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Global Earth Observation System (GEOS): System Capabilities and the Role for U.S. EPA

Recommendations of a Community Panel

Final Report

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U.S. EPA Disclaimer of Endorsement

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Acronyms

ACARS .... Aircraft Communication Addressing and Reporting System
AQ .... air quality
BART .... Biosphere-Atmosphere Research and Training Program
BASC .... Board on Atmospheric Sciences and Climate (National Research Council)
BATS .... Biosphere-Atmosphere Transfer Scheme
BC .... black carbon
CALIPSO .... Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations
CEOS .... Committee on Earth Observation Satellites
CMAQ .... Community Multiscale Air Quality
CTM .... chemical transport model
DBMS .... database management system
DIAL .... Differential Absorption Lidar
DOE .... U.S. Department of Energy
DOI .... U.S. Department of the Interior
ECMWF .... European Centre for Medium-Range Weather Forecasts
EIP .... Ecological indicator prediction
EOS .... Earth Observing System
EOSDIS .... Earth Observing System Data and Information System
EPA .... U.S. Environmental Protection Agency
ESA .... European Space Agency
FACE .... Free-Air Carbon Dioxide Enrichment
FDDA .... four-dimensional data assimilation
GAW .... Global Atmospheric Watch
GCOS .... Global Climate Observing System
GEIA .... Global Emissions Inventory Activity
GEO .... Group on Earth Observations
GeoSCIAMACHY ...... Geostationary Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
GEOSS .... Global Earth Observing System of Systems
GeoTRACE .... Geostationary Observatory for Tropospheric Air Chemistry
GOES .... geostationary operational environmental satellite
GPRS .... General Packet Radio Service
GPS .... Global Positioning System
GTS .... Global Telecommunications System
GURME .... The GAW Urban Research Meteorology and Environment project
HSIP .... Homeland Security Infrastructure Program

IAGOS .... Integration of Routine Aircraft Measurements into a Global Observing System
ICARTT .... International Consortium for Atmospheric Research on Transport and Transformation
IGAC .... International Global Atmospheric Chemistry Project
IGACO .... Integrated Global Atmospheric Chemistry Observations
IGERT .... Integrative Graduate Education and Research Traineeship
IGOS .... Integrated Global Observing Strategy
INTEX-NA .... Intercontinental Transport Experiment-North America
IONS .... INTEX Ozone Network Study
IPCC .... Intergovernmental Panel on Climate Change
IR .... infrared
ITCT .... Intercontinental Transport and Chemical Transformation
ITOP .... Intercontinental Transport of Pollution
JMA .... Japan Meteorological Agency
LAI .... leaf area index
LES/CFD .... Large Eddy Simulations/Computational Fluid Dynamics
LSM .... land surface model
MM5 .... Mesoscale Model, Version 5
MOZAIC .... Measurement of Ozone and Water Vapor by Airbus In-Service Aircraft
NAQP .... numerical air quality prediction
NARSTO-NE-OPS .... NARSTO NorthEast Oxidant and Particle Study
NASA .... National Aeronautics and Space Administration
NCEP .... National Centers for Environmental Prediction
NDVI .... normalized difference vegetation index
NEAQS .... New England Air Quality Study
NEON .... National Ecological Observatory Network
NMHC .... nonmethane hydrocarbons
NMHS .... National Meteorological and Hydrological Services
NMVOC .... nonmethane volatile organic compound
NOAA .... National Oceanic and Atmospheric Administration
NOAH .... Land-surface model developed jointly by **N**ational Centers for Environmental Prediction, **O**regon State University, the U.S. **A**ir Force, and the **H**ydrologic Research Lab of the National Weather Service
NRC .... National Research Council
NSF .... National Science Foundation
OMI .... Ozone Monitoring Instrument
PAN .... peroxyacetyl nitrate
PAR .... photosynthetic active radiation
PBL .... planetary boundary layer

PM............................. particulate matter

PROPHET................. Program for Research on Oxidants: Photochemistry, Emissions, and Transport

QA............................. quality assurance

QC............................. quality control

SCIAMACHY............. Scanning Imaging Absorption Spectrometer for Atmospheric Chartography

SOS........................... Southern Oxidant Study

TOMS........................ Total Ozone Mapping Spectrometer

UCP........................... urban canopy parameterization

USDA........................ U.S. Department of Agriculture

VOC .... volatile organic compound

WMO......................... World Meteorological Organization

WRF .... Weather Research and Forecasting Model

I Introduction

In July 2003, the United States hosted the Earth Observation Summit in Washington, DC (http://www.epa.gov/geoss/index.html). The summit brought together 33 nations plus the European Commission to adopt a declaration that signified a political commitment toward the development of a comprehensive, coordinated, and sustained Earth Observation System to collect and disseminate improved data, information, and models to stakeholders and decision makers. These nations agreed to partner with the U.S. to realize a common goal of establishing an international, comprehensive, coordinated, and sustained Earth Observation System.

Nine months later, in Tokyo, Japan, a second Summit was held and more than 50 nations formally adopted a ten-year implementation plan for a Global Earth Observation System. This Global Earth Observation System of Systems (GEOSS) will help all nations involved produce and manage their information in a way that benefits the environment as well as humanity. GEOSS is a large cooperative effort to bring together existing and new hardware and software, making it all compatible in order to supply data and information at no cost. The U.S. and developed nations have a unique role in developing and maintaining the system, collecting data, enhancing data distribution, and providing models to help all of the world's nations (http://www.epa.gov/geoss/index.html).

On March 9-10, 2004, the U.S. Environmental Protection Agency (EPA) convened a panel of 14 experts in Research Triangle Park, NC, to discuss and make recommendations pertaining to the proposed GEOSS. Table I.1 lists the panel members and their affiliations. The specific charge to the panel was to provide EPA with expert recommendations and guidance concerning opportunities for EPA's participation in GEOSS. Recognizing that other U.S. Federal agencies and other government and non-governmental organizations will also be contributing to the design and implementation of GEOSS, and further recognizing that many related observing initiatives are already in place, the panel was asked to consider unique contributions that could be made by EPA.

Table I.1 List of panel members

Member	Affiliation
Gregory Carmichael	University of Iowa, Iowa City, IA
Mary Anne Carroll	University of Michigan, Ann Arbor, MI
Jason Ching	National Oceanic and Atmospheric Administration (in partnership with the U.S. EPA, Research Triangle Park, NC)
Walter Dabberdt	Vaisala, Inc., Boulder, CO (co-convener)
Jack Fishman	National Aeronautics and Space Administration, Langley Research Center, Hampton, VA
Alex Guenther	National Center for Atmospheric Research, Boulder, CO
Jeremy Hales	ENVAIR, Pasco, WA
Robert Imhoff	Baron Advanced Meteorological Systems, Asheville, NC
Sharon LeDuc	National Oceanic and Atmospheric Administration, National Climate Data Center, Asheville, NC
John McHenry	Baron Advanced Meteorological Systems (co-convener), North Carolina State University (Visiting Scholar), Raleigh, NC
Richard McNider	University of Alabama, Huntsville, AL
Nelson Seaman	Pennsylvania State University (on assignment to NOAA National Weather Service, Silver Spring, MD)
James Szykman	U.S. Environmental Protection Agency (on assignment to NASA Langley Research Center, Hampton, VA)
Anne Thompson	National Aeronautics and Space Administration, Goddard Space Flight Center, Greenbelt, MD

In preparation for the meeting, the panel was given examples of possible approaches to EPA's role in GEOSS. One example involved the special environmental observing requirements—both meteorological and chemical—unique to differing environments: rural and urban, for example, or mountainous and coastal. The special challenges of megacities (in temperate zones and the tropics), and other cross-cutting approaches to environmental monitoring, were encouraged. Similarly, substantive enhancements of existing programs were considered. Also, the panel was asked to consider proposing pilot programs, establishing new or enhanced operational systems, and creating new international coordination mechanisms, if needed. The panel was asked to think about how such observing systems might be directed toward minimizing data gaps across spatial scales, thus helping EPA move toward a more comprehensive observing approach that would not only benefit GEOSS but also EPA's unique domestic mission, including air quality modeling and forecasting.

The agenda devoted approximately one-half day to background presentations, one day to discussion, and one-half day to preparing recommendations. This report describes the discussions of the panel and their recommendations in the following 10 areas:

- Section II: Measurements and sampling
- Section III: Data assimilation
- Section IV: Integrated biogenic assessments
- Section V: Surface characterization and parameterization
- Section VI: Strategies for improved emissions estimates
- Section VII: Special urban challenges
- Section VIII: International air quality forecasting
- Section IX: Testbeds
- Section X: Database management and information systems
- Section XI: Education and outreach

II Measurements and Sampling[2]

A. Leveraging Existing Surface and Upper-Air Measurements

1. Existing surface measurements

From a GEOSS perspective, surface air-quality observations of the criteria pollutants ozone (O_3), carbon monoxide (CO), oxides of nitrogen (NO_x), sulfur dioxide (SO_2), and particulate matter[3] ($PM_{2.5}$ and PM_{10}) are an underutilized yet essential resource. First, however, some limitations of the data need to be acknowledged. From a global perspective, the coverage of surface air-quality data is uneven, and in some regions and sites there are issues related to data quality and accessibility that limit their usefulness. Nonetheless, from the perspective of national needs and opportunities for EPA to contribute to GEOSS, the stations in EPA networks (Figs. II.1-II.6, U.S. EPA AirData, Monitor Locator Map–Criteria Pollutants, http://www.epa.gov/air/data/monloc.html?us~USA~United%20States) represent a ready opportunity. There is good geographical coverage and there are standards in place that assure a reasonable degree of uniformity in instrumentation and data collection and distribution procedures. For clarity, we address the potential of surface air-quality (AQ) data in the short-term and illustrate with reference to a specific pilot (or testbed) project, the NASA/NOAA/NSF summer 2004 INTEX-NA/NEAQS interagency field experiment (discussed in Section II.A.2). In the ten-year outlook of the GEOSS implementation plan, EPA's surface network can be used in a similar way as models scale up from the "U.S. weather range" to a global chemical forecasting capability.

There are two roles that surface data can play:

- In research mode, the surface air-quality data are critical to the development of credible air quality forecast models. The panel reviewed some issues in model representation of surface and boundary-layer processes that would benefit from benchmarking with surface data.

- In an operational mode, it is envisioned that surface air-quality and upper-air observations will be assimilated into models if the data are available in near-real time.

2. Upper-air measurements

Enhancement of the current surface monitoring network for atmospheric trace constituents is important because most emissions enter the atmosphere at or near the surface. However, once emissions enter the atmosphere, differential vertical transport by turbulence, terrain-driven flows, convergence/divergence zones, sea breezes, convection, fronts, etc. lead to complex distribution of chemical species and aerosols that cannot be inferred accurately from surface measurements alone. Moreover, some species such as ozone have large source mechanisms in the upper regions of the atmosphere and can affect surface concentrations through cross-tropopause processes. Long-range (intercontinental and interregional) transport of chemical constituents typically occurs above the surface-based mixed layer. Thus, vertical profiles are necessary to determine three-dimensional distributions of key species, including aerosol speciation, and to understand and forecast the chemistry of the global environment.

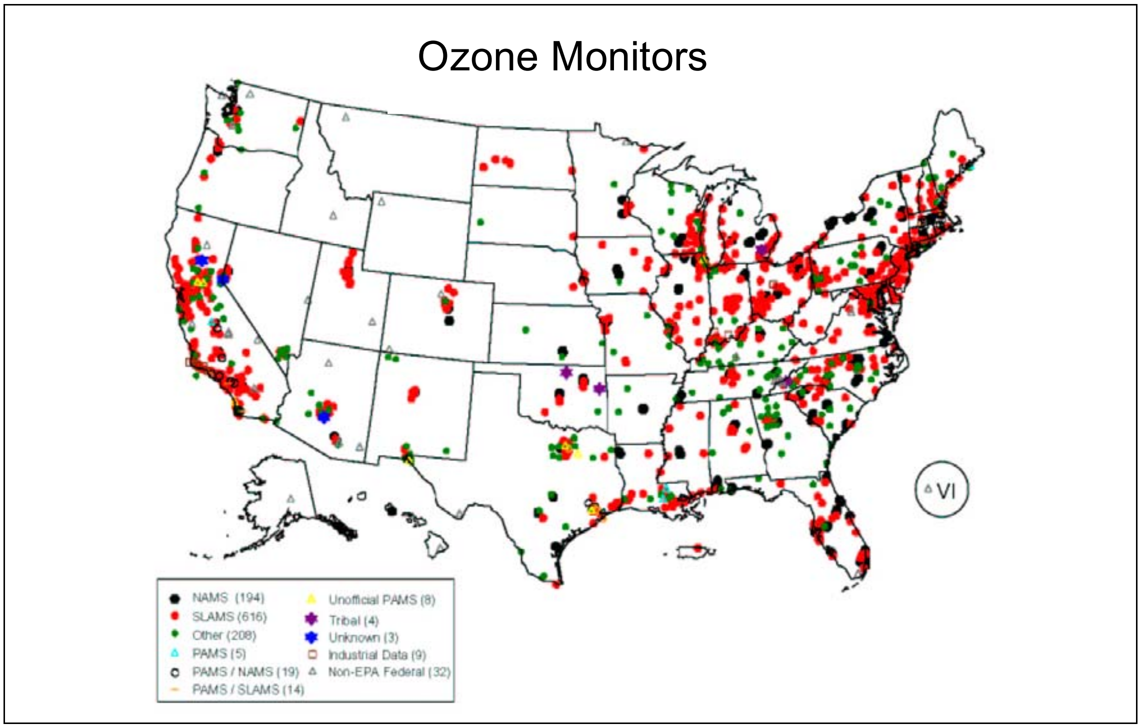

Figure II.1 Surface O_3 monitoring sites in EPA networks.

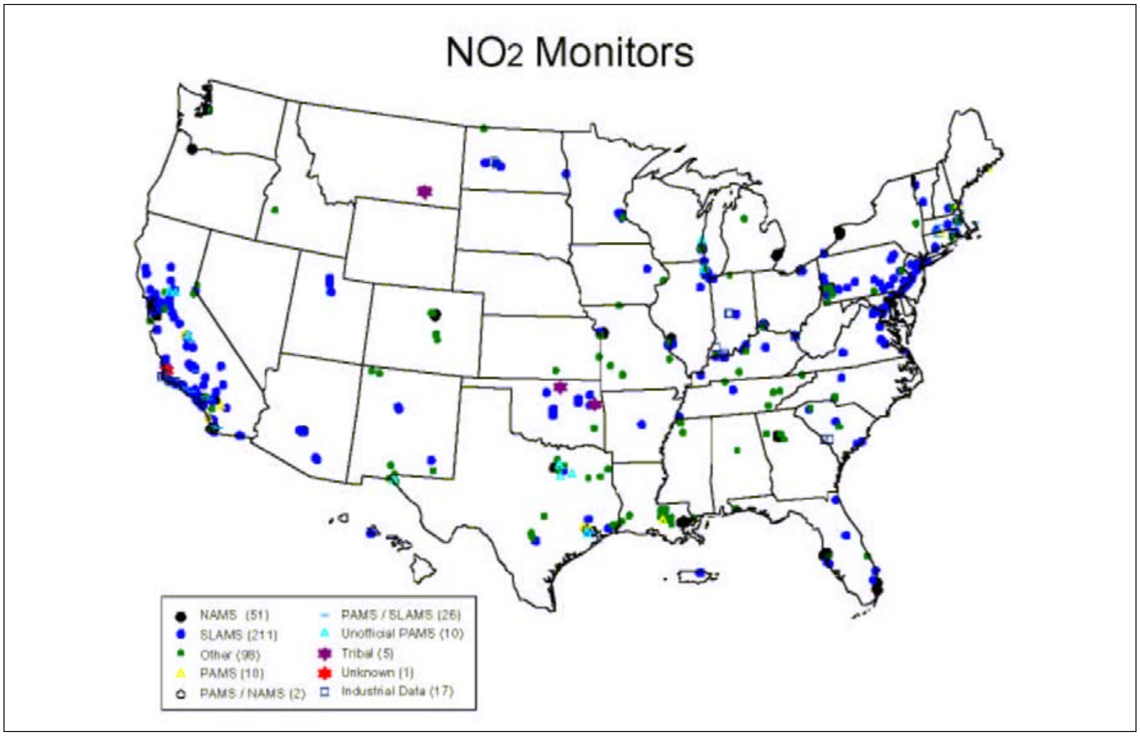

Figure II.2 Surface NO_2 monitoring sites in EPA networks

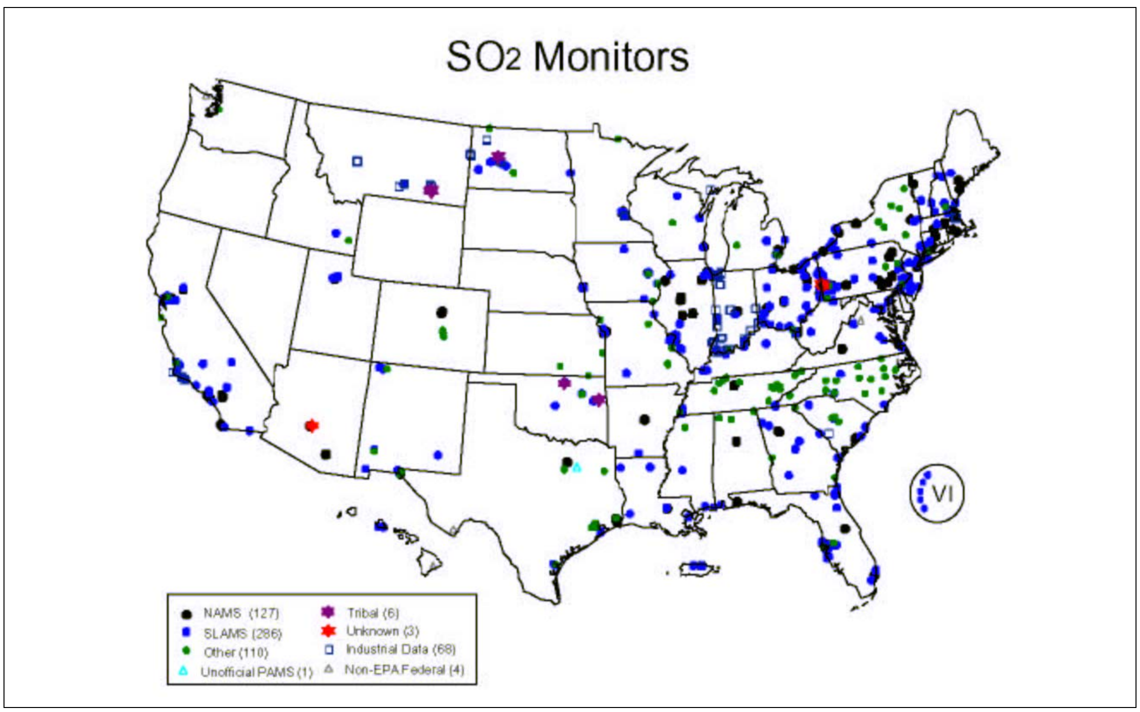

Figure II.3 Surface SO_2 monitoring sites in EPA networks.

