting will help organizations better understand the acute and chronic consequences of accidental or intentional releases of hazardous material into the atmosphere. With that information, they can mitigate risk by reducing exposure, planning effective emergency-response plans, and planning recovery processes from atmospheric and ground releases of hazardous materials. Protective actions may include sheltering in place, evacuation, dispersing potassium iodide tablets to protect the thyroid of children from a radioactive iodine release, and embargoing foodstuffs and food chain contributors (e.g., dairy products contaminated by cows foraging on contaminated grass).

- Forensics. The accurate knowledge of the source term (actual material amounts and physical or chemical makeup) is usually not known in some accidental and most intentional releases of hazardous material into the atmosphere. To determine these source characteristics requires accurately modeling plume concentrations and ground deposition. These simulations are combined with measurements of plume and deposition concentrations to identify source characteristics.

- Wild fires 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 will benefit from early evacuation guidance and smoke protective measures.

**Table 1.** Users and their needs for air quality forecasts are indicated by the check mark.

| | | Forecast Products | | | | | Forecast Period | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Sector | Group or Organization | Regional Daily Maximum | Local or City predictions | Air Quality Index (AQI) | Forecast Uncertainty | Visibility predictions | Human exposure | Short-range (0-48 hrs) | Mid-range (48-168 hrs) | Seasonal Predictions |
| Public | Sensitive Groups | √ | √ | √ | | | √ | √ | √ | |
| | General Public | √ | √ | √ | | | √ | √ | √ | |
| | Outdoor workers/recreation | √ | √ | √ | | | √ | √ | √ | |
| Decision Makers | Air Quality Agencies | | | | | | | | | |
| | Episodic or special sampling | | √ | | √ | √ | | √ | √ | |
| | Emission reductions programs | √ | √ | √ | √ | | | √ | √ | |
| | Health/Air Awareness | √ | √ | √ | | | √ | √ | √ | |
| | Emergency Response | √ | √ | | √ | | √ | √ | √ | |
| | Industry (e.g., Power) | √ | √ | | √ | √ | | √ | | √ |
| | Aviation | √ | | | | √ | | √ | | |
| | Transportation | | √ | | | √ | | √ | | |
| | Health care | √ | √ | √ | | | √ | √ | √ | |
| | Environmental | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| | Forecast and Park Service | √ | √ | | √ | √ | | √ | √ | |
| Media | Television weathercasters | √ | √ | √ | | √ | √ | √ | √ | |
| | Internet Content Providers | √ | √ | √ | | √ | √ | √ | √ | |
| | Newspapers | √ | √ | √ | | √ | √ | √ | √ | |
| Researchers | Air Quality Scientist | √ | √ | √ | | √ | √ | √ | √ | √ |
| | Air Quality Regulators | √ | √ | √ | √ | √ | √ | √ | √ | √ |
| | Field Measurement Studies | √ | | | √ | √ | | √ | √ | √ |

**Table 2.** Air Quality Index (AQI) values, categories, and pollutant concentration thresholds for the criteria pollutants (ozone, $PM_{2.5}$, $PM_{10}$, CO, $SO_2$, and $NO_2$).
Source: U.S. EPA (1999b).

| AQI | AQI Category | $O_3$ (ppb) 8- hour [a] | $O_3$ (ppb) 1- hour | $PM_{2.5}$ (µg/m$^3$) | $PM_{10}$ (µg/m$^3$) | CO (ppm) | $SO_2$ (ppm) | $NO_2$ (ppm) |
|---|---|---|---|---|---|---|---|---|
| **0 - 50** | Good | 0 - 64 | - | 0.0 - 15.4 | 0 - 54 | 0.0 - 4.4 | 0.000 - 0.034 | ([b]) |
| **51 - 100** | Moderate | 65 - 84 | - | 15.5 - 40.4 | 55 - 154 | 4.5 - 9.4 | 0.035 - 0.144 | ([b]) |
| **101 - 150** | Unhealthy for sensitive groups | 085 - 104 | 125 - 164 | 40.5 - 65.4 | 155 - 254 | 9.5 - 12.4 | 0.145 - 0.224 | ([b]) |
| **151 - 200** | Unhealthy | 105 - 124 | 165 - 204 | 65.5 - 150.4 | 255 - 354 | 12.5 - 15.4 | 0.225 - 0.304 | ([b]) |
| **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 | ([c]) | 405 - 504 | 250.5 – 350.4 | 425 - 504 | 30.5 - 40.4 | 0.605 - 0.804 | 1.25 - 1.64 |
| **401 - 500** | Hazardous | ([c]) | 505 - 604 | 350.5 – 500.4 | 505 - 604 | 40.5 - 50.4 | 0.805 - 1.004 | 1.65 - 2.04 |

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

[b] $NO_2$ has no short- term NAAQS and can generate a AQI only above a AQI value of 200.

[c] When 8-hour $O_3$ concentrations exceed 374 ppb, AQI values of 301 or higher must be calculated with 1-hour $O_3$ concentrations.

# 3. The Need for Improved Physical Understanding

## 3.1. Planetary Boundary Layer (PBL)

Much of the Panel's deliberations focused on the structure of the planetary boundary layer and associated measurement and modeling limitations and challenges. The following sections discuss characteristics of the PBL (Section 3.1.1), its importance
in air quality modeling and forecasting (3.1.2), measurement challenges (3.1.3), and interactions with the underlying land surface (3.1.4).

### 3.1.1 Characteristics of the PBL

The planetary boundary layer (PBL) is the lowest layer of the troposphere. The lower boundary of the PBL is in contact with the Earth's surface and it is usually capped aloft by a statically stable layer of varying intensity. The capping inversion is frequently the result of large-scale subsidence that separates the PBL from the rest of the free troposphere. The PBL depth (i.e. the height of the base of the capping inversion) is variable in time and space, and typically ranges up to several kilometers in clear-sky daytime conditions over land. However, the PBL is not always well defined as in the presence of frontal boundaries, deep convection, or multiple low-level inversions.

The so-called mixing or mixed layer can be an important feature of the PBL. By definition (AMS, 2000) it is a "type of atmospheric boundary layer characterized by vigorous turbulence tending to stir and [after travel times of more than 10 or 20 minutes] uniformly mix, primarily in the vertical, quantities such as conservative tracer concentrations, potential temperature, and momentum or wind speed." The turbulence can result from forced convection caused by strong winds or wind shear that generate mechanical turbulence or from free convection due to buoyancy. Buoyantly generated mixed layers are usually statically unstable, caused by heating at the earth's surface or radiative cooling at the tops of cloud or fog layers. Mixed layers may be in contact with the earth surface, and their vertical extent then defines the atmospheric mixing depth. But at other times, particularly at night, mixing 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. In the early morning, the mixed layer is shallow and capped by the remains of the residual stable boundary layer from the previous (clear) night. The so-called residual layer is the middle portion of the nocturnal atmospheric boundary layer that is characterized by weak, sporadic turbulence and initially uniformly mixed potential temperature and pollutants remaining from the mixed layer of the previous day. In mid- to late morning – phase two - the top of the mixed layer grows rapidly through the residual layer as heating eliminates the nocturnal inversion. The third phase occurs in the late morning and afternoon with the presence of a deep convective boundary layer of relatively constant depth (order of 1-2 km). During the ensuing nighttime, the bottom of the surface-based mixed layer is transformed into a statically stable boundary layer by contact with the radiatively cooled surface. The depth, structure and evolution of the mixed layer(s) in urban areas are different than in rural areas as a consequence of changes in the thermal and aerodynamic characteristics of the surface, the flux of anthropogenic sensible heat, and changes in the availability of water vapor. The characteristics of the mixed layer(s) and the PBL are also different over geographic regions with variations in the underlying surface, such as coastal areas, mountainous areas, and irrigated cropland. In contrast to the classic model of mixed-layer evolution, actual mixed-layer structure and variability can be quite different.

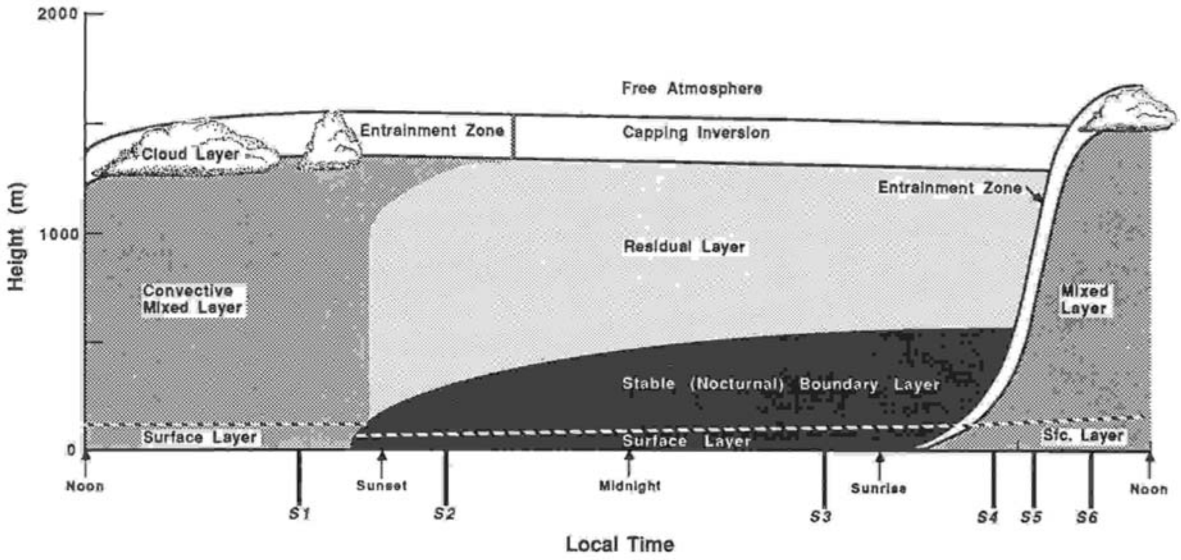

Figure 1. Schematic of mixed-layer evolution (Stull, 1988)

There are a number of scientific challenges associated with the description and prediction of the planetary boundary layer and the mixed layer. The dynamic nature of the PBL (Stull 1988) influences the concentration and residence time of pollutants and hence air quality. However, knowledge of the physical influences on PBL structure (including the presence, extent and intensity of mixed layers), as it changes both spatially over different patchworks of land cover/land use (LCLU), and temporally through the day and the year, are limiting factors in accurately predicting air quality conditions. Given the current sparsity of routine observations of the vertical structure of the PBL, it is essential that there be a nation-wide observing network that routinely monitors with high resolution the diurnal variation of the height and structure of the PBL. Further, it is critical that there be an enhanced capability to numerically model boundary layer structure (e.g. stability, turbulence and wind variability). This necessitates comprehensive observational studies, both intensive short-term programs, and extended long-term monitoring so understanding and model evaluation can consider the spectrum of PBL variability – daily, seasonal and annual. These observations need to be linked to corresponding observations of air quality and chemistry attributes.

### 3.1.2. Importance of PBL in air quality modeling

The height, $z_i$, of the planetary boundary layer (PBL) is particularly important for air quality model forecasts because it: 1) imposes a limit to vertical dispersion, and 2) is a fundamental scaling length for characterizing the neutral and convective boundary layer. The strength of the capping inversion at $z_i$ , the presence of clouds, and the rate of growth (or destruction) of the inversion strongly determine the vertical transport or dispersion of pollutants upward to the free troposphere or downward from the free troposphere to the boundary layer. The magnitudes of these upward and downward 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. Preliminary studies (Ching et al. 1981 and 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 because 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 and several hundred meters for VHF systems). 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 multi-sensor 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 multi-frequency 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. These new technologies need to be brought to bear to more realistically describe and parameterize the stable nighttime PBL and $z_i$.

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 1) thermal inputs, and 2) 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 estimates of $z_i$ uncertainties, which are presently estimated to be about ±30 % in the day and ±100 % at night. These should also account for the not-infrequent situation where there is no $z_i$ and there is 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:

Problem 1) The standard PBL theories strictly apply to what can be classed 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.

Problem 2) There is an important deep layer of the atmosphere above the shallow stable boundary layer that is not included in the standard boundary layer models, which apply to elevations below 5 to 50 m. Pollution plumes are often above this shallow surface layer <u>but</u> <u>still</u> must be modeled. Observations show that, at night, the layer from about 50 m to 1000 m ca 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 may or may not be able to mix through adjacent stable layers. The current EPA regulatory model (ISC3) does not account for these layers and simulates them as a single deep layer with a constant temperature gradient. The newly proposed AERMOD model will account for layers if they are observed but such observations are hardly ever available. Mesoscale models currently do not have adequate vertical resolution to simulate shallow elevated stable layers.

Problem 3) During the night, and at heights above $z_i$ during the day, there can be several shallow inversion layers with mixing layers in between. These can play a large role in vertical transport yet are nearly impossible to forecast. They must be detected by observing systems.

Problem 4) Stable boundary layers (SBL) are known to be intermittent, with periods of low turbulence interrupted by turbulent bursts. Richardson number (Ri) theory can help explain these bursts, since the periods of turbulence are marked by Richardson numbers less than a threshold value (i.e., Ri < 0.25).

Problem 5) As the rural SBL approaches the city it can be eroded by urban-induced thermal inputs and mechanical mixing.

The above SBL issues are being partially addressed by meteorological programs such as CASES–99 (Poulos et al. 2002) and 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 parameterize winds and turbulence above the surface-based SBL. For inputs to air quality models, there is a need for remote sensing devices to estimate vertical profiles of winds, turbulence and temperature in key locations.

### 3.1.3. PBL 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 $z_i$ because it is often ambiguous and the various *in situ* and remote sounders have different sampling limitations (e.g. different radar profilers have different minimum and maximum ranges, and range resolution). Currently, there is no nation-wide network that routinely monitors the diurnal variation of the height and structure of the PBL. The most *comprehensive* measurement system is the NWS upper-air RAOB network, which provides twice daily (00 and 12GMT) *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 U.S. with average separation of 315 km). And these stations only report data for mandatory and significant levels in near real time, although high-resolution data are available in archive mode (height resolution varies from 5 to 30 m depending on the type of sounding system used). Thus the vertical and temporal resolution of the operational RAOB data is poor for the determination of mixing layer depth and its diurnal evolution. Boundary-layer UHF wind profilers are better matched to the PBL monitoring requirements and are beginning to become more numerous, although 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). The frequency of aircraft soundings available at major airports is much greater than the RAOB network, but the height resolution is poorer.