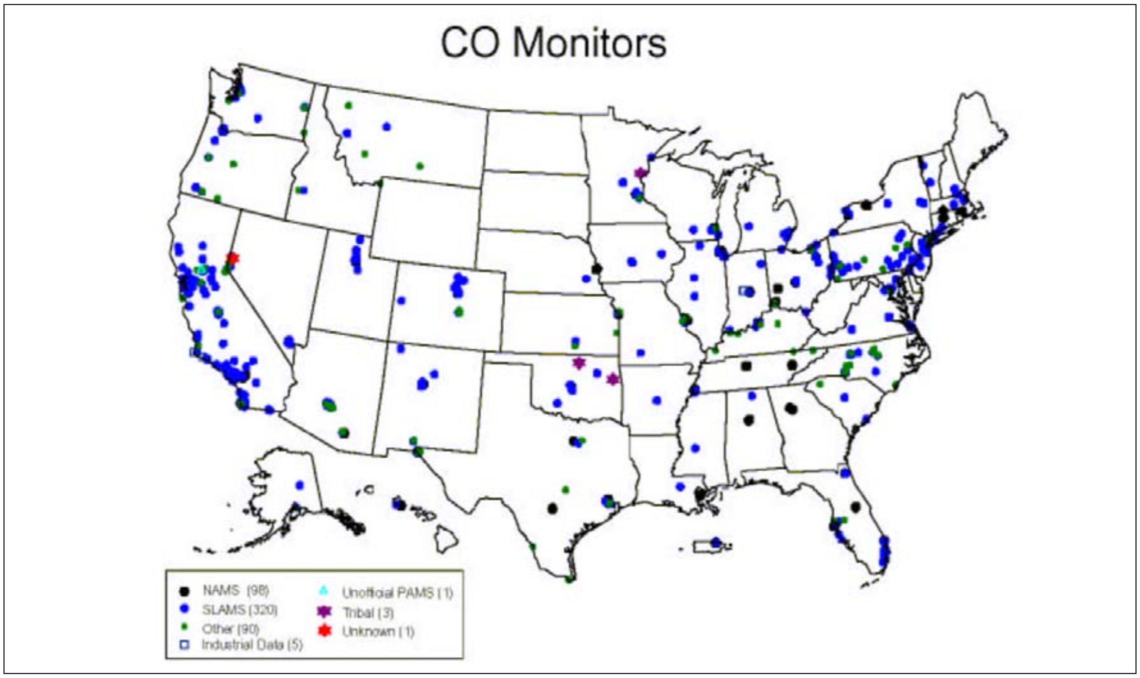

Figure II.4 Surface CO monitoring sites in EPA networks.

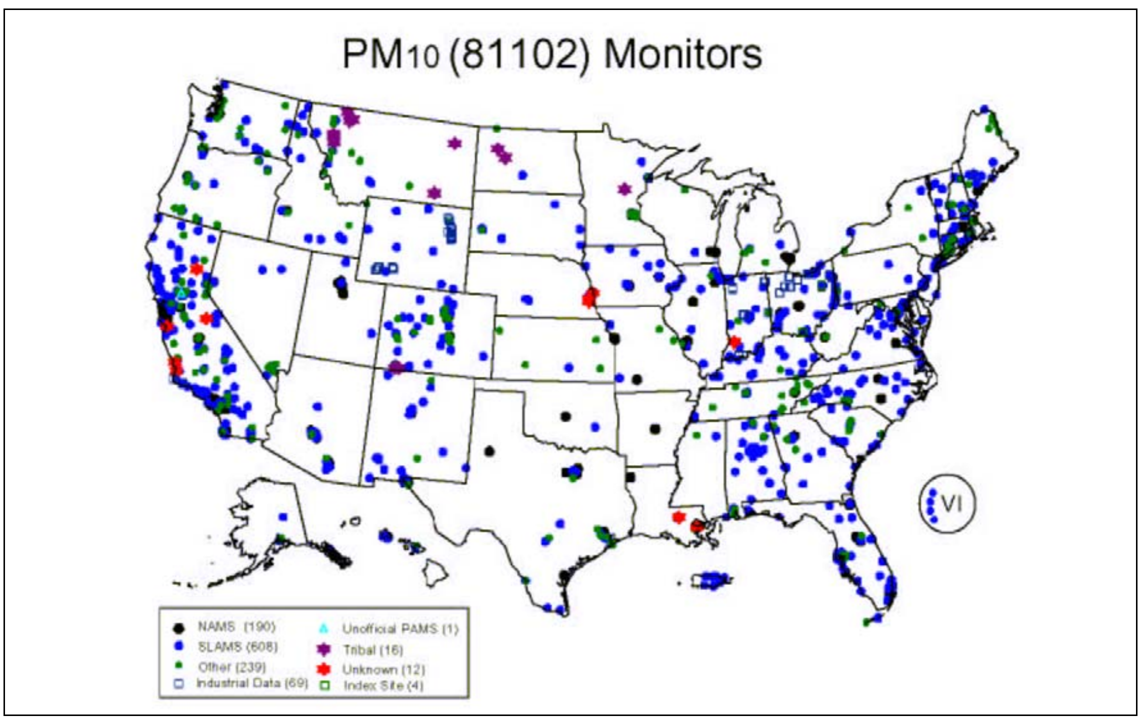

Figure II.5 Surface PM_{10} monitoring sites in EPA networks (81102 is AIRS parameter code).

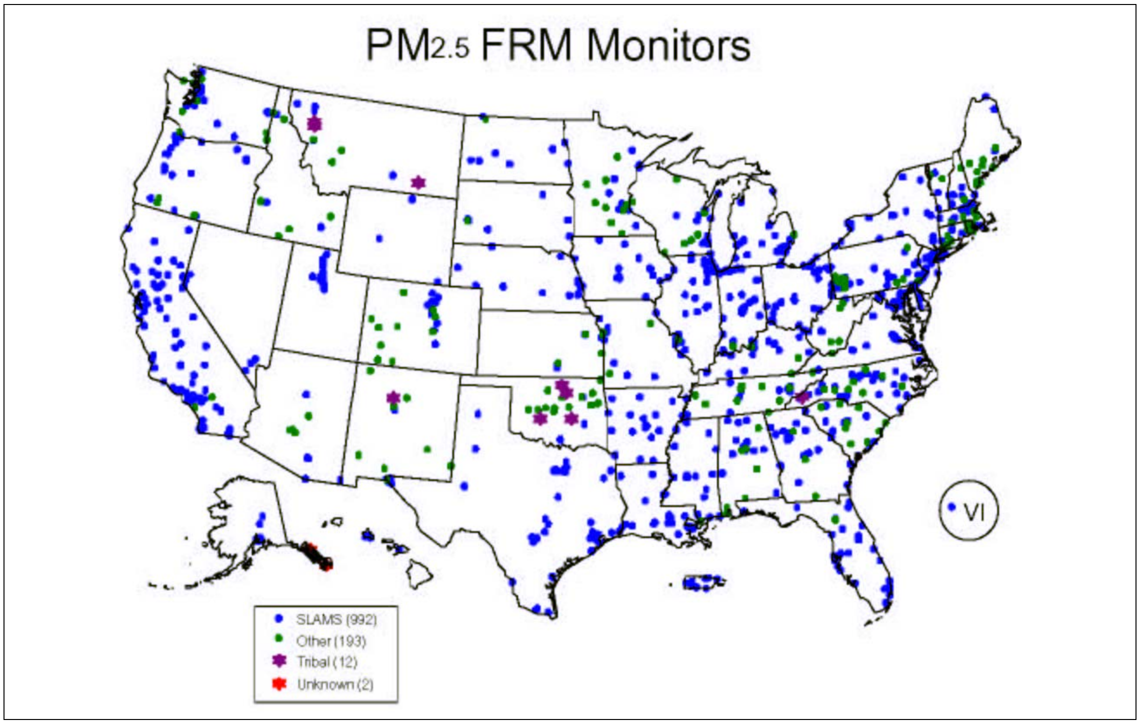

Figure II.6 Surface $PM_{2.5}$ monitoring sites in EPA networks (FRM is Fed Ref Method).

The paradigm for interaction of observations and models feeding into forecasts for policy decisions is summarized in Fig. II.7. The figure illustrates how the surface air-quality data and an assimilation model will interact during INTEX-NA/NEAQS, the Intercontinental Transport Experiment-North America/New England Air Quality Study[4]. This multi-agency (NASA, NOAA, NSF), multiplatform (aircraft, ground-based, shipboard) field campaign is designed to study the evolution of eastern North American air pollution and its export to Europe (http://cloud1.arc.nasa.gov/intex-na/) The experiment is taking place during the summer of 2004 at major staging points in the Midwest and New England. Data from the EPA's AIRNow program (http://www.epa.gov/airnow/) will be used to evaluate the performance of regional and global chemical transport and chemistry models and to support operational decisions. Decisions that the models will support include the planning of flights of multiple aircraft and launching of ozonesondes for the INTEX Ozone Network Study (IONS; see http://croc.gsfc.nasa.gov/intex/intex_ozonesonde.html). IONS will provide a coordinated set of ozonesonde data over eastern North America. Aircraft will be directed toward pollution plumes for further model verification and the collection of comprehensive chemical data to address process questions. Post mission, the aircraft, ozonesonde, and AIRNow data will be re-assimilated in the chemical transport models (CTM) and analyzed for model improvements and to address the scientific goals of INTEX-NA/NEAQS. Clearly, the use of AIRNow in INTEX-NA/NEAQS provides a test for EPA's contribution to both a GEOSS-type international scientific endeavor and a data–model–decision-support paradigm for national chemical forecasting. The international aspect of INTEX-NA/NEAQS is its role in the International Global Atmospheric Chemistry Project/Intercontinental Transport and Chemical Transformation (IGAC/ITCT), an umbrella program that includes Canadian and European participation during the summer 2004 sampling period. INTEX-NA/NEAQS may also serve as a valuable testbed for the joint EPA-NOAA operational air-quality-forecasting program that will provide one- to two-day forecasts of surface ozone and fine particles.

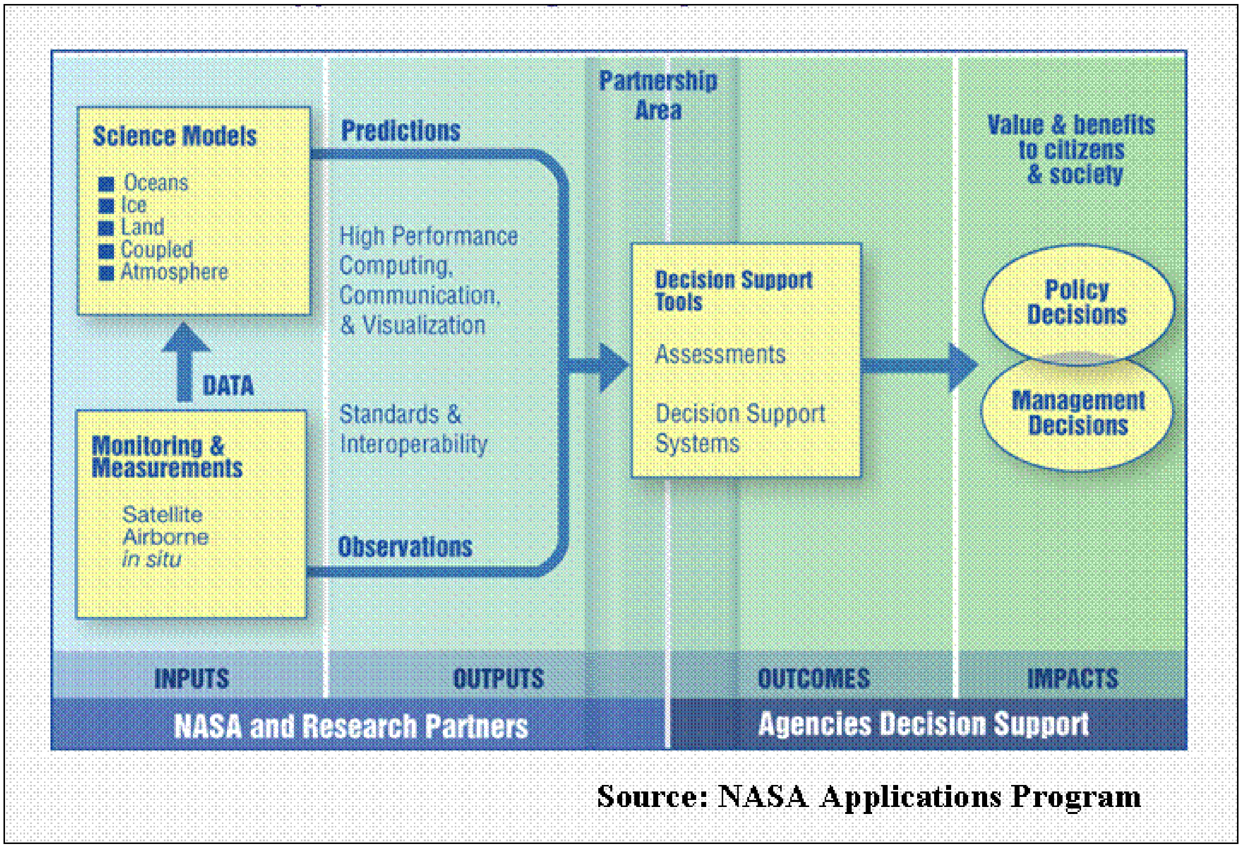

Figure II.7 Paradigm for interaction of observations and models feeding into forecasts for policy decisions.