Better utilization of all current boundary-layer observations, together with additional measurements, will improve model predictions of PBL structure. Models alone, without improved observations, cannot improve PBL simulations and forecasts. To do this we will need to conduct observational studies, both intensive short-term programs and more importantly extended long-term operational monitoring so understanding and model evaluation can consider the spectrum of PBL variability – daily, seasonal and annual. These observations need to be linked observations of PBL physical characteristics and corresponding air quality and chemistry attributes.

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). It is important that explicit attention is given to the method used by models to derive mixing height (e.g. Bianco and Wilczak 2002).

A further issue related to spatial resolution arises when comparing observed and modeled mixing heights. The nature of the surface from which $z_i$ measurements are determined (the source area) is time dependent as is the mixing height itself (Cleugh and Grimmond 2001). If the area is relatively homogeneous, then the mixing height source area may be fairly uniform (Zutter et al. 2002). However if the area is more heterogeneous, then there may be some patchwork of the surface, such as exists in many urban areas (Cleugh and Grimmond 2001). This complexity of the surface needs to be considered both in interpreting observations and evaluating models. Measurement campaigns must investigate the spatial variability of PBL structure through time and space, and relate $z_I$ variability to surface variability.

Recently, there have been intensive campaigns to investigate the PBL under specific meteorological conditions. For example the summertime ESCOMPTE/CLU campaign in Marseilles (Cros et al. 2002), and the Urban 2000/VTMX stable boundary layer study in Salt Lake City (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 the examples cited here the urban setting is in complex terrain, an important issue to be addressed. PBL behavior under a wider variety of meteorological conditions with continuous data collection remains to be addressed.

### 3.1.4. Land-Surface Modeling

The evolution and vertical mixing of the daytime boundary layer is largely forced by surface heating. Surface net radiation is partitioned into turbulent fluxes of sensible and latent heat as well as soil heat flux and heat storage in soil, vegetation, and anthropogenic materials. The portion of the net radiation that becomes latent heat is determined by soil evaporation, vegetative evapotranspiration, and evaporation from wet surfaces. Land-surface models (LSMs) that explicitly include these processes along with prognostic simulation of soil moisture in several layers are often included in mesoscale meteorological models (e.g. Chen and Dudhia 2001a; Xiu and Pleim 2001). The realism of PBL processes, including PBL height and mixing and ground level temperature and humidity, can be greatly enhanced through the use of an LSM (Pleim et al. 2001; Xiu and Pleim 2001; Chen and Dudhia 2001b). Inclusion of an LSM and an associated dry deposition model been shown to significantly affect air quality model results such as ozone concentration (Pleim and Byun 2001).

While LSMs adds important physics to meteorology and air quality model systems, there are also additional data requirements: land use, vegetation, and soil type. In addition, soil moisture initialization is a critical issue. Without realistic soil moisture fields, especially at root depth, LSMs generally add more error than skill. One approach to this problem is to run "off-line" LSMs, often referred to as Land Data Assimilation Systems (LDAS) 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. Another approach is indirect nudging where atmospheric observations, such as surface air temperature and humidity, are used to "correct" the soil moisture (e.g. Bouttier et al. 1993; Giard and Bazile 2000). Satellite observations of skin temperature tendencies can also be used to adjust soil moisture and surface heat capacities (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 stomatal models are based directly on calculations of photosynthesis rates (e.g. Berry and Farquhar 1978; Collatz et al. 1991). These models are less empirical than their predecessors since stomatal response to sunlight and temperature are described by photosynthetic reaction mechanisms. Dependence on humidity and soil moisture, however, are still empirical. 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 ingredient in realistic land-surface modeling is 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. These schemes have the advantage of being responsive to year-specific conditions but do not account for differences among plant species and ecosystems. Crop models that describe growth according to environmental conditions are also used in some models, but these schemes usually require planting date. More direct information of vegetative state can be derived from satellite data (e.g. 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, particularly by tree species. Thus, advances in surface-air exchange modeling largely depend on development of more sophisticated, high-resolution land-use and vegetation data.

Surface (with sub-surface) schemes need to be evaluated in conjunction with the PBL estimates. In particular, the urban environment is an area where the need for air quality forecasts is great and where relatively little attention has as yet been devoted to evaluating surface schemes. In the recent past a number of new 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). After a thorough identification of the urban surface schemes currently available, it will be necessary to evaluate the schemes across a wide variety of conditions.

### 3.2. Urban Meteorology for Air Quality Models

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 ADMS model (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 non-homogeneity 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 m to 1000 m) regime deals with plumes that grow to encompass several buildings in the lateral dimension 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 account for "hold-up" of plume material within wakes or cavities behind buildings (e.g. Dabberdt et al. 1994). The heating effects on building walls may 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 km to 10 km) where the pollutant plumes extend laterally to cover several blocks and vertically so that 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 u* in addition to the sensible heat flux and turbulence using standard boundary-layer formulas. The fourth spatial regime is the urban region (10 km to 100 km), encompassing the central business district, the suburbs, and the 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.

Methods to aggregate fluxes from a patchy landscape to an effective model grid-cell averaged value, and its relationship to effective average surface characteristics are discussed, among others, in Mason (1988), Claussen (1991), Blyth et al. (1993), Schmid and Bünzli (1995), Bünzli and Schmid (1998) and contributions to a special issue of the Journal of Hydrology (e.g., Michaud and Shuttleworth 1997). The sensitivity of modeled wind velocity and momentum flux in mesoscale meteorological models to the aggregation of grid scale effective values has been explored by Hasager and Jensen (1999) and Pielke et al. (1996) among others. Results from these studies show that surface characteristics over the entire model domain should be obtained at the scale of the (variable) landscape fractionation. This database should then be used to aggregate effective surface fluxes to the scale of the model resolution.

### 3.3 Clouds and Cloud Processes

Clouds are critical in understanding and predicting air quality, yet remain one of the largest sources of uncertainties in air quality modeling. The role of clouds is complex as they impact air quality (AQ) in four areas: 1) the planetary boundary layer (PBL), 2) photochemistry, 3) surface characteristics, and 4) pollutant transport. The magnitude of the impact is dependent upon the cloud characteristics, i.e. their depth, breadth and lifetime and their microphysical characteristics. An additional factor that further complicates the interaction of clouds with AQ is the effect that anthropogenic constituents have on the clouds, e.g., aerosols that act as cloud condensation nuclei (CCN), or light absorbing aerosols that alter the thermodynamics of clouds. These effects are non-linear and as yet not well understood. Numerous modeling studies have shown potentially large effects of cloud processes 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 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 at the present time.

Cloud microphysical processes (e.g. nucleation, condensation, evaporation) 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 (e.g. processing of organics), but may be of considerable importance to the transformations and ultimate fate of pollutants upon rainout or re-evaporation. 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 typically impact ambient AQ in a positive direction, i.e. their presence is thought to usually decrease the level of those atmospheric constituents that are considered to have adverse effects on the environment, e.g. ozone, nitrogen oxides, hydrocarbons and particles. As there has been little research in this area, however, that assumption is speculative at this point, based on the limited, available evidence and the current understanding of cloud thermodynamics and microphysics. [At the same time, cloud processes can have negative impacts on the environment and human health as, for example, in the case of acid rain and washout of radionuclides].

As discussed earlier, air quality is highly sensitive to the structure of the planetary boundary layer, i.e. its thermodynamic stability, distribution of water vapor and other trace gases and the fluxes of heat, mass and momentum. Clouds will significantly alter this structure and increase the difficulty of accurately characterizing and forecasting the state of the boundary layer. The degree with which clouds alter the PBL will depend upon the forcing mechanisms that form the clouds, e.g. 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 changes in the vertical profiles of temperature and humidity. And the radiative properties of clouds, i.e. their albedo, modify the radiant energy that heats the air and surface.

Photochemistry is sensitive to the flux of UV radiation. Clouds scatter or absorb this radiation depending upon their albedo. Thin clouds may actually increase photochemical reactions as a result of multiple scattering, but more often 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 cloud that they cover, but their altitude and geometry with respect to the solar zenith angle will also determine the subsequent impact on radiative fluxes. 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. And 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, i.e. droplets form on aerosols and then grow by condensation, deposition, coalescence or aggregation to precipitation sized hydrometeors. Some aerosols, however, are also removed by collision and collection with hydrometeors. The detailed physics of these two processes are still under investigation and more research is needed before the relative contribution to scavenging from both of these mechanisms can be quantified. Aerosols and some gaseous species are removed by deep convection that produces strong updrafts. The depth of such clouds may vary from less than one kilometer to more than ten kilometers. Clouds may transport aerosols horizontally if these clouds form on CCN from one region and then advect to another region.

Air quality forecasting in the presence of clouds is difficult because of the multiple, non-linear ways in which clouds interact with other parameters that affect traditional AQ. Forecasting the effects of intense releases of chemical, biological or nuclear materials in the presence of clouds (both precipitating and non-precipitating) is equally or perhaps more difficult. Present understanding of these interactions is limited as little research has been done these areas. And whereas there is 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, CCN supersaturation spectra, and regional meteorology, e.g. frontal systems, larger scale winds, etc. Much of this information is missing or sparse in those regions where AQ forecasts will be made.

Given the impediments that currently limit our ability to incorporate clouds into AQ forecasts, 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 AQ components, i.e. 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. These programs should be conducted at multiple sites with different latitudes, topography and chemistry. The data from these projects would be used to refine the models recommended in (1).
3) New approaches for parameterizations (convective, boundary layer, microphysics schemes) should be tested and developed. One example would be schemes that are based on ensemble techniques or on a combination of ensemble and data assimilation techniques (Grell and Devenyi 2002).

# 4. Need for Improved Capabilities for Estimating Uncertainty and Predictability and for Evaluating Models

## 4.1 Modeling

Current model evaluation and uncertainty assessment tools are inadequate to support quantitative AQ forecasting and thus require improvement and augmentation.

### 4.1.1 Common operational and predictive tools

On-going community modeling efforts using, for example the Community Multiscale Air Quality Model (Models3/CMAQ, designed as a long-term air quality planning tool) and the Weather Research and Forecasting Model (WRF, developed as a mesoscale research and forecasting tool, designed to include full "online" chemical capabilities) should be incorporated as fully as possible in the effort to accelerate the development of an operational air quality forecasting model and the research associated with it. As was done in the development of the WRF model, the meteorology and chemistry communities should collaborate on all phases of the development of this common operational model, which should include a 4-D 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. This sort of assessment is required to reach a greater understanding of the uncertainties associated with each modeled process. As well, new parameterizations or improvements to existing parameterizations could be tested more efficiently and without any dependence on the native modeling system. Progress made could then be quantified in terms of the change in prediction metrics. Through this platform, researchers' contributions could be integrated into the common operational model more effectively —sometimes directly— and efficiently. This would assure continuous flow of the latest state-of-the-science into the common operational model. A data archiving/mining facility attached to the platform would facilitate sharing available data, which is particularly important for data assimilation research.

### 4.1.2 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 potentials. 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. If implemented in an online meteorology-chemistry model, such as the WRF model, adaptive grids may help resolve important dynamic and chemical (emissions, reactivity, etc.) 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. Since the number of nodes is constant, refinement in one region is accompanied by coarsening in other regions. This results in optimal use of computational resources for a more accurate solution throughout the simulation. 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 applied to reactive flows (Srivastava et al. 2001a) and to the simulation of a power-plant plume (Srivastava et al. 2001b). In all 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 than the adaptive grid solution. Finally, the algorithm was incorporated in a comprehensive air quality model and an ozone episode was simulated, as shown in Figure 2.

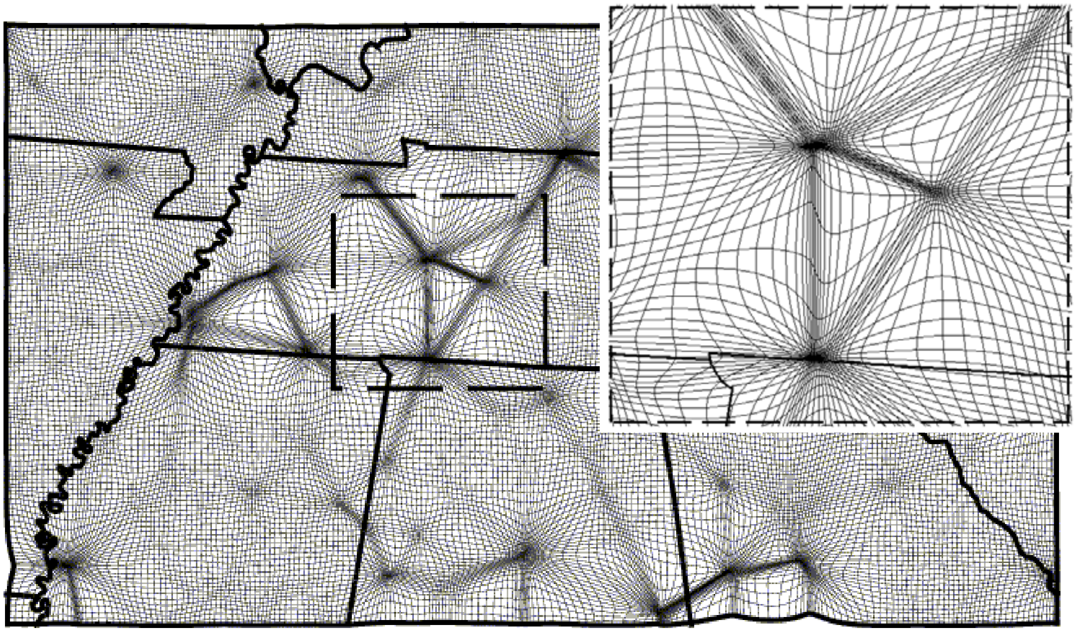

Figure 2. Snapshot of the dynamic grid in a simulation of an ozone episode in the Tennessee Valley (Odman et al. 2002). The grid is adapting to NO concentrations; this leads to clustering around urban and power plant plumes as shown in the insert. Grid lengths vary by two orders of magnitude between the largest and smallest cells. The $O_3$ mixing ratios predicted by the adaptive grid model were much closer to observations than the fixed grid, even when the latter used four times as many grid nodes. This was due to superior resolution of the urban and point source plumes in the adaptive grid simulation.