Options for *in situ* chemical profiling are limited at present, with two types of approaches used. Ozonesondes, launched with standard radiosondes, are the only routinely deployed instrumentation. About 100 stations globally (the U.S. currently has four) launch ozonesondes regularly (2-4 times/month) and transmit their data to the World Ozone and UV Data Centre archive in Toronto, operated by Environment Canada (http://woudc.ec.gc.ca/e/ozone/ozonecanada.htm). The transmittals are for archival purposes, not real-time operational use. The IONS augmentation of soundings in summer 2004 involves combining profiles from a dozen operational sites with forecast fields to predict pollution flow across eastern North America. With a relatively modest investment, the IONS approach could become operational during the peak pollution season. The second *in situ* dataset for chemical profiles is from the Measurement of Ozone and Water Vapor by Airbus In-Service Aircraft (MOZAIC) activity (http://www.agu.org/pubs/crossref/1998/98JD00977.shtml) that collects ozone, CO, and water vapor data from five Airbus A340 in-service aircraft. Observations made at cruise altitude (10-12 km) of long-haul flights will be added to thousands of profiles developed from the landings and takeoffs at cities around the world (http://www.gmes.info/library/files/Forum%20Reports%20and%20Contributions/3rd%20GMES%20FORUM/Parallel%20Session%203/3F_PR3_Cammas_Presentation.pdf). A successor program to MOZAIC, IAGOS (Integration of routine Aircraft measurements into a Global Observing System) (see http://www.aero.obs-mip.fr/mozaic/Conferences/Mozaic2004/Nedelec-MIIIFMPack1.pdf), is due to begin in 2005. This program will result in near-real-time profiles being archived at some point in the next several years.

Research efforts are expected to bring additional vertical profiling on-line in the near future (1-5 years). These options may include inexpensive ozonesondes, chemical-sensing laser technologies used in an Aircraft Communication Addressing and Reporting System (ACARS) (see Moninger et al., 2003), and ground-based lidars. New lightweight, low-cost sensors under development offer an opportunity to turn routine twice-daily radiosondes into ozonesondes at an affordable cost. Such advances may be feasible in two to five years.

Laser technology has led to current deployment of new, highly accurate *in situ* water vapor sensors for use in the ACARS instrument package carried on many commercial aircraft. At present, commercial aviation sampling utilizes low-cost, low-maintenance meteorological packages on long-haul aircraft (with profiles typically from larger cities). Instrumentation of regional jets would greatly enhance the data base. It is anticipated that *in situ* laser technology can be adapted to low-cost, low-maintenance sensors for ozone, CO, and other chemical species. This approach will require five to eight years of development and testing, but offers the important advantage of being able to tap into existing platforms and telecommunications. Lidars capable of remotely sensing profiles of ozone and several other constituents have been under development for at least 30 years. While considerable progress has been made, it is apparent that further effort is needed to improve the accuracy of lidar profiles. Two limitations to lidar are its expense and inability to sense through clouds. Thus, this technology may not be feasible for fully filling gaps left by other components of a multisensor, upper-air network for chemistry.

Vertical profiling of atmospheric chemicals can benefit greatly when combined with concurrent satellite measurements that give column totals and, as research continues, may yield at least some information about vertical distribution (see later discussion in Section II.C). On the other hand, the next generation of satellite data can be expected to give 10-km horizontal resolution for the chemistry of the atmosphere (http://aura.gsfc.nasa.gov/). To use these data effectively, an *in situ* measurement system is needed to provide vertical detail at sufficient intervals in space and time. These *in situ* data can be combined with satellite data to yield good-quality 3-D analyses over broad regions and eventually on the global scale. The combination of satellite and *in situ* measurements using advanced data assimilation techniques mimics methodologies that have proven successful for analyzing diverse types of meteorological data.

3. Ground-based mobile platforms

As discussed above, commercial aircraft routinely act as platforms from which automated observations of meteorological variables are made and reported in flight and during ascent or decent. Automated systems now in the early stages of development may be able in the next two to six years to provide measurements of ozone, CO, and other chemical species using low-cost *in situ* laser technology. At the earth's surface similar opportunities exist based on the same technology. Already, GPS systems are carried on commercial trucks and trains. Environmental sensor packages are being added to these to provide up-to-date information about the temperature conditions of roadways and tracks and the ambient air. The same low-cost laser technology envisioned for use aboard aircraft could be adapted for these surface vehicles as well. Compared to passenger-carrying aircraft, mounting remote-sensing equipment on trucks or trains raises far fewer safety concerns and certification requirements. The potential number of vehicles that could be so equipped is potentially very large and their distribution is widespread. Equipping several major fleets of trucks with nationwide markets would effectively provide a continuous stream of chemistry data that includes all urban areas in the U.S. and the major connectors between them. Such a wide-ranging database, coupled with the existing (e.g., AIRNow) and future fixed networks, would provide a far more representative look at nationwide air quality than is possible today, and might also be assimilated into CTMs.

B. Satellites for Air Quality: Current and Future Technologies

Satellite-based tropospheric trace-gas and aerosol measurements are a recurring theme in the Integrated Global Observing Strategy (IGOS) (see http://ioc.unesco.org/igospartners/; also Barrie et al., 2004) that can be used by EPA to support its mission of improving understanding of the impacts of air pollution. Coupled with global chemical data assimilation systems, these measurements may provide the initial and boundary condition information that is necessary to properly constrain regional air quality forecasts (see Fig. II.8). Use of current and future satellite tropospheric trace-gas measurements should therefore be an important component in developing a national air quality forecasting and assessment capability.

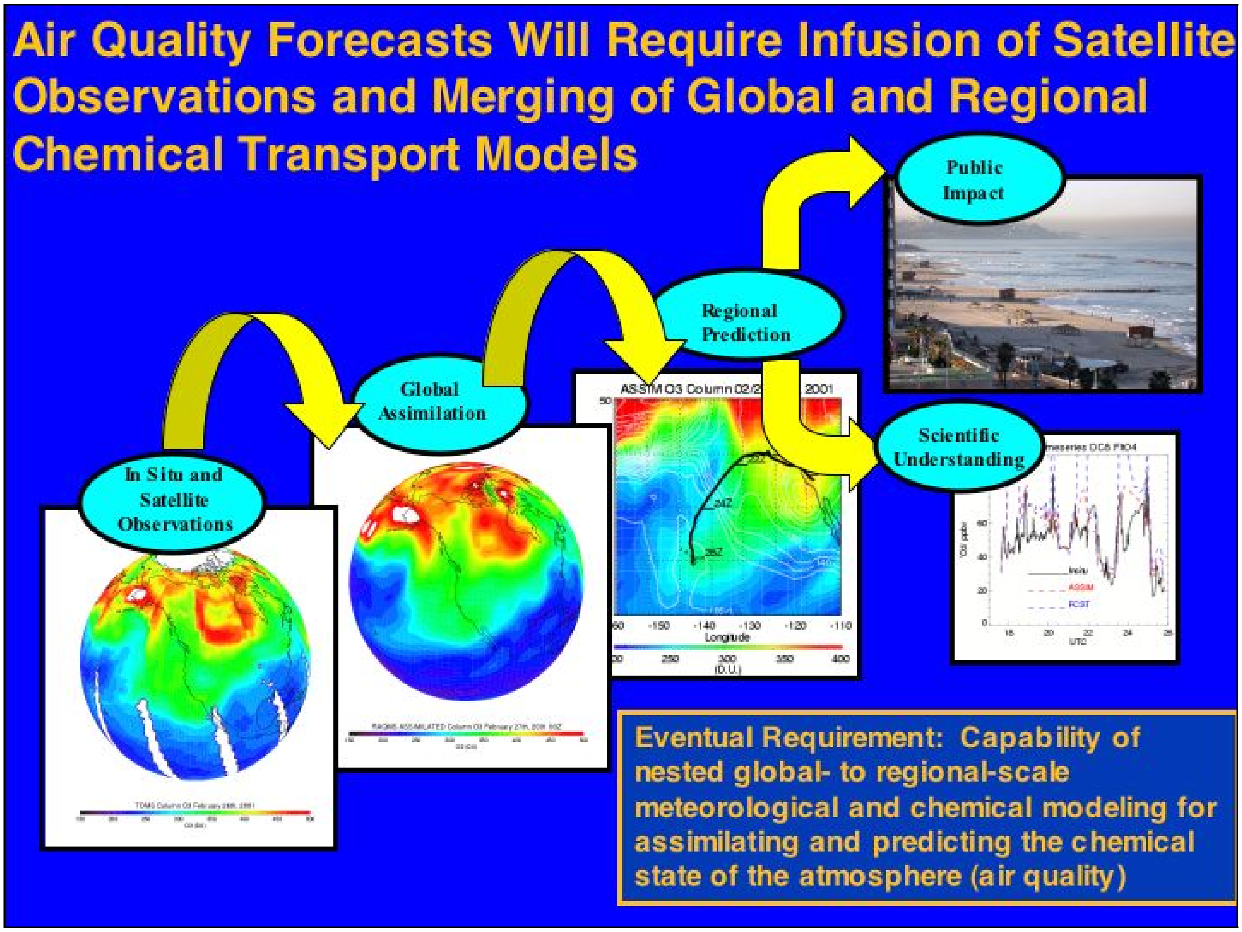

Figure II.8 Schematic diagram outlining the use of satellite measurements in conjunction with *in situ* observations in an assimilation system that can be used both in a decision-support system and for providing useful scientific information for assessment and global change studies.

Table II.1 at the end of this section briefly describes existing, planned, and feasible satellite-based tropospheric trace-gas measurements by NASA and the European Space Agency (ESA). The existing and planned measurements are made from low Earth orbit, providing a swath of data during each orbit with individual measurements on spatial scales of tens to hundreds of kilometers. Future measurement systems that are feasible with current sensor technology include geostationary trace-gas measurements such as the proposed GeoTRACE (Geostationary Observatory for Tropospheric Air Chemistry) instrument, which would provide continuous coverage at high horizontal resolution. (GeoTRACE was proposed to NASA's New Millennium and Earth System Science Pathfinder Programs, but was not selected). Figure II.9 compares the pixel size that could be obtained from such a geostationary platform with the pixel sizes from the existing Total Ozone Mapping Spectrometer (TOMS) instrument and the Ozone Monitoring Instrument (OMI), which was successfully launched on NASA's Aura satellite on July 15, 2004. Although the GeoTRACE proposals included pixel sizes on the order of 5 km^2, it is technically feasible to build an instrument with a "zoom" capability that would be able to generate pixel sizes as small as 1 km^2 for use in detailed specific studies of urban environments.

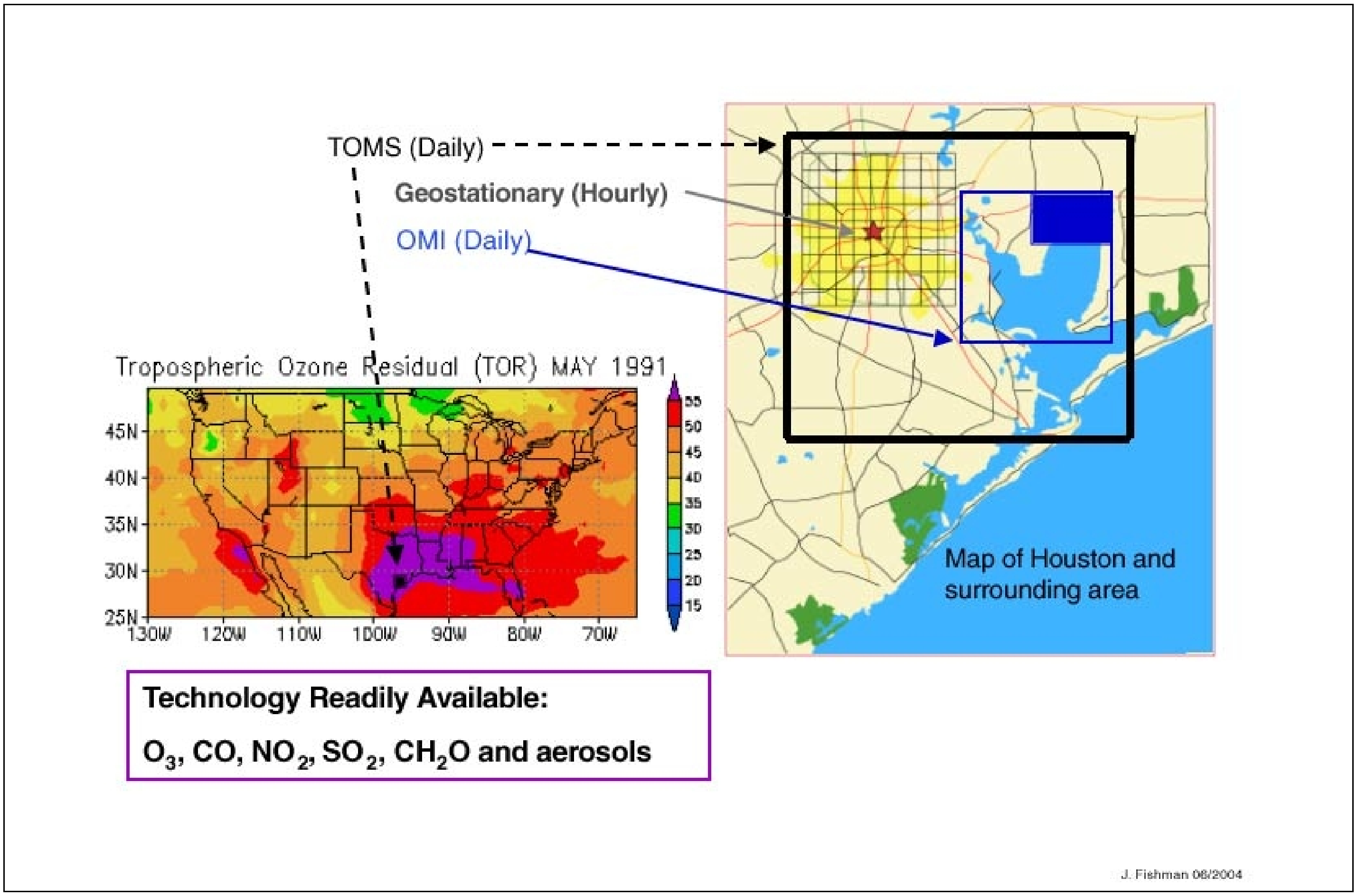

Figure II.9 Diagram illustrating a satellite-derived depiction of tropospheric ozone over the United States and comparing the pixel size used to generate the data using TOMS with pixel sizes that could be available from the planned OMI and proposed GeoTRACE satellites over the Houston metropolitan region. The solid blue pixel is the smallest size pixel that will be provided by OMI; the open blue box is the product that will be generated by the tropospheric ozone algorithm, which averages eight pixels. Units on the TOR color contour plot are Dobson Units and depict the integrated amount of ozone in the troposphere (courtesy of Dr. Jack Fishman, NASA Langley Research Center).

Satellite based measurements of O_3, NO_2, SO_2, HCHO, CO and PM may be available over the next five years from ESA's SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography) and NASA's Earth Observing System (EOS) Aura mission. However, these polar orbiting satellites provide data with sampling frequencies of at best once per day, are unable to resolve diurnal variations in trace-gas concentrations, and have significant data gaps in persistently cloudy areas. Trace-gas measurements from geostationary orbit are the best way to mitigate these sampling issues. High-horizontal-resolution geostationary measurements could provide critical constraints on urban-scale air quality predictions, emission databases (through inverse modeling), and would be ideal for model validation.

Enhanced vertical resolution can be obtained using active remote sensing techniques. The first of these instruments is CALIPSO (Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations), a lidar that will provide ~100-m resolution of aerosols and clouds. Differential Absorption Lidar (DIAL) systems have shown that ozone and water vapor can be measured from aircraft, and are in the development stage for deployment on satellites. Incorporating these high-resolution vertical profiles into a comprehensive spatially coherent distribution through the use of geostationary measurements can be achieved through assimilation techniques.

Effective utilization of new and existing satellite data sets for air quality prediction will also require the development and evaluation of a broad range of global modeling and data assimilation tools of varying complexity. These tools are consistent with the recommendations of the IGOS theme report on atmospheric chemistry measurements (IGACO: Integrated Global Atmospheric Chemistry Observations; see Barrie et al., 2004). Furthermore, the IGACO strategy recognizes the importance of regional networks feeding into a global observing network. Thus, as part of implementing the Group on Earth Observations (GEO) findings, we endorse the specific recommendation of IGACO "to proceed with the immediate implementation of satellites in support of air quality applications. In particular, priority should be given to a satellite system that includes geostationary instruments since only these offer the necessary time and spatial resolution to support air quality forecasting."

C. Recommendations Concerning Measurements and Sampling

- AIRNow is an excellent, underused resource for the GEOSS scientific community and for the emerging U.S. air quality forecasting effort. Its use in these two regimes is imperative.

- Vertical *in situ* profiling and satellite retrieval of chemical constituents, with evolving data coverage and potential technology improvements, should be an integral part of a GEOSS data initiative that will benefit EPA in the next decade and beyond. Vertical profiles must be increased in number and frequency, at least during peak pollution season. Three-dimensional observations will need to be made by EPA, other U.S. agencies, and the international community. For EPA's modeling and chemical forecasting efforts, these data will have to be available in near-real time.