An alternative approach to grid refinement is grid enrichment (Tomlin et al. 1997). In this approach an unstructured grid is used and cells are added as they are needed and 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 have the meteorological and air quality models running in parallel and operating on the same grid that is adapting to a mix of dynamic and chemical state variables in which resolution errors may be large. There is a need to develop adaptation criteria that would lead to the most accurate air quality forecasts. Such criteria may be developed and evaluated by comparing their individual improvements over fixed, uniform grid forecasts.

### 4.1.3 Improved verification and evaluation metrics

The numerical comparison of model predictions with observed field data provides only a partial means for assessing model performance. Due to the limited supply of evaluation data sets, there are severe practical limits in assessing model performance. For this reason, the conclusions reached through science peer reviews and supportive analyses have particular relevance in deciding whether a model can be applied in the circumstances defined by the model evaluation objectives. Thus it is concluded that model evaluation involves:

- Science peer review.
- Diagnostic and performance evaluations with data obtained in trial locations and, if possible, evaluation of performance in the circumstances of the intended applications.
- Supportive analyses (modeling system verification, sensitivity and uncertainty analyses).

- The completion of each of these components requires that specific model goals and evaluation objectives be defined.

#### 4.1.3.1. Sensitivity studies

In air quality forecasting, uncertainties in the model initial state, emission and deposition rates, and boundary values, to name only a few, must be considered. The meteorological and AQ modeling components have been studied largely as separate systems. However knowledge of key uncertainties and feedbacks between the meteorological and air quality components is critical to further improvements AQ forecasting. Using quantitative metrics, 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, and 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 evaluating sensitivities and uncertainty, including ensemble studies, direct sensitivity analysis and adjoints. A mathematical framework of the adjoint parameter estimation, identifiability and regularization issues with applications to meteorology and oceanography are described by Navon (1998). 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.

#### 4.1.3.2. Verification

We use the term "verification" in the sense of 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," since only a portion of the natural variability is simulated by the modeling system. The "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 bases), propagation of measurement and input uncertainties (which can be amplified due to nonlinear effects), and differences arising from the fact that Nature contains more variability than characterized by 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 pseudo-ensembles for evaluation of short-range dispersion models (American Society for Testing and Materials D6589 2001), but this is an evolving area of research that has yet to address evaluation of meso-scale meteorological or air quality models employed in the characterization of the fate of reactive species.

Evaluation of models can be envisioned as a multi-step process. Since evaluation data is limited in extent, and models are routinely employed for situations not well covered in the evaluation data, a science peer review of the models is essential. Sensitivity studies can reveal aberrant behavior, and uncertainty studies help qualify a model's predictions. Since uncertainties propagate forward in a prediction model, it is helpful to assess performance (with correction of flaws when possible) 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.

It is concluded that development of standardized "physics-based" evaluation metrics are needed. It is important to realize that the frequency distributions of the observations and predictions are inherently different, having different sources and reasons for variance. 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. An ultimate goal is thus to develop a series of "physics-based" metrics that allow objective statistical tests to be made of whether differences seen in results obtained from alternative models can be deemed significant. From such statistical comparisons, "measures of success" can be then developed.

#### 4.1.3.3. Quantifying Uncertainty

Uncertainty in model predictions arises from use of input that does not meet the assumptions upon which the modeling is based. For instance, a grid model is expecting specification of volume average values for say ambient temperature or wind information for each cell in the simulation, but may actually receive instead values extrapolated from point measurements. Similarly, evaluation models have spatial mismatch problems (Masson et al. 2002). These differences in what the model expects and what it receives will cause the model predictions to deviate from providing an estimate of the ensemble average for the conditions that actually exist. Modern air quality models are systems of models, and standard methods for characterizing model uncertainty have yet to be agreed to (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 which 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 samples.

In addition, several promising ensemble techniques have been developed to represent the uncertainties in meteorological weather predictions (for example 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. Uncertainties in the deterministic models are caused by:

*1. The equations in the model do not fully capture ALL processes occurring in the atmosphere*.

The equations in a meteorological model deal primarily with wind, temperature, and moisture. Some of the equations in the model are highly non-linear and the full calculations cannot be processed in time for real-time forecasting. Therefore, some of the more complex terms in the equations are parameterized (typically atmospheric processes in the boundary layer like convection, friction, heat exchange etc.).

*2. The model can not resolve atmospheric processes and features smaller than certain thresholds.*

For example, in a 10 km grid point model, any feature smaller than 10 km is not resolved. Therefore, the model misses any change that occurs between grid points. Over time these errors accumulate and eventually become the dominant signal in the model output.

*3. Limited availability of initial data*

Meteorological observation are not available at every model grid point over the globe horizontally or vertically. Remotely sensed satellite and radar based observations are also limited either horizontally or vertically.

### *4. Limited Accuracy of initial data*

Lorenz (1963) found that truncating the accuracy of model initialization produced "errors" which grew in magnitude and effected the forecast output. Observations and model initialization techniques currently do not produce the accuracy needed to avoid these chaos type errors.

To account for these errors listed above, 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 System (EPS) provide ranges of scenarios that may occur, as well as helping to identify the most likely result. Research indicates that an ensemble comprised of different models will likely offer better results than an EPS from one model (Toth 2001). Several operational EPS and their output are currently available (see Tracton and Kalnay 1993 for short range ensembles; and Toth 2001 for medium range ensemble forecasts).

Ideally the EPS will produce significant differences in solutions whose forecast distribution match 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 the most of the forecast variability caused by initial conditions uncertainties. 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 Seigmund (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.

### 4.1.3.4. Limits of Predictability

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 to be seen in nature. This imposes a limit, that 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 degrees, as they proceed downwind, and seldom is this angle larger than 20 degrees. With such narrow plumes, even a 2-degree 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 hours 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 1/4 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 larger than 1/4 of the plume's total width. The uncertainty in characterizing 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 limits our ability to deterministically characterize the time series of concentration values that will be experienced at any one location.

#### 4.1.3.5. Performance Measures and Criteria for Model Acceptance

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. There are some performance measures available (e.g., fractional bias, geometric variance, figure of merit) but they are not universally used or accepted. And 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 persons who have worked on this topic and regulatory agency representatives. The goals of the workshop would be to 1) present examples of current work on model performance measures and acceptance criteria, 2) suggest a set of agreed-upon interim measures and criteria, and 3) setout 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.

## 4.2 Assimilation tools

Quantitative aspects of model-based atmospheric chemistry analyses and forecasts are hampered by the fact that comprehensive CTMs are often poorly constrained due to a variety of reasons including: incomplete emissions information; lack of key measurements to impose initial and boundary conditions; missing science elements; and poorly parameterized processes. Improvements in the analysis capabilities of CTMs require them to be better constrained through the use of observational data. The close integration of observational data is recognized as essential in weather/climate analysis and forecast activities, and this is accomplished by a mature experience/infrastructure in meteorological data assimilation. By data assimilation we refer to the process by which model predictions utilize measurements to produce an optimal representation of the state of the atmosphere.

Assimilation techniques fall within the general categories of variational (3D-Var, 4D-Var) 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 3D-VAR method the observations are processed sequentially in time. The 4D-VAR generalizes this method by considering observations that are distributed in time. These methods have been successfully applied in meteorology and oceanography [Navon, 1998], enabling both meteorological forecasts and the production of meteorological analysis several times a day. These analyses have proved invaluable in understanding the atmospheric circulation and monitoring and assessing changes in the circulation on both long and short timescales. However, these techniques are only just beginning to be used in non-liner atmospheric chemical models. When chemical transformations and interactions are considered, the complexity of the implementation and the computational cost of the data assimilation are highly increased.

## 4.3 IT Infrastructure

AQ forecasting is characterized by immense complexity and large data sets. There are needs for ready access to model forecasts products, and databases that enable the automatic retrieval of background concentrations and observational data, and construction of application specific data sets (such as those for assimilation).

### 4.3.1 Web-based interfaces

Near-real-time access to remotely sensed and directly measured data is needed for model initialization; e.g., land cover, SST, soil moisture, meteorological data, as well as for setting initial and boundary conditions such as satellite derived aerosol and aerosol quantities. 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, isosurfaces, 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.

### 4.3.2 Visualization tools

Visualization tools will play an important role in the realization and utilization of AQ forecasts. The size and complexity of the analysis data sets have greatly increased over the last decade are expected to continue to grow. Tools that integrate advanced visualization hardware and interactive software to create collaborative virtual environments that allows the user to create, view, navigate, and interact with data, models, and images in an immersive 3-D environment, are needed. The future may rely more on virtual reality tools for atmospheric applications. For example, recently personnel from the Atmospheric Sciences Data Center (ASDC) at NASA's Langley Research Center have developed new tools (the Virtual Global Explorer and Observatory (VGEO) software) and these have been used in the recently completed NASA TRACE-P field experiment, a major activity within NASA's Earth Science Enterprise [(GTE) http://www-gte.larc.nasa.gov]. This experiment demonstrated how model products from multiple models and observations from a variety of platforms could be merged together and visualized in a single virtual environment.

The intimate connection between measurements and models in atmospheric chemistry research can be illustrated through the example of large-scale field studies. Aircraft experiments, involving multiple aircraft and as many as 100 scientists, play an important role in atmospheric chemistry. Aircraft experiments are designed to characterize atmospheric chemistry and transport in association with features of specific scientific interest (e.g., transport of pollutants in association with frontal outflow) and to test certain aspects of our understanding. The difficulty in planning such experiments lies in the fact that features of interests are usually transient in nature. Flight planning relies on forecasting what features of interest are in the region and where they are expected to be at the time of the flight. Traditionally, flight planning has relied on meteorological forecasts alone. CTMs are just beginning to be used in forecast-mode to enhance flight planning by enabling the representation of important three-dimensional atmospheric chemical structures (such dust storm plumes, and polluted air masses associated with large cities or widespread biomass burning events) and how they evolve over time. With this added information, it is hoped that the expensive field-deployed resources (facilities and people) can be employed/utilized more effectively, and science successes maximized. CTM forecasts play the additional important role of providing a contextual representation of the experiment, and facilitate a quick analysis of the field results. The data obtained along the flight tracks for specific experiments (of typical duration of 8 hrs) provide the “real” representation of the atmosphere at those specific points in time and space. The models predict the time evolution and three-dimensional structures within the entire region of operation during the proposed measurement period. When measured and modeled data are viewed together, the context of the observations is elucidated. For example, one can see the sources of the air mass intercepted and measured by the aircraft and where it was headed. In addition, when viewed over the entire field period (typically weeks), the combined data set of measured and modeled quantities allows

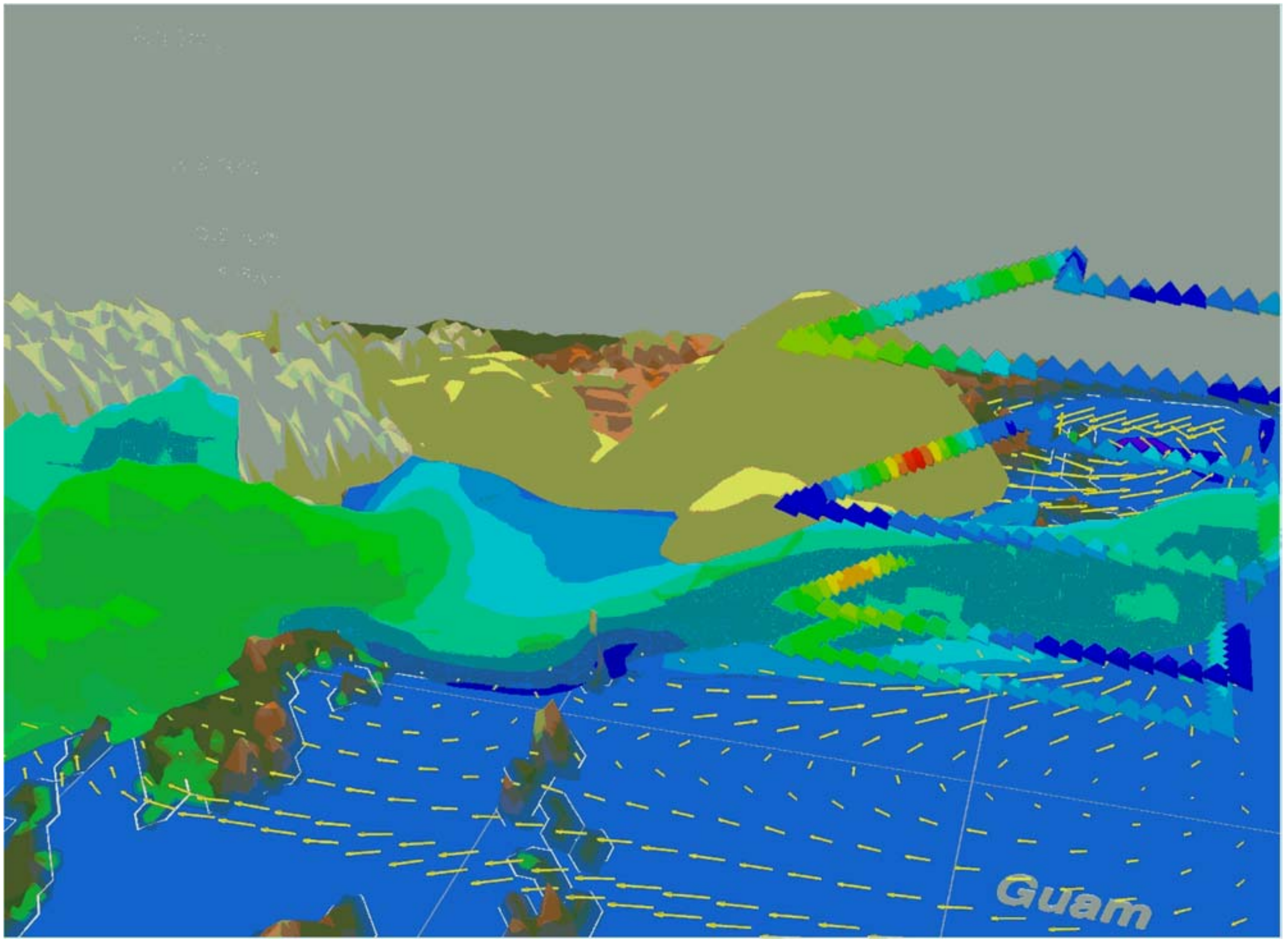

**Figure 3.** Visualization helps the integration of measured and modeled data. Shown are measured CO along the airplane's flight path, the brown isosurface represents modeled dust (100 ug/m3), and the blue isosurface is CO (150 ppb) shaded by the fraction due to biomass burning (green is more than 50%).

for an assessment of how typical the observed features are (i.e., is the observed feature unusual or do events like it occur with some regularity). This is illustrated in Figure 3, above, where modeled dust and CO distributions are shown along with a flight path and measured CO values.