- The optimal observing strategy, as endorsed by the Committee on Earth Observation Satellites (CEOS) (http://www.ceos.org/) and the Global Climate Observing System (GCOS) (http://www.wmo.ch/web/gcos/gcoshome.html), needs to incorporate satellite observations, soundings, measurements from commercial platforms, and AIRNow-type surface data, together with assimilation modeling to give a 3-D picture in near-real time. Highest priority should be given to ensuring that an optimal observing system is in place to support this strategy. As part of the implementation of the GEO findings, we support the specific recommendation of IGACO "to proceed with the immediate implementation of satellites in support of air quality applications. In particular, priority should be given to a satellite system that includes geostationary instruments since only these offer the necessary time and spatial resolution to support air quality forecasting."

Table II.1 Selected past, current, and future remote sensing instruments used to determine the amounts and distributions of constituents in the troposphere

Instrument	Name	Vertical extent of measurement	Horizontal resolution, domain	Temporal revisit	Target constituent/ property for air quality	Platform (operation period or future launch schedule)
Current and past instruments						
GOME*	Global Ozone Monitoring Experiment	TR and ST	40 x 40 km^2, 40 x 320 km^2 swath	Once every 3 days	Tropospheric columns for O_3, NO_2, BrO, SO_2, HCHO, clouds, and aerosols	ESA-ERS-2 (1995-present)
MODIS	Moderate Resolution Imaging Spectroradiometer	Surface to space	0.25-1 km , 2330 km wide swath	Once every 1-2 days	Aerosol column optical thickness, aerosol type (sulfate, biomass burning) over land	NASA Terra (1999), NASA Aqua (2002)
MISR	Multi-angle Imaging SpectroRadiometer	Surface to space	0.275-1.1 km, 141 x 563 km^2 swath	Once every 9 days	Aerosol properties (angular radiance dependence)	NASA Terra (1999)
MOPITT	Measurement of Pollution in the Troposphere	TR columns, layers	22 x 22 km^2, 22 x 640 km^2 swath	Once every 3 days	Total column of CO, CH_4 ; CO layers	NASA Terra (1999)
SCIAMACHY*	Scanning Imaging Absorption spectrometer for Atmospheric ChartographY	TR and ST	30 x 60 km^2	Once every 6 days	Tropospheric columns for O_3, NO_2, CO, BrO, SO_2, HCHO, clouds, and aerosols	ESA Envisat (2002-present)
TOMS*	Total Ozone Mapping Spectrometer	Total O_3 Column	~100 km	Daily	Total O_3 column	Nimbus 7 (1978-1993), Meteor 3 (1991-1994), Earth Probe (1996-present)
Future instruments scheduled to be launched						
OMI*	Ozone Monitoring Instrument	ST profiles, TR columns	12 x 24 km^2	Once per day	Tropospheric columns for O_3, SO_2, HCHO, NO_2, and aerosol	EOS Aura July 2004
TES	Total Emission Spectrometer	ST profiles, TR layers	26 x 42 km^2	~Once every 2 days	Tropospheric columns for 0_3, NO_y, CO, SO_2, CH_4	EOS-Aura July 2004
CALIPSO	Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations	ST profiles, TR profiles	0.3 x 0.3 km^2	Not operated continuously	Aerosol density and radiative properties	NASA CALIPSO (September 2005)

Instrument	Name	Vertical extent of measurement	Horizontal resolution, domain	Temporal revisit	Target constituent/ property for air quality	Platform (operation period or future launch schedule)
Anticipated future instruments						
GeoTRACE	Geostationary Observatory for Tropospheric Air ChEmistry	TR layers	4 x 4 km^2, 8000 x 4000 km^2 (entire North American continent)	Once per hour	Tropospheric columns for O_3, NO_2, SO_2, HCHO, CH_4, clouds and aerosols;: tropospheric columns and layers for CO	Potential future Earth Probe
Geo-SCIAMACHY	Geostationary SCanning Imaging Absorption spectrometer for Atmospheric ChartographY	TR layers	25 x 25 km^2, entire Earth disk, European view	Twice per hour	Tropospheric columns for O_3, NO_2, H_2O, SO_2, HCHO, CH_4, CO, clouds, and aerosols	Potential future ESA mission

*For several of instruments (GOME, SCIAMACHY, TOMS, and OMI), total column amounts are measured and tropospheric quantities are determined using an independent measurement to subtract the integrated stratospheric amount of the trace constituent. This “residual” methodology provides an integrated tropospheric column].

III. Data Assimilation[5]

A fundamental, widely recognized problem in air quality forecasting is the lack of complete 3-D chemical data with which to initialize air quality forecast models. Even if some data are available (such as surface ozone), it is not clear at present how to balance the chemical system with these chemical data, although new applications of four-dimensional data assimilation (FDDA) should be applicable (Carmichael et al., 1999). Most current air quality forecast methods re-initialize meteorology but keep chemistry on the grid from previous forecasts. However, unless the pollutant fields are totally dominated by short-term local production, this technique is inadequate; initialization of the previous chemical fields is critical to forecast success. Without some connection to reality, forecast errors in the chemistry continue to grow. While new profiling and satellite measurement techniques might improve chemical initialization in the future, these types of remotely sensed data are likely to be limited for at least the next five or more years.

A. Physical Data Assimilation

One partial solution to the lack of chemical data is to try to minimize forecast errors in the chemistry through a physical data assimilation preforecast period. While chemical data for assimilation are scarce, there is a wealth of physical *in situ* and satellite data that can be used to improve modeling of the physical atmosphere. *In situ* data assimilation techniques have used meteorological observations to recover critical parameters, such as soil moisture (e.g., Pleim and Xiu, 1995). New satellite data assimilation techniques have been developed and initially tested as part of EPA control strategy *a posteriori*-type simulations to specify data on finer scales than those available from terrestrial meteorological observations. These have been used to retrieve critical parameters to modeling the physical atmosphere, such as surface moisture (McNider et al., 1994), stomatal resistance (Jones et al., 1998) and surface grid-scale heat capacity (McNider et al., 2004) using geostationary operational environmental satellite (GOES) infrared (IR) skin temperature tendencies.

Model-predicted clouds are highly parameterized, and their spatial position and optical properties are subject to large error. GOES-derived insolation and albedo can be used in place of modeled clouds to improve model performance (Diak and Gautier, 1983; McNider et al., 1995a). Finally, photolysis fields can be specified using GOES broadband transmittance and IR cloud-top temperatures in photolysis models (McNider et al., 1998).

In physical data assimilation, the strategy is to use all available physical observations from the previous day to constrain the physical atmosphere as close as possible to reality. The chemical forecast is then rerun with this new physical atmosphere. This new chemical state is used as the chemical initial conditions for the next true air quality forecast period. Ideally, this 24-36-hr assimilation period reduces the chemical initialization errors. This is especially critical in the near future where chemical data are not going to be available to reduce chemical initialization errors.

There is a pressing need to conduct research to develop optimal physical data assimilation techniques for re-creating the physical atmosphere to improve the chemical initial conditions. This would include testing and refining satellite and *in situ* data assimilation techniques in an operational mode. Special tests in a simulated operational mode could be carried out against special observation periods in the air quality community, such as NARSTO-NE-OPS (NorthEast Oxidant and Particle Study; Philbrick et al. 2002), TEXAQS2000 (http://www.utexas.edu/research/ceer/texaqs/), Southern Oxidant Study (SOS) 1999 (http://www.etl.noaa.gov/programs/1999/sos/), and New England 2002 (http://www.al.noaa.gov/neaqs/)

B. Chemical Data Assimilation

Forecasts of atmospheric chemical concentrations are increasingly important. At the moment, a variety of methods (statistical, expert systems, and CTM-based) are used to forecast regional air quality and support air pollution abatement strategies (over 120 cities in the U.S. are issuing air pollution forecasts). An increased ability to forecast air pollution has important societal benefits. Furthermore, the use of chemical forecasting in support of comprehensive atmospheric chemistry and air pollution studies is becoming the standard mode of operation. Forecasting also provides one of the best model evaluation opportunities, as the model cannot be tuned in advance. There is a pressing need to develop and evaluate data assimilation tools in order to improve the accuracy and lead time of chemical forecast products. This area of research needs to address the assimilation of *in situ* (surface, aircraft, etc.) and remotely sensed (lidar and satellite) chemical concentrations (and column-integral data) in the preparation of chemical forecasts. It also needs to address the question of the optimal chemical measurement strategies for making chemical forecasts.

One aspect should focus on the creation of applications testbeds that consist of airsheds with excellent measurement networks, as they provide an ideal opportunity to evaluate the effectiveness of data assimilation on model performance. A systematic evaluation of the impact of the assimilation of individual chemical species and sets of species on model prediction skills (see Daescu and Carmichael, 2003) could be performed. An important outcome of such research would be to test and demonstrate the operational aspects of assimilation tools, and also to provide guidance on what species to focus assimilation efforts on in order to improve operational forecasts of air quality.

Another key element in chemical data assimilation is the sparseness of chemical measurements, in contrast to the established infrastructure of meteorological measurements (e.g., surface observation networks, the global radiosonde network, and a host of dedicated satellite observations) that are assimilated into meteorological models. The number of observations available for chemical assimilation is typically several orders of magnitude smaller than the number of variables in the model. Thus, the spatial and temporal distribution of the observations plays 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. The assimilation tools can be effectively used to help design such chemical measurement strategies. Specifically, effort must be devoted to applying assimilation tools to the problem of optimal network design and adaptive measurement strategies (see Daescu and Carmichael, 2003).

C. Data Assimilation and Emissions

Another important aspect of data assimilation relates to emission estimates in support of air quality forecasting (this includes anthropogenic heat emissions as well as conventional pollutant emissions). Emissions often represent the most significant source of model uncertainty. The assimilation and adjoint techniques potentially developed in this type of research could be deployed to optimally estimate the emissions. Biomass burning is an excellent example of the critical role of emissions. Air quality in many parts of the world is negatively impacted by emissions associated with biomass burning activity. The forecasts of the smoke intensity and future location of the plume depend explicitly on the location and magnitude of sporadic fires. Assimilation of satellite data on fires, burned area, and tropospheric constituents such as CO and aerosol optical depths can be used to produce optimal estimates of these emissions.

Measurements provide a means to evaluate the quality of the estimated emissions. As discussed in Section VI, the standard method of using measurements and models to assess emissions is to (1) start with an emissions inventory constructed from activity data and emission factors (i.e., a bottom-up approach); (2) run the chemical transport model in the forward mode and compare predicted values with the observations; and (3) attempt to draw inferences about the emissions inventory from the degree of agreement between the predicted and observed values; i.e.,

Input emissions → Run CTM model → Produce predicted fields →
Compare predicted with observed → Draw emission inferences

The above sequence can of course be reversed, starting with the observations and then using the model to estimate the emissions needed in order to have the model-predicted fields match (in some optimal manner) the observations (i.e., inverse emissions modeling). The inverted emissions can then be compared with the *a priori* (bottom-up) estimate and inferences drawn (e.g., Kasibhatla et al., 2002; Palmer et al., 2003). In these studies, inversions using surface observations of CO identified the need for significantly larger biomass (~100% higher), and biofuel and fossil fuel sources (~50% higher) of CO in Asia. These large differences in estimated emissions are not limited to Asia. Recent studies in Houston, TX (i.e., the Houston 2000 study) have found that emission estimates of key reactive hydrocarbons must be increased by a factor of 5 to match calculated levels of ozone to observed levels.

Uncertainty enters into all levels of emission estimates. It is widely recognized that emissions inventories, models, and ambient air measurements are all uncertain, so perfect matching of the observed and predicted means is not expected. However, our limited capabilities to formally bring these uncertainties into analyses and assessments cause evaluations of the consistency between the modeled and observed distributions to remain qualitative only. It is necessary to develop a more formal data analysis and assimilation framework to enable a quantitative evaluation and estimate of emissions for use in air quality forecasting. Figure III.1 illustrates the analysis needed to meet this research need.

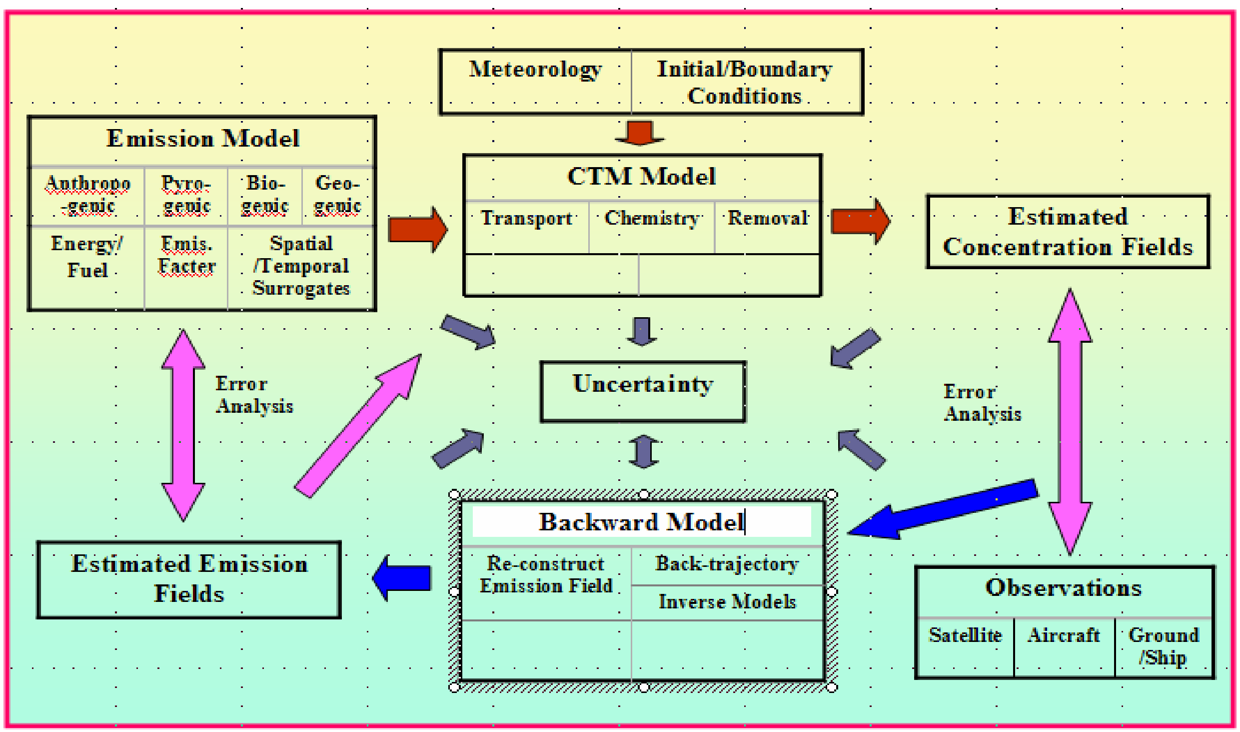

Figure III.1 Improvements in the quantification of emissions requires creative combinations of bottom-up and top-down approaches.

D. Recommendations Concerning Data Assimilation

EPA, within the GEOSS framework and in partnership with NASA and NOAA, should embark upon a research plan that emphasizes the development of advanced data assimilation capabilities in air quality modeling. The research elements should focus on developing general computational frameworks to facilitate the close integration of measurements and models in CTM systems. These techniques and analysis tools should be applied to the interpretation of observational data, the design of optimal observing systems, and forecasting activities. The following research activities are envisioned:

- Develop and explore various techniques for data assimilation.
- Apply and test these techniques in campaign mode (field study), in both forecasting and post-analysis mode.
- Apply the methods to targeted measurement systems (satellites, surface sites, airborne and volumetric systems, etc.) to evaluate information content in measurements and sensitivity in the model-world, and to aid in the design of observation strategies to improve chemical forecasting capabilities. For example, given finite resources, is it better to increase the number of surface sites or to add measurements of additional parameters at a few existing sites, or is there perhaps more benefit in obtaining information above the surface through vertical soundings, lidar, etc.? These are important, fundamental questions in the design of measurement systems.
- Further develop and apply these techniques for use in inverse analysis to produce better estimates of emissions.
- Develop testbeds for data assimilation, including incorporation of techniques into the Weather Research and Forecasting (WRF) system and other models identified for operational use, and to test research as well as operational aspects of data assimilation.

IV. Integrated Biogenic Assessments[6]

A. Discussion

Development of effective predictive tools for environmental quality and human health requires a comprehensive understanding of the earth system. The biosphere component is a source and sink of particles and gases that affect air quality. Biosphere-atmosphere emission and deposition rates are strongly influenced by direct (land management) and indirect (climate change) human activities. Volatile organic compounds (VOCs) and CO emissions from live and decaying vegetation, nitric oxide (NO) emissions from soils, and emissions of particles, CO, NO, and VOCs from fires are important for air quality, and emission inventory methods/models are available for generating inputs to air quality models. The models that predict emissions are currently being driven by satellite-derived variables, and there is considerable potential for future improvements.