### 4.4 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. However, data on surface energy budgets and fluxes over regionally representative surfaces would also be very useful for testing and refining models. 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 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, including short-range (a few km or less) short-term (a few hours or less) predictions typical of the toxic or otherwise hazardous releases common to emergency response needs and longer-range longer-term forecasts more typical of air quality forecasting needs. For short-range short-term cases, fairly rapid (one minute 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 cross-wind and along-wind locations. Detailed information on local wind fields, e.g., from a horizontal array of sonic anemometers to resolve the time-varying 3-dimensional mean and turbulent wind components, even under light wind conditions, is also required. For longer-range cases, lower spatial and temporal resolution data will generally be adequate and 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 and land use and vegetation distribution data, and the synoptic situation.

Surface databases need to reflect the temporal scales of surface characteristics (e.g., albedo, substrate heat conductance and heat capacity, soil water potential, roughness length, or drag coefficient), 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 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-term duration. Indeed, the number of observations available for chemical assimilation is typically several orders of magnitude smaller than the number of variables in the model.

As 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 the design of observational strategies to support these efforts. Data assimilation tools can be effectively used to help design such strategies. While applications to atmospheric chemistry 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 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 semi-permanent 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 towers 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 archival. 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 pre-processors of air quality models. Ideally, especially in the case of forecasts of acute events (e.g., emergency response forecasting), pre-processors would be kept in a continuous “idle” mode, regularly running in background in the anticipation of an unforeseen emergency event.

Emergency response forecasting is likely to be especially important within an urban area, so detailed information on building distributions and geometry, location of significant local vegetation (e.g., tree rows or hedges) that can steer the local flows, surface and air temperatures, and emission characteristics (release mode, release rate, release temperature and momentum, release quantity, and material type) are essential. In terms of testing 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 $CO_2$ 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 $CO_2$ concentration, and a host of soil and vegetation parameters.

# 5. Recommendations

## 5.1 PBL- and Mixed-Layer Characterization

5.1.1 In urban areas, $z_i$ is enhanced by about 20% during the day due to thermal inputs. Similarly, urban mixing height values may not collapse at night due to 1) thermal inputs, and 2) mechanical mixing by building obstacles (e.g. Ludwig and Dabberdt 1973). There is a pressing need to include estimates of $z_i$ uncertainties, which are presently estimated to be about ±30 % in the day and ±100 % at night. These should also account for the not-infrequent situation where there is no $z_i$ and there is just a gradual approach to the free troposphere.

Recommendation:

- Research efforts are needed to better estimate the temporal and spatial variability and uncertainty of $z_i$ for input to urban air quality models.

5.1.2 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.

Recommendation:

- There is still a strong need to parameterize winds and turbulence above the shallow surface-based stable boundary layer. For inputs to air quality models, there is a need for remote sensing devices to estimate vertical profiles in key areas.

5.1.3 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 $z_i$ because it is often ambiguous and the various *in situ* and remote sounders have different sampling limitations (e.g. different radar profilers have different minimum and maximum ranges, and range resolution).

Recommendation:

- Given the current scarcity of routine observations of the vertical structure of the PBL, it is essential that there be a nation-wide observing network that routinely monitors with high resolution the diurnal variation of the height and structure of the PBL. Methods should be explored to exploit and supplement existing measurement systems, such as profilers, radar, RAOBs and aircraft.
- Further, it is critical that there be an enhanced capability to numerically model boundary-layer structure. To do this there is the need to conduct observational studies, both intensive short-term programs and more importantly extended long-term monitoring so understanding and model evaluation can consider the spectrum of PBL variability – daily, seasonal and annual. These observations need to be linked to observations of PBL physical characteristics and corresponding air quality and chemistry attributes.

### 5.2 Land-Surface Modeling

Generally, the refinement of input data and data assimilation are among the most important factors in the improvement of short-term forecasts at meso- or regional scales. The urban environment is an area where the need for air quality forecasts is large and where relatively little attention has as yet been devoted to evaluating surface schemes. After a thorough identification of the urban surface schemes currently available, it will be necessary to evaluate the schemes across a wide variety of conditions.

Recommendations:

- Vegetation and land use databases need refinement to provide better plant speciation rather than just broad land-use classes (e.g. deciduous forest, or dry crops). Different crops have very different minimum stomatal resistances, different canopy heights and roughness lengths, and different growing seasons. Different deciduous and coniferous tree species also have important distinctions particularly with regard to biogenic emissions. Speciation will also help to distinguish between plants with different photosynthetic chemical mechanisms (C3 or C4), which is critical for the latest stomatal models. In urban areas, there is the added complexity of the heterogeneity of the vegetation over small areas.
- Improving resolution and accuracy of land-use data are also quite important. Comparisons of several commonly used land-use databases show large discrepancies. For example, in a 1000 x 1000 km$^2$ area centered on Nashville, TN, total forest ranged from 52% to 72% (Pierce et al. 2002). Resolution far greater than the model grid resolution is also important since most models have some kind of accounting for subgrid land-use composition.
- Seasonal and interannual vegetation variations need to be better represented. Wilson et al. (2000) showed large effects of seasonal and interannual variability on energy fluxes. Vegetation variations have similar effects on chemical dry deposition. Various satellite and modeling approaches are being developed as discussed in Section 3.1.4.
- The largest effects on surface energy and chemical fluxes on a week-to-week time scale are caused by the spatial and temporal variations in soil moisture. Indeed, modeling the soil moisture is one of the main reasons for including an LSM in a model system. In urban areas we have the added complexity of including human controlled irrigation patterns, which are both spatially and temporally variable (Grimmond and Oke 1986; Grimmond et al. 1996). However, soil moisture initialization is critically important for realistic model simulation. Alternative techniques for off-line (LDAS) and on-line approaches are outlined in Section 3.1.4. The best solution may be a combination where real time observations are assimilated into an on-line LSM in a pre-forecast initialization period. This approach will depend largely on advances in precipitation, skin temperature, and solar radiation observations and their close-to-real-time availability.

### 5.3 Clouds and Cloud Processes

Clouds are critical in understanding and predicting air quality, yet remain one of the largest sources of uncertainties in air quality modeling. The role of clouds is complex as they impact air quality (AQ) in four areas: 1) the planetary boundary layer (PBL), 2) photochemistry, 3) surface characteristics, and 4) pollutant transport.

Recommendations:

- Removal of aerosols by scavenging occurs when cloud systems precipitate. Nucleation scavenging is thought to be more common, i.e. droplets form on aerosols and then grow by condensation, deposition, coalescence or aggregation to precipitation sized hydrometeors. Some aerosols, however, are also removed by collision and collection with hydrometeors. The detailed physics of these two processes are still under investigation and more research is needed before the relative contribution to scavenging from both of these mechanisms can be quantified.

- Given the impediments that currently limit our ability to incorporate clouds into AQ forecasts, 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 AQ components, i.e. PBL structure, surface characteristics, photochemistry, aerosol evolution, and cloud formation on the time scales important to AQ forecasts; and 2) Field programs are needed to study cloud formation and microphysics in large urban areas. These programs should be conducted at multiple sites with different latitudes, topography and chemistry. The data from these projects would be used to refine the models recommended in (1).

### 5.4 Modeling Capabilities

5.4.1 A common operational air quality forecasting model and a common predictive modeling platform are needed to support air quality forecasting (4.1.1).

Recommendations:

- Combine current modeling efforts and products to develop a common operational air quality forecasting model with fully coupled physical and chemical processes. The design should include a 4-dimensional data assimilation capability and extensions that facilitate data assimilation research.

- Develop a common predictive modeling platform for parameterization testing and evaluation and to most effectively integrate researchers' contributions and the latest state-of-the-science parameterizations and capabilities into the common operational air quality forecasting model.

- Develop ensemble prediction capabilities to provide improved model uncertainty information.

- Develop a data archiving/mining facility to facilitate sharing of available data.

5.4.2 Nesting or adaptive grid technology may be needed to support air quality forecasting (4.1.2).

Recommendation:

- Conduct tests to establish the extent to which use of adaptive grids affects computational resource allocation and/or resolve dynamic and chemical features.

5.4.3 Improved verification and evaluation metrics are needed to support air quality forecasting and forecast model evaluation. Improved techniques to quantify model uncertainty are needed for air quality forecasting. (4.1.3).

Recommendations:

- Conduct sensitivity studies to quantify uncertainties and feedbacks between meteorological and air quality modeling components. Ensure that a variety of approaches are used (e.g., ensemble, direct analysis and adjoints).

- Explore the utility of ensemble techniques to provide probabilistic information for air quality forecasts.

- Develop evaluation metrics that diagnose the characterization of physical processes and allow objective statistical tests to be made to determine the significance of differences seen in results obtained from alternative models.

- Convene workshop(s) to address uncertainty quantification, limits of prediction, performance measures, and criteria for model acceptance.

### 5.5. Assimilation tools (4.2)

5.5.1 Spatial data assimilation tools are needed to support air quality forecasting and forecast model evaluation.

Recommendation:

- Integrate observational network and model design activities to ensure that the scale of representativeness of surface flux data matches the scale of model resolution.

5.5.2 Meteorological and chemical data assimilation tools are needed to support air quality forecasting and forecast model evaluation.

Recommendations:

- Ensure that data assimilation tools are used in the design of observational strategies.

- Identify and prioritize strategies to ensure that comprehensive CTMs are better constrained.

### 5.6 IT Infrastructure

5.6.1 Improved web-based interfaces are needed to support air quality forecasting and forecast model evaluation (4.3.1).

Recommendation:

- Develop web-based interfaces to support the automatic retrieval of observational data, construction of application-specific data sets, and ready access to forecast model products. Ensure that this activity is conducted in parallel with activities designed to improve the air quality forecasting system.

5.6.2 Improved visualization tools are needed to support air quality forecasting and forecast model evaluation (4.3.2).

Recommendation:

- Develop tools that integrate advanced visualization hardware and interactive software to create collaborative virtual environments that allows the user to create, view, navigate, and interact with data, models, and images in an immersive 3-D environment.

## 5.7 Observations (4.4)

5.7.1 Improved databases of surface parameters (e.g., albedo, substrate heat conductance and heat capacity, soil water potential, and roughness length or drag coefficient) and boundary layer exchange observations are needed to support air quality forecasting, emergency-response modeling and forecasting, and forecast model evaluation. These need to be regularly updated given the nature and rate of land use and land cover changes due to such activities as urban sprawl.

Recommendations:

- Create a central data assimilation hub with support for routine telemetry for data input, operational data processing and archival facilities and capabilities, and access for routine community use of data products (including emergency response).
- Begin by taking advantage of on-going measurements at sites associated with the AmeriFlux and FLUXNET programs. Lessons learned in the initial stages of working with these data sets can inform implementation of a long-term high spatial resolution observations network.

5.7.2 Improved databases of chemical composition are needed to support air quality forecasting and forecast model evaluation.

Recommendations:

- Identify and prioritize a suite of radioactive, relatively long-lived, and shorter-lived species characteristic of various anthropogenic and biogenic sources to be used as tracers of transport.
- Determine the level of spatial and temporal resolution needed for each species and identify areas where measurements are needed.
- 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 data can be obtained at several heights above the surface.
- Augment existing field sites with instrumentation as needed and generate a protocol for assessment of data quality (e.g., exchange of calibration sources, calibration procedures, and interference and artifact tests).

5.7.3 Improved predictability at small temporal and spatial scales is needed to support air quality forecasting, emergency-response modeling and forecasting, and forecast model evaluation.

Recommendations:

- Ensure that data having the spatial (horizontal and vertical) and temporal (daytime and nighttime) resolution needed to run and evaluate air quality forecast models used for both short-range, short-term and longer-range, longer-term predictions are obtained. (This must be a key part of activities associated with recommendation #2.) Preliminary measurements with high spatial and temporal resolution will likely be needed to determine the appropriate spatial and temporal resolution of sensors to adequately sample important features.
- Enhance instruments currently used to make observations of turbulence, PBL-structure and surface forcing parameters with instruments that have improved detection limits, are linear over the full range of ambient values, are capable of making higher-resolution measurements, and can directly measure some variables that are currently parameterized.

- A significant measurement 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 multi-sensor systems that use UHF profilers to address the long-range challenges and optical or acoustic profilers to sample the very lowest nocturnal layers. Also, emerging multi-frequency 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. These new technologies need to be brought to bear to more realistically describe and parameterize the stable nighttime boundary layer and $z_i$.

- Add related instrumentation to existing sites and expand the number of measurement sites to provide adequate spatial coverage for air quality forecasting at small scales. This effort should be an integral part of the activities recommended above (recommendation #2). Serious consideration should be given to the expanded use of *in situ* and remote sensing devices to obtain representative point, line and volumetric measurements of winds, turbulence, and temperature.

- Enhance the physical parameterizations in air quality model meteorological pre-processors 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, retain existing capabilities for operating models using lower resolution data.

- Incorporate flexible data assimilation schemes with powerful capabilities for data interpolation and/or effective aggregation into air quality models to more efficiently and effectively handle differences in model and data scales to optimize use of surface data.

5.7.4 A long-term diagnostic network is needed to support air quality forecast model evaluation.

Recommendation:

- Design and install a network of sites with sufficient density in the horizontal and towers and/or remote sensing options to obtain vertical data for air quality model evaluation. This diagnostic network should be operated for a long period of time to allow the study and evaluation of seasonal and annual variability. (This activity should be an integral part of the activities associated with the recommendations in section 1, above.)

- For the near-term, set up a system that includes operational data processing and telemetry to a central assimilation hub for use of the continuous energy balance, momentum flux, temperature profile, humidity, and soil and vegetation parameter measurements made at flux observation tower network sites.

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