A predictive capability for air quality requires a full understanding of anthropogenic and biogenic inputs and processes in addition to meteorology and atmospheric chemistry. The factors controlling variations in emissions from terrestrial ecosystems include

- land cover (e.g., leaf area, leaf age, vegetation type, fuel loading, and soil type);
- land use and land management practices (e.g., burning, harvesting, thinning, fertilizing, irrigation);
- exposure to ecological stresses (e.g., drought, flooding, pollutants, herbivory, and disease); and
- weather and climate (e.g., temperature, solar radiation, winds, humidity, and precipitation).

All of these driving variables can and should be available from a global earth observation system.

Although a complete understanding of ecosystem processes is not yet in hand, it is critically important that we understand the extent to which air quality affects ecosystem processes and vice versa. Furthermore, a comprehensive predictive capability for air quality can be achieved only through integrated studies of interactions involving the atmosphere, biosphere, and anthrosphere. Focused integrative efforts require expertise in several disciplines, such as boundary-layer dynamics, atmospheric chemistry, plant physiology, soil biochemistry, microbial ecology, hydrology, and ecosystem processes. Developing appropriately comprehensive science plans is challenging, as achieving a truly interdisciplinary strategy requires integrated and creative thinking and flexibility. These plans must fully recognize the limitations of current knowledge bases and assumptions. Such plans must also foster experimental design that promotes assessments of the impacts and feedbacks of multiple stresses.

Long-term, integrated field measurement programs are required in order to quantify:

- atmospheric inputs and their effects on biogenic emissions;
- biogenic emissions and their roles in ecosystem processes and atmospheric photochemistry;
- ecosystem response to chronic and episodic stresses and atmospheric feedbacks; and
- impacts of multiple stresses and feedbacks.

Reactive nitrogen emissions and atmosphere-ecosystem-atmosphere feedbacks (Fig. IV.1) are an example of important anthrosphere-atmosphere-biosphere interactions that can significantly affect air quality. Nitrogen is a limiting nutrient and it plays a central role in regulating the structure, function, and composition of terrestrial ecosystems. As reactive nitrogen levels increase in the atmosphere and in terrestrial and aquatic ecosystems, interactions between nitrogen effects and pollutant feedbacks on carbon uptake and biogenic emissions are of growing importance. However, the coupling of nitrogen deposition to the carbon cycle and to atmospheric photochemistry is not yet fully understood and is not adequately represented or even included in current models. As the Intergovernmental Panel on Climate Change (IPCC) has stated, "studies of the combined effect of air quality, nitrogen, elevated CO_2 and carbon cycling are needed before we can answer the interrelated questions of separability, attribution and stability in the growing number of regions affected by changing atmospheric chemistry" (Intergovernmental Panel on Climate Change, 2003).

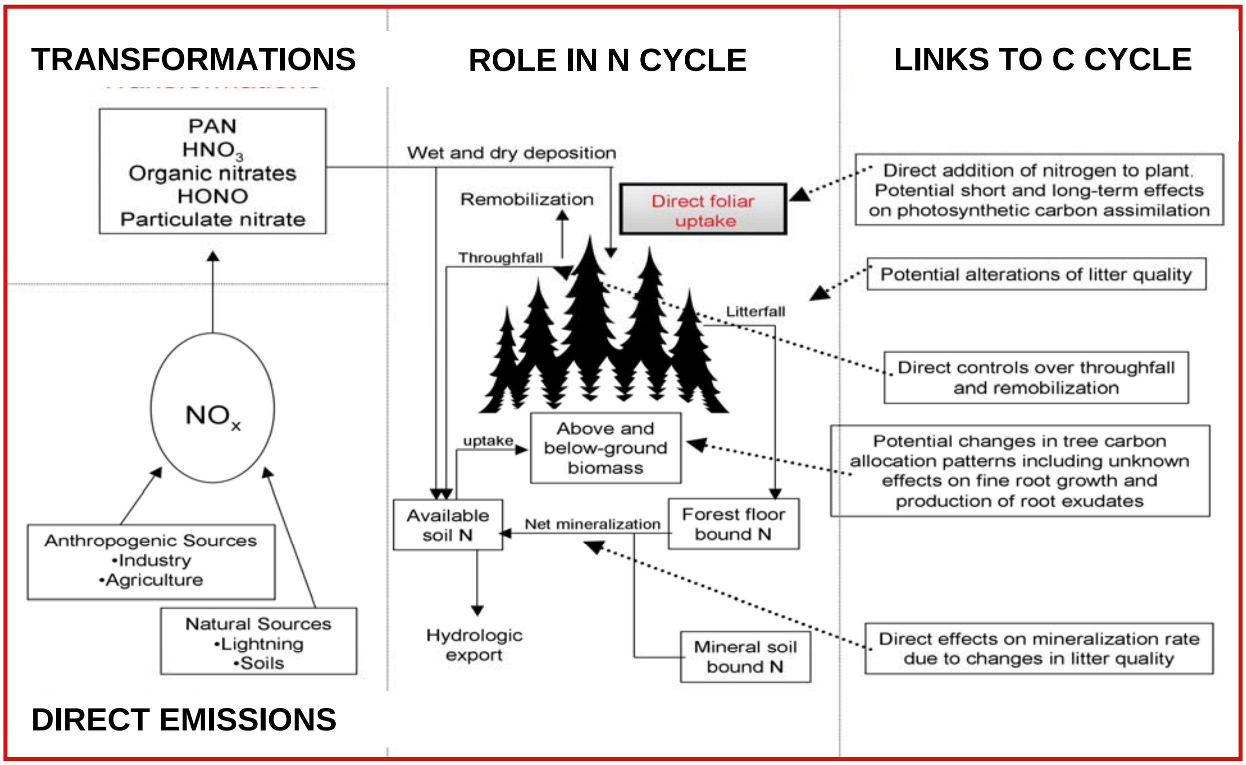

Figure IV.1 A schematic of the "life cycle" of gas-phase nitrogen, including dominant emissions sources, tropospheric transformations, role in the overall nitrogen cycle, and important linkages to the carbon cycle (Carroll et al., 2003)

Process studies are valuable tools, and significant progress has been made through such investigations at a number of sites—for example, Hubbard Brook, Harvard Forest, Blodgett Forest, the Program for Research on Oxidants: Photochemistry, Emissions, and Transport (PROPHET) site of the University of Michigan Biological Station, and Duke Forest (e.g., Goulden et al., 1996; Hirsch et al., 1996; Pardo and Driscoll, 1996; Goldstein et al., 2003, 1998; Munger et al., 2004, 1998; Lefer et al., 1999; Faloona et al., 2001; Hurst et al., 2001; Pippin et al., 2001; Thornberry et al., 2001; Aber et al., 2002; Apel et al., 2002; Driscoll et al., 2003; Spaulding et al., 2003; and Di Carlo et al., 2004). Similarly valuable are manipulation studies involving open-chamber and open-air fumigation experiments, such as those conducted at the Free-Air Carbon Dioxide Enrichment (FACE) sites. For example, studies at the Aspen FACE site in Rhinelander, WI, involving elevated O_3 and elevated CO_2, are significantly advancing the understanding of atmosphere-forest interactions. In each of the above examples, significant infrastructure is in place, and in many cases a number of important environmental parameters are continuously measured (e.g., Dickson et al., 1998; Karnosky et al., 2003, 2002, 1999, 1998; Curtis et al., 2000; Isebrands et al., 2001; King et al., 2001a,b; Holton et al., 2003).

The understanding of whole ecosystem function has greatly improved through flux measurement networks. For example, FLUXNET (Fig. IV.2) is a global network involving 216 micrometeorological tower sites where eddy covariance methods are used to measure the exchanges of CO_2, H_2O, and energy between terrestrial ecosystems and the atmosphere (http://www.daac.ornl.gov/FLUXNET/fluxnet.html). Data are also collected on site vegetation, soil, hydrologic, and meteorological characteristics, and the sites are operated on a long-term and continuous basis. Within the United States, the AmeriFlux network (sites are shown in Fig. IV.2) has been established to quantify the magnitude of net annual CO_2 exchange in major natural and managed ecosystem/biome types, to determine the response of CO_2 fluxes to changes in environmental factors and climate changes and to elucidate the processes controlling CO_2 flux and net ecosystem productivity (http://public.ornl.gov/ameriflux/).

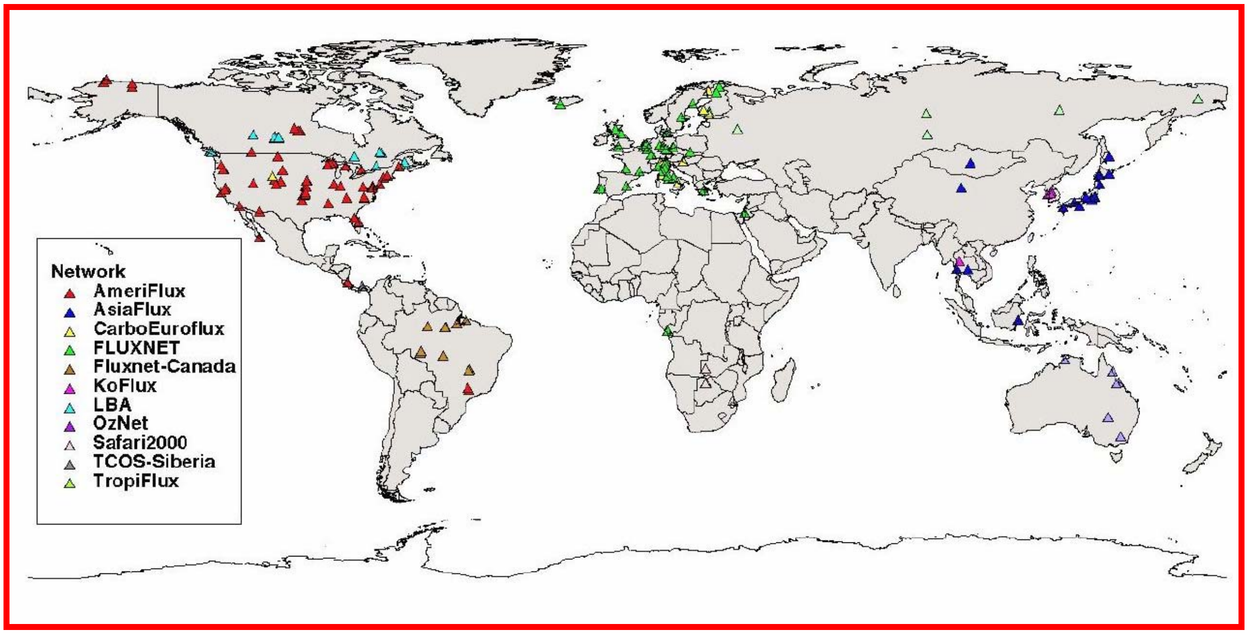

Figure IV.2 Locations of FLUXNET sites (http://www.fluxnet.ornl.gov/fluxnet/maps.cfm)

Rather than starting from scratch, the establishment of measurement sites and networks for air quality forecasting and for further investigations of atmosphere-ecosystem interactions should be accomplished by leveraging on existing sites and networks whenever possible. Existing sites and networks could, in many cases, be expanded (e.g., to include chemical species measurements, or to add manipulation studies) and extended in the vertical or horizontal. Furthermore, participation in—or leveraging on—the development of the National Ecological Observatory Network (NEON), should be considered as an effective strategy in developing the measurement networks that are required for air quality forecasting and other goals of the global observing program. NEON, as proposed by NSF, would establish a national platform for integrated studies and monitoring of environmental parameters at all spatial and temporal scales (e.g., National Research Council, 2004).

B. Recommendations Concerning Integrated Biogenic Assessments

- As EPA develops its GEOSS Science Plan, it should adopt a process that requires interdisciplinary strategies and flexibility, recognition of the limitations of current knowledge and assumptions, and an experimental design that promotes assessments of the impacts and feedbacks of multiple stressors.

- This Science Plan should include a multiple-site network made up of a variety of experimental investigations, including monitoring, process studies, and manipulation studies.

- This Science Plan should strongly leverage on other national networks (e.g., AmeriFlux) and sites where process studies are underway, and other national infrastructure investments, such as NEON.

V. Surface Characterization and Parameterization[7]

A. Introduction

Land surface characterization is critical to the prediction of temperature, moisture, boundary-layer heights, and wind fields. In turn, these physical aspects impact the emission, production, loss, and concentration of air pollutants and their precursors. Many of the characteristics needed are not routinely observed, and some are as much model heuristic as they are physical parameter. Because of the heterogeneity in land surface characteristics, even parameters that are measured (e.g., temperature) are not at sufficient resolution to guide model results or be used for evaluation. Thus, it is critical to air pollution predictions that land surface characterizations be made as robust as possible using available information. Satellite data, because of its high resolution and broad coverage, provide a potential source for describing land use and its physical behavior. Also, in a global context it may be important that models and techniques be developed to use products from a GEOSS measurement system, since such models would be transferable to many locations.

B. Specification of Parameters

Simple land surface models (LSMs) such as Blackadar (1979) used bulk parameters such as thermal inertia and moisture availability to characterize the behavior of the land surface. Complex LSMs, such as the Biosphere-Atmosphere Transfer Scheme (BATS) (Wilson et al., 1987), or the NCAR model (Chen and Dudhia, 2001), are based upon intertwined physical and biological processes that are used to predict the thermal and moisture fluxes at the surface. The more complete land surface models can also include basin-scale hydrologic models (McHenry and Peters-Lidard, 2002; Crosson et al., 2002). All of these models have several parameters that can potentially be prescribed by geostationary and polar-orbiting satellite platforms:

- Albedo
- Insolation
- Photosynthetic active radiation (PAR)
- Leaf area index (LAI)
- Biomass heat capacity
- Land/water boundaries
- Vegetative fraction
- Land-use classification

Some of these parameters are direct radiative quantities (e.g., albedo, insolation, PAR); they are thus highly suited for measurement by radiometric instruments on satellites, and have substantial histories of success (e.g., Gautier et al., 1980; Diak and Gautier, 1983). The most direct and perhaps most important parameter for air quality modeling may be insolation. Current meteorological models have a difficult time specifying the radiative properties of clouds and predicting clouds in the right place and time, yet this parameter is critical to boundary-layer development and temperature prediction. Satellites, on the other hand, are well suited to specifying the reflective radiative properties of clouds and land surfaces and thus can make robust measurements of albedo and insolation.

C. Simple Land Surface Models

Simple LSMs, those without extensive vegetative canopy and hydrological submodels, can be constrained to match satellite observations of temperature with other information specified by observations, such as planetary boundary layer (PBL) height (Brutsaert et al., 1993; Diak and Whipple, 1995). Also, simple land surface models can be constrained during dynamic assimilation periods

(McNider et al., 1994, Pleim and Xiu, 1995; see also Section III of this document). For the simple land surface models, the scientific objective is to use satellite data to partition sensible and latent heat fluxes without describing the physical and biological details of how this partitioning comes about. Tests have been made using GOES tendencies down to 4 km to recover moisture availability and bulk heat capacity (McNider et al., 1994). Multiple passes of polar orbiters might be used to provide higher resolution products if conditions can be assumed to be steady during the time tendencies are calculated from polar-orbiting satellites (Carlson, 1986).

D. Complex Land Surface Models

Complex land surface models including basin-scale hydrologic models can potentially be constrained to match satellite observations during assimilation periods. Here the objective is to specify as well as possible the different parameters needed in the land surface scheme, but use satellite observations in an assimilation period to constrain the model to match direct observables. For example, all land surface models in the end produce a radiative or skin temperature, T_s. The outward flux from the surface, $\varepsilon\sigma T_s^4$, is a direct observable by the satellite in clear window channels (with some atmospheric correction). This satellite measurement can then be used to adjust parameters in the model so that the model $\varepsilon\sigma T_s^4$ agrees with the satellite $\varepsilon\sigma T_s^4$ or so that tendencies in these quantities agree. Several parameters that are important to the land surface that can perhaps be specified or constrained by satellite observations are given below:

- *Stomatal Resistance:* Through stomatal release, plants control a considerable fraction of the moisture flux, especially in humid climates. Specifying the details of the plant physiology and associated parameters is difficult. However, stomatal resistance for plant canopies can perhaps be recovered by use of midmorning satellite skin temperature tendencies (Jones et al., 1998). Other methods, such as those of Carlson (1986), using polar orbiter data may be applicable.

- *Surface Evaporation:* Surface evaporation is critical to the partitioning of latent and sensible heat in land surface models. Bulk available moisture for bare soil or from leaf surfaces can be recovered by use of midmorning satellite skin temperature tendencies (Wetzel et al., 1984).

- *Root-zone Moisture:* For complex land surface schemes, root-zone moisture is critical to specifying the partitioning of latent and sensible heat fluxes in surface energy budgets. Root-zone moisture for vegetated surfaces has been recovered using *in situ* surface temperature and moisture (Pleim and Xiu, 2003, 1995). This technique can perhaps be expanded to use satellite skin temperatures.

- *Thermal Inertia/Heat Capacity:* The thermal inertia of surfaces in models is very important in determining the rate at which the model surface heats or cools. This is especially true of the rate of cooling in the nocturnal boundary layer. Carlson et al. (1981) outlined a technique for recovering thermal inertia using multiple passes of polar-orbiting data. Mesoscale model grid-scale heat capacity or thermal inertia can potentially be recovered using evening skin temperatures (McNider et al., 2004).

- *Leaf Area Index:* Leaf area is related to stomatal evapotranspiration rates. In the past, surface modelers have utilized the type of *in situ* information available in heavily instrumented forests, such as LAI as a parameter related to evapotranspiration. However, satellites cannot directly measure LAI, so some relation between the satellite observable and LAI must be constructed. A more direct path would be to relate the satellite observables to transpiration rates. This may be a future path, as GEOSS observations become more readily accessible and processed.

- *Soil Surface Moisture:* Surface moisture in soils is important to evaporation rates and thus to the partitioning of latent and sensible heat fluxes. Microwave techniques (Lakshmi et al., 1997) have promise for directly measuring moisture in bare soils. However, characteristics such as soil type, vegetation, etc. make some of the current measurements difficult to interpret and use in model formulations.

E. Use of Direct Satellite Measurements

The land surface is responsible for a large part of the losses of air pollutants from the atmosphere. For long-term simulations it is critical that the deposition losses be correctly specified. Vegetation and especially the stomatal uptake of pollutants are important, and satellites can be used to help specify vegetative parameters such as LAI. Further, since stomatal uptake is highly related to evapotranspiration through open stomata (Finklestein et al., 2000), satellite estimates of evapotranspiration may be useful.

F. Characterization of Heterogeneity

1. Sub-grid variability

Models by necessity deal with integral averages over a model grid. In general, first-order closure models are unable to characterize sub-grid-scale variability, especially variability due to heterogeneity in surface forcing. High-resolution satellite data at a finer scale than the model grid have the potential to examine the variation in skin temperature across the grid. This may be especially important in understanding the context of a single *in situ* measurement in the grid domain.

2. Land/water interfaces

Coarse-grid models have difficulty handling land/water boundaries for complex coastlines. Satellite remote sensing may help define the integral effect of the coastline in the model.

3. Leaf-out

One of the most critical factors in land surface modeling is the timing of leaf-out in the spring (Fitzjarrald et al., 2001). This is a function of soil temperature, sun angle, etc. Satellite data can detect and define this critical parameter.

G. Parameter Sensitivity

Theoretical studies are needed to understand land surface model behavior as a function of model parameters in order to determine when parameter retrieval strategies might be successful and when they might fail. This requires an analysis of the coupled atmosphere-surface system as a function of parameters (Wetzel et al., 1984; Carlson, 1986; Diak, 1990; Henderson-Sellers, 1993). In the past, this was done using multiple model runs as sensitivity analyses. Today, the mathematical community has highly sophisticated bifurcation analysis techniques that use numerical continuation to trace out parameter dependence. These techniques (McNider et al., 1995b) can find critical regimes where assimilation might fail because of steep gradients in parameter dependence or even multiple solutions.

H. Recommendations Concerning Surface Characterization and Parameterization

The physical atmosphere is important to the fidelity of air pollution simulations, whether in control strategy testing or in air quality forecasting. In case studies, satellite data have been shown to improve the quality of air quality simulations. With this in mind, we make the following recommendations:

- Current geostationary data products and polar orbiter data products should be more widely used in air quality forecasting endeavors to improve the specification of the land surface and insolation fields.

- For processes that have fast temporal changes, such as solar insolation and moisture availability, it is recommended that greater emphasis be placed on geostationary products.

- A specific infrastructure recommendation is for EPA and NASA to support a satellite processing center that can make satellite products available to the public-, academic-, and private-sector modeling communities.

- While newer polar-orbiting instruments have recently been the focus of research in both NOAA and NASA, geostationary observations offer a unique ability to specify many of the critical parameters needed in air quality models. Under GEOSS, NASA and EPA should put more emphasis on developing tools, data products, and satellite archives for the enhanced use of geostationary data.

VI. Strategies for Improved Emissions Estimates[8]

A. Inventory Methodology and Uncertainties

Developing accurate emission estimates is critical to atmospheric chemistry studies and to the design of effective air quality forecasting and environmental management strategies. Quantifying emissions is very difficult, as the estimates depend on the quantity and quality of the fuel used, the manner in which it is consumed, and what control technologies are utilized. In North America and Europe, emission estimates have been under development for several decades, and while estimates of certain species are believed to fairly certain (e.g., SO_2), others still remain problematic (e.g., nonmethane hydrocarbons [NMHC] from industrial sources). Further complicating the issue is that the chemistry of the atmosphere is controlled by total emissions, so natural emissions such as biogenic emissions, as well as those from biomass burning, *must be quantified,* as discussed in Section IV.

Emission inventories are usually developed using a bottom-up approach, where information on energy use is combined with emission factors. The details of inventory development, estimation of uncertainties, and a summary of previous emission estimates are presented in Streets et al. (2003). The emissions of a particular species are estimated as a product of the activity rate, the unabated emission factor, and the removal efficiency of any applied emission abatement technologies, using the following equation:

$$E_{j,k} = \sum_{l.m.n} A_{j,k,l,m}\ ef_{j,k,l,m}\ \left(1-\eta_{j,l,m,n}\alpha_{j.l.m.n}\right) X_{j,k,l,m,n}$$

where *j,k,l,m,n* = species, region, sector, fuel/activity type, abatement technology; E = emissions; A = activity rate; ef = unabated emission factor; η = removal efficiency of abatement technology n; α = maximum application rate of abatement technology n; and X = actual application rate of abatement technology n. A large number of parameters are needed to define and characterize each source, fuel, and sector category. Uncertainties enter into all aspects of the emissions estimates, and as a result the inventories are highly uncertain.

Estimates of uncertainty in Asian emissions are shown in Fig. VI.1 and VI.2 below. The first figure depicts results involving three source categories (biofuels, biomass burning, and fossil fuel), and 52 regions/countries. Each source category was further broken down into fuel type (e.g., dung, agricultural waste, and wood in the biofuel category, and different grades of coal, oil, gas, and diesel, etc. in the fossil sector). Uncertainties in U.S. emissions fall between those for Japan and Other East Asia.

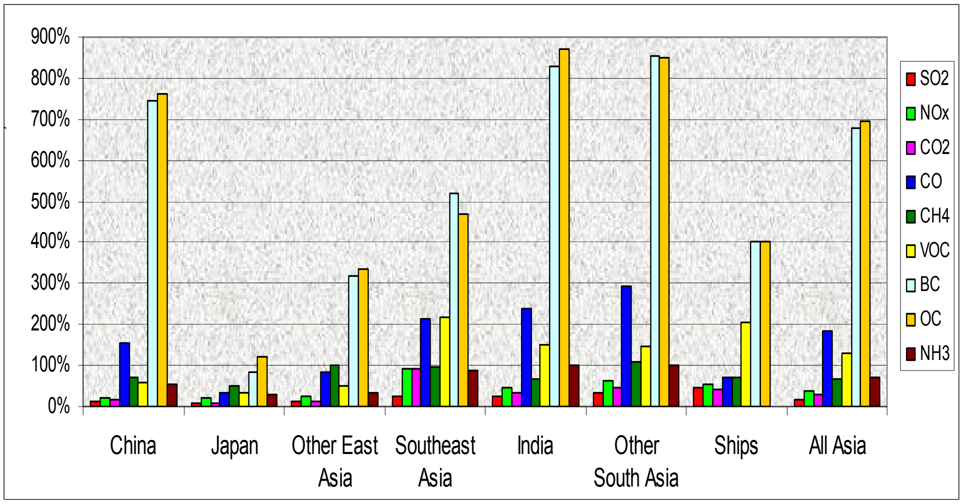

Figure VI.1 Uncertainty results from an Asian chemical transport modeling example utilizing emissions information from 27 chemical species (8 major species and 19 nonmethane volatile organic compounds [NMVOC] subspecies). The percentages on the y-axis indicate uncertainty in the emissions estimates.

Emissions of black carbon (BC; Figure VI.2), a key air pollutant linked directly to health effects and an important constituent of global warming, has an uncertainty of 100%-300%. There are clear needs to improve the accuracy and reduce the uncertainty in emission estimates. This requires improved methodologies, expanded and updated observations, and closer integration of observations and models. These issues are expanded below.

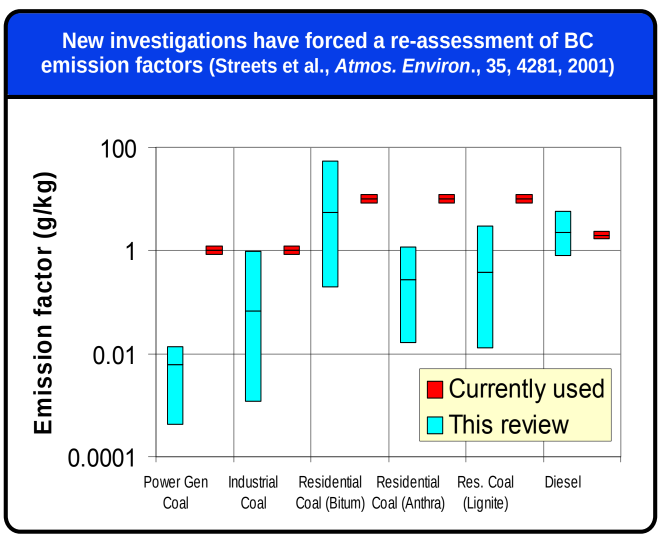

Figure VI.2 The variations in emission factors in the reported literature. These variations constitute an important contribution to the uncertainty of modeling results.

B. Dynamic Models of Surface-Atmosphere Exchange of Air Toxics, Ozone, Particles, and their Precursors

Estimates of the exchange of gases and particles between the earth surface and the atmosphere are critical components of the models used to predict atmospheric distributions of air pollutants. Past estimation efforts have generally used static emission inventories to provide inputs for air quality models. The next generation of air quality models needs to incorporate dynamic emission models that directly couple the physical, chemical, and biological components of the earth system. Dynamic emission models are required to simulate potential earth system feedbacks and should provide more accurate predictions of future emissions. A requirement of an effective global earth observation system is that it provides the inputs needed for dynamic emission models.

Dynamic emission models should be used for both urban and rural landscapes. Models should integrate the various emission types (e.g., fires, biogenics, mobile sources, point sources) so that the activity of one source is reconciled with each of the others. The landscape databases used for these emission models (e.g., urban, industrial, agriculture, forest) should be harmonized with each other and with the land surface component of weather and climate models used to determine transport and dispersion.

The emission and uptake of an individual biological organism can be modeled using a metabolic approach that describes the key controlling processes. This has been extended to the ecosystem level and used to describe biogeochemical cycles, including surface-atmosphere gas exchange, on regional and global scales. The same approach should be adapted to describe urban metabolism and predict pollutant emission from entire cities and regions. The spatial resolution required for categorizing areas into landscapes with different emission potentials is not well known but is probably 1 km or higher. Satellite-based global 1-km land cover databases are already available and are expected to be improved in the future.

The components of an integrated dynamic emission and uptake model include (1) databases of georeferenced surface characteristics, (2) driving variables that are calculated online by the weather and chemistry models, and (3) model components that describe the response of emissions and uptake to weather and air quality and that are directly coupled with the weather and chemistry model components. The result is an earth system model where weather, air quality, and surface chemical exchange are coupled.

C. Top-Down Emissions Methods

Satellite observations may provide a means of real-time assessment of emissions using a top-down approach. Using present-day satellite capabilities, column-integrated information can be obtained with a resolution of better than 50 km (see Section II). This information could be used to assess integrated emissions on this scale and thus might be used to validate how well the inputs into models agree with the integrated amounts used in the models. The important trace-gas species that can be measured from space are CO, HCHO, NO_2, and SO_2. CO, NO_2, and SO_2 are criteria pollutants, and NO_2 is an important precursor to ozone formation, another criteria pollutant that can also be measured from space. The measurement of formaldehyde (HCHO) on this scale from the OMI, GeoTRACE, and GeoSCIAMACHY satellites is expected to provide important insight into the integrated amount of isoprene released, since its oxidation is the dominant source of HCHO in the background atmosphere.

Coincident measurements of NO_2, CO, and HCHO will help define urban versus rural emissions by examining the ratios among these species. The use of regional/global-scale satellite information can be used to identify widespread transient emissions, such as those from wildfires and prescribed burning for land clearing. Plumes from such events can likewise be tracked and then separated from localized inputs into regions.

In addition to satellite observations, *in situ* measurements are required to directly validate the processes included in dynamic emission models, for two reasons: (1) such measurements are needed for chemical species that are not presently measured by satellites; and (2) the concentration distributions of reactive gases observed by satellites are the integrated product of emissions, deposition, transport, and chemistry, and so are not a direct validation of surface fluxes. There have been substantial advancements in direct flux measurement techniques (e.g., eddy covariance) for particles (numbers and chemical composition) and gases (speciated VOC, NO, peroxyacetyl nitrate [PAN], NO_y, NH_3, ozone), but continued improvements are required to enhance the accuracy and reliability of some techniques. Flux measurement systems deployed on above-canopy (for forests) or building (for urban) towers can be used to validate model predictions of diurnal, seasonal, and interannual variations. Aircraft-based systems can be used to validate predictions of regional distributions.

D. Recommendations Concerning Strategies for Improved Emissions Estimates

- Global earth observations, including both satellite observations and *in situ* measurements, should be used in a top-down approach to validate and improve emission models.

- High-resolution global-scale databases of driving variables should be provided by the global earth observation system in order to replace the current, static emission inventory approach for both biosphere and anthrosphere sources with dynamic emission models that are coupled within weather and air quality (earth system) models.

VII Special Urban Challenges[9]

A. Background

Air quality predictions and assessments are of great value in addressing health concerns in urban environments, home to the majority of the world's populations. It is important that the information provided on urban air quality be accurate and at a scale commensurate with the needs of population exposure. Air quality variations are scale dependent. For a variety of reasons, the scale dependency will differ for different air pollutant species. Air quality modeling provides the tools to generate information needed for regulatory implementation and for driving human health exposure assessments; however, the model resolution must be scaled appropriately to the urban application. Pollution episodes are typically associated with stagnating, weakly forced meteorological fields. In such situations, control of the flow and ventilation is dominated by the local conditions. The size of pollution hot spots and spatial gradients in urban areas are on the order of 1 km. It is very important to model at the scale of the problem.

A next-generation prototype modeling paradigm for urban areas is based on a hybrid modeling approach. The Community Multiscale Air Quality (CMAQ) modeling system (U.S. EPA, 1999), with modeling at grid sizes of ~1 km and concentration distribution functions describing within-grid variability, is being developed and tested in Houston and Philadelphia (Ching et al., 2004). The latter study in Philadelphia considers both sub-grid source contributions and inherent chemical variability due to photochemistry in a turbulent mixing environment. The meteorological and emission preprocessors to CMAQ will benefit by being better "urbanized" (e.g., ~1 km grid scale) for more accurate gridded transport, flux, and dispersion modeling.

For general meteorological modeling, the treatment of surface characteristics is typically based on land use classes. Urban simulations generally apply a roughness approach based on dominant land use class. In high building density regions of urban areas, introduction of canopy modeling parameters is being investigated to provide more accurate modeling of flows and emission sources. The presence of buildings, impervious surfaces (roads, parking lots, etc), landscape greens and water bodies in urban areas strongly influences the meteorology, especially under weakly forced flow conditions. Recent investigations explore replacing the dominant land use method for estimating roughness with canopy-drag modeling. They incorporate a land surface model for improved modeling of soil moisture (degree of dryness, and spatial heterogeneity of land use types). These tests resulted in more realistic simulations of transport and dispersion fields in urban areas. This was achieved by incorporating gridded flux parameters that introduce the effects of urban structures and canyons consisting of canopies of buildings, trees, roads, and other urban features (Dupont et al., 2004; Otte et al., 2004). However, it is noted that generating the urban canopy parameterizations (UCPs) for operating these advanced models requires specialized databases with high-resolution building and ancillary information. Such databases are rapidly becoming available from photogrammetric methods and airborne lidar mapping imagery, although extrapolations are still needed in data-poor regions. The quality of the gridded UCPs depends on the level of detail of the input data on urban features. With the introduction of UCPs in models, new modeling issues arise, such as (1) the need to distinguish between mixing within, above, and between canopy and above-canopy layers; and (2) the need for advanced numerical filtering of spurious numerical perturbations. It is anticipated that refinements to current community multiscale modeling systems such as the Mesoscale Model Version 5 (MM5) will be extended to the next-generation WRF modeling system, currently under development.

B. Building on the Current State of Knowledge

Given that fine-scale urban building databases are becoming available for most major metropolitan areas (e.g., the 133-city Homeland Security Infrastructure Program [HSIP] Study database), the panel recommends development of gridded sets of UCPs for all major metropolitan areas. There is also a need to evaluate the sensitivity of urban model predictions to the complexity of different urban canopy parameterizations. In addition, in view of the proliferation of detailed fluid modeling studies within urban canyons, there is the opportunity to link urban mesoscale models with Large Eddy Simulations/Computational Fluid Dynamics (LES/CFD) models. Advanced treatments of underlying surfaces in canopy models are being developed and tested. Such models, coupled with urban canopy databases, provide a capability for predicting changes in urban climate due to changes in urban morphology. These advanced systems will provide a basis for better understanding the feedbacks between urban built areas, heat emissions, and local meteorology; between urban air pollution and atmospheric chemistry and radiation; and between urban and regional scales.

C. Opportunities

Given the need for advancing the next generation of urban-scale modeling, EPA is undertaking activities leading to a capability for fine-scale air quality modeling in urban areas (Ching et al., 2004); this effort is based upon many of the new advancements described above. The activities include specifying and characterizing variability in meteorology, emission, and air quality fields. This work is motivated in large part by the need to explore and build upon the merits of linking air quality model outputs to exposure models for performing risk-to-health assessments. Such a capability will require additional inputs and also activities to test and evaluate these emerging capabilities. The GEOSS program can contribute in the areas of model inputs and model evaluation in urban modeling, using data from satellite, aircraft, and mobile sampling platforms as well as surface and vertical profile information.

Regarding fine-scale meteorology and air quality modeling, satellites can provide fine detail (~1 km grid resolution for complete urban domain-wide characterization of the normalized difference vegetation index [NDVI] and surface radiance [skin temperatures]) for evaluation of urbanized mesoscale model predictions. This information will provide diagnostic evaluation of how well urban models predict surface energy budget partitioning. Specialized analyses of satellite data can provide information on key parameters such as urban-scale albedo, land-use parameters such as surface heat capacity, and perhaps information on surface gradients and temporal variations of surface moisture across the urban domain.

Information on regional scales for criteria pollutants and air toxics from satellite studies can provide either input or confirmatory details regarding pollutant inflow, and confirmatory details regarding the modeled outflow from urban areas.

The use of aircraft platforms that measure surface radiance parameters can provide fine-scale characterizations for more spatial detail where heterogeneity in the urban land surfaces is pronounced. Airborne and ground-based lidar systems can provide spatial variability of some pollutants such as ozone and SO_2 for model evaluation and emission estimation purposes. Aircraft and surface mobile sampling can provide a basis for characterizing and determining the within-grid pollution variability. Surface monitors and vertical profiles from fixed sampling sites will provide a vertical dimension to model evaluation in urban areas. Implementation with prototype testbeds in specific urban areas will facilitate testing many modeling, observing, and data assimilation approaches. Extension to other urban areas and megacities can proceed once the advanced neighborhood-scale urban modeling paradigm is developed, tested, and evaluated from these testbeds.

D. Recommendations Concerning Special Urban Challenges

The information base required to support, maintain, and improve air quality management in urban areas will become increasingly complex and comprehensive, given the growth and change in population and in urban size and surface characteristics. Air quality forecasting, exposure, and risk assessments and urban planning will require advanced monitoring and the introduction of new, innovative modeling concepts, including assessments of the pollutant variation at model sub-grid scales. Critical to the design of this information base is a recognition and understanding of the variety of scales that influence meteorology, emission source dispersion, and subsequent air quality, and the roles played by individual and sets of urban morphological structures.

Careful planning, partnerships, and collaborations among EPA, NASA, and NOAA can achieve considerable advancements toward meeting future urban air quality related health and environmental goals. The panel recommends exploring such partnerships. We also recommend creating urban testbeds to develop, improve, and evaluate urban data needs, measurement and sampling strategies, and modeling methods.

VIII International Air Quality Forecasting[10]

A. Introduction

EPA can make a vital and lasting contribution to GEOSS through (1) the contribution of observations from existing and planned platforms; (2) new strategies for observation and four-dimensional atmospheric-chemical data assimilation; (3) advancing concepts for characterizing emissions; and (4) improvements in data sharing and management. At the same time, the GEOSS effort would benefit substantially from a major focus on the emerging fields of numerical air quality prediction (NAQP) and ecological indicator prediction (EIP). Here we discuss only NAQP, but EIP is a logical extension that would move beyond a strictly atmospheric focus to an emphasis on the whole earth system.

B. Air Quality Forecasting: A Brief U.S. History

EPA has been involved with state- and local-agency programs to provide operational air quality forecasts since about 1996 (U.S. EPA, 2004). To date, these programs have relied on forecaster experience and a range of computer-based forecast tools to develop operational forecasts. These tools have primarily consisted of statistical-correlation approaches developed and refined by either commercial or academic providers. In the late 1990's, the ability to produce numerical-photochemical-model based forecasts in real-time was developed (McHenry et al., 1999, 2004), and this approach has become an important new tool, assisting many state forecast agencies. In 2001, NOAA launched an "early start" pilot program to evaluate existing numerical tools that could be used for an emerging Federal air quality forecast model effort (McHenry et al., 2004; McKeen et al., 2003). By 2003, EPA and NOAA entered into a partnership to operate a modeling system based on NOAA's operational Eta mesoscale meteorological model (Janjic, 1994) and EPA's CMAQ model (U.S. EPA, 1999). This system is currently being tested at the National Centers for Environmental Prediction (NCEP) for the Northeast U.S. and is targeted for deployment over that domain in September 2004 (Davidson, 2003). NOAA has announced a five-year plan to expand the domain to encompass the entire U.S. and eventually add fine particles to the numerical forecast model while migrating toward a WRF-based system (WRF WG11, 2004).

C. Air Quality Forecasting: Current International State of the Art

Several European Union countries, Canada, and Australia currently have air quality (AQ) forecasting capabilities. Canada and Australia have both deployed NAQP systems ahead of the numerical efforts occurring in both the private and public U.S. sectors. These initiatives have been driven by the more localized transnational air quality issues intrinsic to Europe, by the stricter Canadian public health standards for ozone, and by pollution problems unique to Australian coastal cities. Many other countries are also developing or contemplating forecasting capabilities, including statistical and box-model-based urban approaches. Countries participating in the GEOSS effort should be extensively surveyed to understand how these forecast systems, along with systems based in the U.S., can contribute and serve as foundations for further development and deployment of new measurement and improved forecast-modeling capabilities in GEOSS.

There are many opportunities to partner this GEOSS initiative with other international activities. One good example is the GAW Urban Research Meteorology and Environment (GURME) project (see http://www.cgrer.uiowa.edu/people/carmichael/GURME/GURME.html), a new World Meteorological Organization (WMO) activity under the auspices of the Global Atmospheric Watch (GAW). It was initiated at the 1999 WMO Congress at the request of the National Meteorological and Hydrological Services (NMHSs) with the goal of enhancing the capabilities of the NMHSs related to urban air pollution. One important objective of GURME is to build "capacity" related to meteorological and AQ forecasting for urban environments. Toward this objective, GURME has organized a series of AQ forecasting workshops. The objectives of these workshops are as follows:

- Obtain an overview of the current operational air quality forecasting tools and their requirements, including measurement needs;
- Obtain an overview of the current status of relevant research that can be expected to improve operational models in the next few years;
- Develop recommendations for the direction of improving air quality forecasting; and
- Present the above information in such a way that it is useful for NMHSs that are starting or developing their air quality forecasting activities.

A breadth of perspectives has been sought, from those with ongoing AQ forecasting efforts and those with interests in initiating and/or expanding activities. Meetings have been held in China, Moscow, Malaysia, Mexico, and Chile.

Some of the important findings that have emerged from these GURME workshops are the following:

- There is growing experience and interest in air quality forecasting.
- Air quality forecasting and management share a common science-base.
- Improvements in AQ forecasting will come from (1) better understanding of local situations and key processes (e.g., local winds, boundary-layer dynamics); (2) increasing accuracy in the meteorological forecasts; (3) the act of doing—increased experience will lead to enhanced capability; and (4) improvements in emission estimates.
- Resolution matters in many circumstances, but there are limits to when increasing resolution increases forecast quality.
- Simple statistical models can outperform complex numerical models at present in AQ-data-rich cities, but there are additional reasons to pursue numerical grid-based models.
- Emissions data are an important but not a limiting factor in *beginning* AQ forecasting.
- Tools commonly used to improve meteorological forecasts need to be explored in the air quality forecasting arena (e.g., data assimilation, ensemble forecasts).
- Satellites are a key element of air quality forecasting systems, as they hold promise for providing key information that can be used anywhere around the globe.
- There are barriers (perceived and real) to initiating and sustaining AQ forecasting activities.
- There are a variety of tools for forecasting air quality, but the many tools can present a confusion of choices when deciding how to get started in forecasting.
- It is of critical importance to define the reasons why air quality forecasting activities are undertaken, and to define the roles of the end-users and the various institutions involved.

These workshops have resulted in common recommendations calling for:

- An emphasis on capacity building, and the need to undertake additional capacity building/training initiatives focused on air quality forecasting
- Assistance in fostering national coordination, specifically focused on interfacing the meteorological and AQ communities
- Articulating and advocating the necessary and complementary roles of research and operations

D. The Challenges

There are four major challenge areas that must be addressed to achieve successful international system of observations and modeling: basic infrastructure, meteorological characterization, emissions characterization, and global NAQP systems.

1. *Challenge1: Basic infrastructure*

The complexity of air quality forecasting is greater than that of weather forecasting. While nations have been active in weather forecasting for many decades, air quality forecasting is in its infancy. Advances in air quality forecasting will greatly benefit from interagency and international collaboration. EPA is in a position to make important contributions to and benefit from partnerships with GEOSS countries that have air quality issues resulting from industrialization and urbanization (urban megacities and downwind rural areas) and who share an interest (and have expertise) in air quality forecasting. EPA, in collaboration with other U.S. agencies (e.g., NOAA, NASA), partner nations, and the private sector should work toward the development of testbeds, data sharing, and even technology transfer.

A focus on international air quality forecasting could become an application *par excellence* of the global GEOSS enterprise, enabling participating nations to more accurately assess and warn of the impacts of adverse air quality, including traditional criteria pollutants, particles, and toxics. Integrated approaches that provide downscaling from global-regional scales through the mesoscale to the urban scale could be most useful. Global models would be run to provide boundary and initial conditions for simple and complex regional-to-urban air quality models, with statistical models serving as a baseline and for bias correction. This focus would encourage "in kind" data sharing among GEOSS participants.

There are at least four basic infrastructure challenges that must be addressed if GEOSS is to make a substantive contribution to the international air quality forecasting enterprise.

Societal receptivity

Implementation of a successful and sustainable international forecasting focus within GEOSS will depend on overcoming numerous societal challenges, such as

- adequate financial commitment;
- a commitment to public air-quality education, access to information, and outreach to affected communities;
- appropriate governmental infrastructure to make and distribute air quality forecasts; and
- decision-making and/or policy structures to deal with incentives, regulations, and penalties.

Measurement and monitoring networks

Implementation of reliable and extensible air quality forecasting depends upon an adequate real-time meteorological and air quality measurement capability. Such data streams could be an important contribution of GEOSS. More advanced (upper air, remote sensing) capabilities could emerge as EPA testbeds develop. Also, continuously improving forecast capabilities, including development of chemical data retrieval and chemical data assimilation, could be a valuable technology transfer contribution of GEOSS.

Computing environments

The capacity to obtain, manage, and sustain the hardware, software, and networks needed to collect and disseminate ground-based monitoring data and possibly to initialize, run, archive, and disseminate information from forecast models is a critical infrastructure requirement for any GEOSS-based NAQP system in a participating country.

Personnel expertise

Expertise is needed to successfully deploy and maintain ground-based monitors and their data streams; to produce and disseminate public forecasts; and to install, run, and manage forecast model software and forecast products.

2. *Challenge 2: Meteorological characterization*

Air quality forecasting requires a basic meteorological infrastructure. In situations where there is limited local information, regional- to mesoscale and even urban-scale meteorological data streams may be provided by downscaling of NAQP forecasts. These NAQP products can provide increasing value with respect to accurate air quality forecasting, because they improve the skill of high-resolution meteorological forecast models. Collection and utilization of meteorological observations within GEOSS, from platforms managed by a partner country, is the second challenge.

3. Challenge 3: Emissions characterization

Projects like the Global Emissions Inventory Activity (GEIA) project (Graedel et al., 1993) have contributed estimates of global emissions at relatively coarse scales, probably not sufficient for the higher-resolution modeling systems needed for effective air quality forecast guidance. Traditional inventories may exist within sovereign national borders but may be reserved for a variety of reasons; contribution of such databases to GEOSS may or may not be practicable. Therefore, the third challenge is to develop methods to characterize the emissions that provide overall forecast value but do not impinge upon the sensitivities of participating nations.

4. Challenge 4: Global NAQP systems

The goal of numerical air quality prediction within GEOSS is to provide a system that produces and disseminates a routine set of information in near-real time, utilizing current and next-generation environmental observations and forecasts flowing into and from a global GEOSS database. The National Research Council Board on Atmospheric Sciences and Climate (BASC) encouraged the U.S. to develop such a routine forecast capability within its borders (see http://books.nap.edu/books/0309064155/html/R1.html#pagetop). Global extension of such a capability would be a significant undertaking that presents challenges to the best technology currently available anywhere. These challenges include computational requirements; observational requirements (including development of initial conditions using data assimilation); gaps in process understanding (including linkages between the weather, the chemistry of the atmosphere, and the biology of the oceans and land surfaces); feedbacks between weather and both biogenic and anthropogenic emissions (including energy production); information systems management and network bandwidth; and others on global-to-local scales.

E. Opportunities

The challenges involved in forecasting air quality address a number of gaps that the panel felt were important to the overall EPA participation within GEOSS: (1) lack of ability to properly characterize (analyze) the 3-D state of the chemistry of the atmosphere at any time; (2) lack of knowledge of emissions on a global scale; (3) lack of robust approaches to assimilate current observations of pollutants into 3-D coupled or uncoupled atmospheric chemical models; and (4) lack of urban-zone meteorological measurements. However, the nature of these gaps and the challenges they pose evoke promise central to the purpose of GEOSS itself: adoption and successful implementation of a global-to-local NAQP-to-EIP system-of-systems could mark the long-term success and viability of GEOSS.

A number of significant GEOSS opportunities present themselves to EPA, listed below. Out of these opportunities could come a refined understanding of the role of anthropogenic and biogenic effects on the environment, and what can be done to forecast and minimize the impacts.

1. Linkage of existing and new air quality and environmental measurement systems (both *in situ* and remote) contributing to the GEOSS data streams, including urban-zone meteorological and chemical measurement systems.

2. Development of new approaches for characterizing emissions, including inverse and dynamic (urban metabolism) methods; and top-down, remote-sensing (retrieval) techniques.

3. Deployment of common protocols for data communication, archiving, and dissemination for both observations and model products.

4. Development of the ability to reliably characterize the quality of the air in 3-D space at any given time, anywhere on the globe.

5. Development of multiscale NAQPs in collaboration with other U.S. agencies, participating GEOSS countries, and the private sector.

F. Benefits

Integrated (from many measurement platforms) data streams to GEOSS, enhancing the ability to observe the earth's environment.

1. Improved methods for characterizing emissions in differing environments (urban, rural) using novel methods, leading to better emissions estimates and modeling methods.

2. Access to multipollutant, multiplatform observations under a common data protocol in both real time and through historic archives.

3. Capacity-building to accurately characterize air quality globally, enhancing our ability to understand the effects of local and regional emissions on local and regional air quality.

4. Increased ability of the U.S. and partner nations to respond to air quality issues in real time through increasingly reliable forecasting. Development of NAQPs within GEOSS will lead to better fundamental science, better modeling, and in the long run, better public policy. This will improve local abilities to correctly model and characterize effects of industrialization and emerging economies while also improving local ability to enhance response approaches designed to meet local needs and protect public health.

G. Recommendations Concerning International Air Quality Forecasting

EPA should identify numerical air quality prediction as a primary focus for GEOSS.

1. EPA should encourage development of U.S. testbeds—urban and rural—which would, with the involvement of other U.S. agencies, the GEOSS international community, and the private sector, involve an end-to-end focus for GEOSS. This would incorporate development of :

    - Integrated data streams from existing and emerging observing platforms.

    - New, validated methods for emissions characterization.

    - The ability to properly characterize the 3-D chemical and meteorological state of the atmosphere.

    - Nested global-to-local numerical air quality prediction forecast tools.

The testbeds would also provide a mechanism for technology transfer to interested participating nations through bilateral and/or commercial arrangements. Testbeds are discussed in more detail in Section IX.

IX. Testbeds[11]

A. Definition

A testbed is seen as a facility that enables and expedites the development of observational, modeling, and dissemination methods and their transfer from research to operations. As such, it is a system that is established for evaluating the components of modeling and observing systems (instruments, sensors, locations of sensors, NAQP and data assimilation models, data communication, etc.), the configuration of the observing systems, the data quality methods, end-user applications, and data and forecast-product dissemination methods.

B. Need for Testbeds

A testbed is a device for effecting the achievement of GEOSS goals, thereby providing a proof-of-concept for GEOSS tools, mechanisms, and relationships. Testbeds can be for the short term, but the main emphasis here is for longer-term maintenance of such a system to provide for establishing baseline configurations, and for homogeneity and continuity of products from future systems. Data management for these systems is critical for successful utilization, and thus there is linkage to recommendations on data management (see Section X). In principle, testbeds can cover various spatial scales (e.g., urban, global) and include all aspects of observing, data transfer, processing, analysis, assimilation, modeling, and distribution of data and products.

C. Recommendations Concerning Testbeds

The panel recommends that EPA, in the context of GEOSS, promote and lead the establishment of testbeds, and cooperate with other agencies in operating and maintaining them. The number and scale of the testbeds need to be chosen using modeling tools and considering the range of key GEOSS and EPA applications. Further, EPA should seek to take on a leading role in developing testbed requirements, configurations, and evaluation criteria. As a minimum requirement, both an urban-scale and a rural-scale testbed should be developed. EPA should take the lead in establishing the urban testbed(s). The rural testbed(s), on the other hand, should be established jointly, considering the needs of multiple agencies and the location of existing networks and coverage of satellite and radar. The items that are listed in Section IX.D, which are activities that would be enabled by the development of testbeds, can be used to examine and define the cross-agency benefits that would be supported by testbeds. Agencies that should be part of this effort are EPA, NASA, NOAA, DOI, DOE, USDA, and NSF, and possibly others.

Actions that are required in developing effective testbeds include:

- Develop methods and strategies for determining optimal 3-D measurement-network configurations for both chemical and meteorological variables (one approach is to over-sample with the testbed and evaluate design strategies, such as data denial experiments).

- Test alternative sampling strategies (e.g., adaptive sampling; aircraft vs. balloon soundings vs. remote sensing-based mobile sampling strategies using public vehicles or commercial vehicles).

- Test data assimilation methods (including network design applications).

- Test new instruments and measurement systems (e.g., low-resolution aircraft AQ soundings vs. high-resolution balloon soundings vs. continuous, high-resolution remotely sensed profiles), both for chemical (gases and particles) and supporting meteorological measurements.

- Test data communications, telemetry strategies (e.g., Internet vs. GPRS [General Packet Radio Service]) cell phone vs. dedicated network) and common formats and protocols (refer to recommendation on data management in Section X.C).

- Test alternative "business models" for acquiring and maintaining measurement, communications, and database systems, for providing forecasts and other services, and for distributing data to intermediate and end users. In other words, use the testbed to determine how to make the system financially viable.

- Evaluate various strategies for domestic applications and for international applications in developing, third-world countries.

- Explore synergies with other applications, such as emergency response, weather forecasting, and public information.

- Contribute to model development, evaluation, and data analysis methods, and to development and testing of new and improved data assimilation models.

- Test alternatives for capacity building, e.g., training, education, documentation (refer to recommendation on education and outreach in Section XI.B).

- Provide opportunity for science investigations and quality data sets for "exploratory" science questions.

- Develop and test effective means for disseminating to end users various air quality and other environmental data, including forecast products.

- Create mechanisms for establishing effective relationships among the public, private, and academic sectors.

X. Database Management and Information Systems[12]

A. Background

Several past efforts to build and operate more limited environmental data-management systems provide a valuable experience base for this effort. The meteorological community has a long history of archiving and disseminating meteorological variables, most notably using a system developed starting in the1960s by the national hydrological and meteorological services and space agencies and coordinated by the WMO, in order to integrate measurements important to weather prediction and climate. Today a system of land-based networks and satellites deliver observations of physical variables such as temperature, pressure, winds, precipitation, and humidity in near-real time through the Global Telecommunications System (GTS) to weather-forecast centers around the world. Furthermore, it provides comprehensive data sets consisting of real-time and non-real-time observations to a data archive, which is accessible for re-analysis using models at the NCEP, the European Centre for Medium-Range Weather Forecasts (ECMWF), the Japan Meteorological Agency (JMA), and elsewhere.

Although integrated data-management and dissemination systems for air quality chemistry lag that for meteorological variables noted above, inroads are being made. The WMO Global Atmosphere Watch (GAW) program, for example, is attempting to construct a distributive data archive to host data from its reporting stations as well as pertinent information from external sources. The GAW data system provides a relatively slow turnaround time for data reporting.[13] GAW has directed considerable thought and planning toward data quality assurance (QA) and quality control (QC). However, associated problems stemming from the diverse, multinational client community have impeded the archive's development process. As another example, the North American Research Strategy for Tropospheric Ozone (NARSTO) maintains a data archive, housed on the NASA Earth Observing System Data and Information System (EOSDIS) system, containing a variety of chemical and meteorological measurements generated from its field studies, as well as selected model-output data. As with GAW, NARSTO's data archive provides relatively slow data turnaround. Obtaining input data in the required formats from a diverse user community is a major challenge for the NARSTO archive, requiring substantial effort from NARSTO's data-management personnel. Design of the proposed GEOSS system must take this experience base into careful consideration, incorporating desirable features and designing-out the difficulties encountered by existing management systems. Below we list several guidelines to assist with this design process.

B. Guidelines for General Design Features

The GEOSS database management system (DBMS) should be designed to provide widespread, free user access, and should be cognizant of ongoing plans by other organizations as well of experiences by current and former systems. In particular:

- The system should be compatible with general features of the proposed IGOS data-management system design, augmented as discussed below (see Fig. X.1

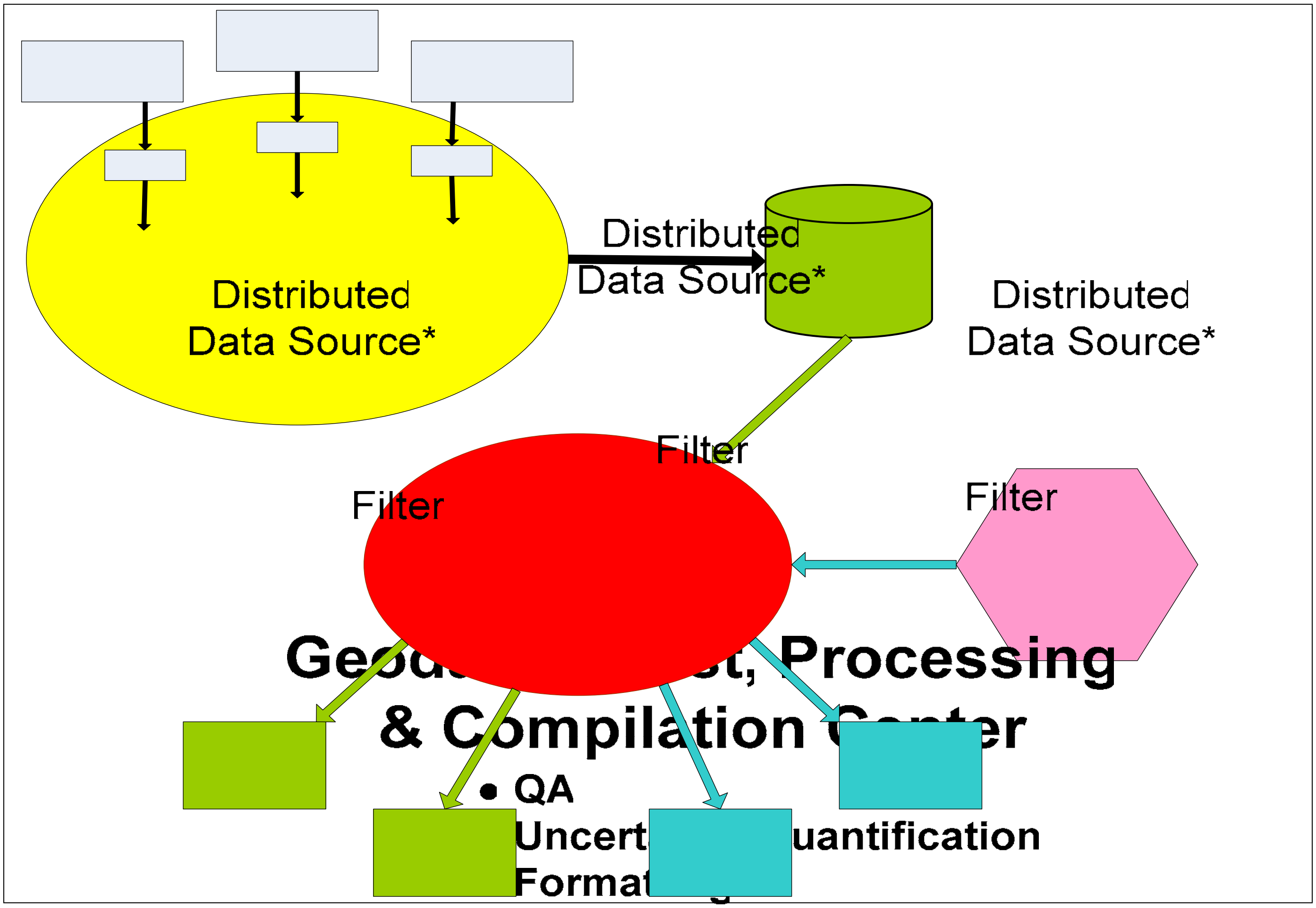

Figure X.1 Schematic of GEOSS database management system (*Examples of Distributed Data Sources include EOSDIS, NOAA, WMO/GAW, NARSTO)

- The facility should operate as a hybrid between a central and a distributed DBMS. All data should be stored on and be directly assessable from the system. However, the DBMS should be linked formally with external bases, which feed new data to the system online through the DBMS input filters (discussed below).

  - The system should have well-posed and defined data-storage formats and data-entry protocols, which are sufficiently flexible to accommodate all types of geodata, including stationary, moving, point, and path measurements, as well as metadata.

- The system should encourage high levels of quality assurance (QA) and quality control (QC). Rather than stimulating QA and QC levels, however, the DBMS should quantify and post precisely defined uncertainty levels associated with each data set. Quantitative uncertainty-level estimates should be established by standing expert teams, operating as components of the DBMS.

- The system should encourage adherence to its data-entry protocols and formats by various input entities, but should not rely on this adherence. Instead, the DBMS should, as a routine internal function, create *input filters* that automatically reformat data from specific sources to adhere to the DBMS protocols. In the case of near-real-time data, these should take the form of online “hot filters,” which operate continuously.

C. Recommendation Concerning Database Management and Information Systems

EPA, cooperating jointly with NASA and NOAA on an equal-partner basis, should participate in a three-agency initiative to design, implement, operate, and sustain the central GEOSS database management system. The central DBMS will serve as the heart of the composite GEOSS complex. It is imperative that this system function to expectations and be used extensively by the world community for its intended purpose. If it succeeds, many of the other GEOSS components will succeed as well and will grow in utility over time. The DBMS effort’s successful implementation will be a major contribution to GEOSS and to the world community. EPA will benefit directly by using the GEOSS resource to implement its mission responsibilities, a situation that will be enhanced by its central role in system design and management.

XI. Education and Outreach[14]

A. Discussion

To be successful, a comprehensive and integrated global observing program requires personnel with expertise in the following areas:

- Scientific understanding
- Instrument and model development, optimization, and verification
- Platform development, optimization, and management
- Hypothesis development
- Experiment design
- Sampling strategies and techniques
- Data archiving, management, and communication
- Technology transfer

Existing (traditional) doctoral degree programs meet the needs of individuals who will not be required to work at the interface of multiple disciplines. For example, any number of science and engineering degree programs produce Ph.D.'s having the expertise required to address science questions that focus on atmospheric dynamics or atmospheric chemistry or water quality or ecosystem dynamics (whether via satellite measurements, surface measurements, or modeling studies). In contrast, few doctoral degree programs adequately prepare their graduates to knowledgeably and effectively work at the *interface* of disciplines. This represents a critical gap—one that compromises the successful development of an integrative global observing program.

For example, expertise in forest ecophysiology, atmospheric chemistry, microbial ecology, and boundary-layer dynamics is needed when designing an experiment addressing the effects of air pollutants on biogenic VOC emissions and subsequent oxidant photochemistry. For a newly minted Ph.D. to work effectively on such a problem, he/she would require expertise in one of these areas and sufficient understanding of the other disciplines to bring the appropriate expertise to the project and to effectively interact with multidisciplinary colleagues (or, with colleagues from multiple disciplines) on experiment design and data analysis and interpretation. Scientific leadership on integrated issues requires a similar breadth of understanding and appreciation of the critical environmental parameters, ecosystem processes, and/or science questions.

NSF has embarked on a major effort to produce Ph.D.'s having a multidisciplinary perspective. The Integrative Graduate Education and Research Traineeship (IGERT) Program currently involves ~115 interdisciplinary graduate degree programs at universities across the country. However, there are drawbacks: only a few of these programs involve the environmental sciences, the programs are "expensive" for universities (full tuition costs are not covered and indirect costs are only 8%), and long-term NSF funding is not an option. Therefore, there is a critical need for innovative efforts focusing on educating the future cadre of interdisciplinary scientists needed for a dynamic global observing program. Furthermore, a change in funding strategies is needed to support the development and sustainability of interdisciplinary doctoral degree programs, i.e., a new program outside traditional graduate fellowships.

One useful model of a successful program is the University of Michigan's Biosphere-Atmosphere Research and Training Program (BART). The program involves a residential "immersion" cornerstone experience involving research; fundamentals workshops on global and climate change, boundary-layer meteorology, atmospheric chemistry, plant physiology, forest ecophysiology, aquatic ecosystems, biogeochemical cycles, and experimental design and statistics; policy and industry perspectives workshops; seminars; reading groups; discussions of professional ethics and grantsmanship; and a significant evaluation component involving an external advisory committee and a professional program evaluator. Students have an atmospheric mentor and a biospheric mentor, and their research must be truly interdisciplinary.

B. Recommendations Concerning Education and Outreach

The panel recommends that EPA (and other U.S. GEOSS participating agencies) play a major role in preparing interdisciplinary scientists for participation in the global observing program. EPA could take the lead in defining degree program elements, possibly including a science policy dimension. It is recommended that significant effort be devoted to program evaluation, as producing successful interdisciplinary scientists is in itself a new area of education research. A long timeline must be embraced in order to assess a program's merits. Timely evaluation is critical for program success, and the program's impact cannot truly be known until the degree of interdisciplinarity and the resulting contributions are evaluated several years after graduation.

XII. Summary of Panel Recommendations

The panel's recommendations to EPA concerning its future role in GEOSS are summarized below according to high-level thematic element. Important details are provided in the various sections of this report. The reader is encouraged to consider the entire report when evaluating the scope and focus of the individual recommendations. This summary simply seeks to provide an overview of their broad nature; it is not prioritized.

- EPA should adopt air quality forecasting as a major focus of its contributions to GEOSS.

- Urban air quality forecasting should receive special emphasis, especially urban needs pertaining to characterizing sub-grid-scale processes and variability.

- Development, improvement, and testing of data assimilation schemes for air chemistry demand additional effort within GEOSS.

- Improved, dynamic emissions inventories are very important, and need to consider multiple aspects: urban, rural, anthropogenic, and biogenic.

- A focused effort is needed to design and establish multisensor 3-D measurement networks and observing strategies for air chemistry, meteorology, and surface characteristics (bootstrapping on existing meteorological measurement networks).

- Additional effort is required to improve the use of current and future satellite data for air quality forecasting, dynamic emissions inventories, and surface characterization.

- Testbeds are a critical component in the development of a successful GEOSS program and the transfer of technology from research to operations; EPA has much relevant experience and should take a leading international role.

- EPA, in cooperation with NASA and NOAA, should participate in the design, implementation, operation, and support of a central real-time GEOSS database management system.

- EPA (and other U.S. GEOSS participating agencies) should play a major role in preparing future interdisciplinary scientists for participation in local, regional, and global observing programs.

- GEOSS will be extremely beneficial to the global community for its ability to transfer technology to developing countries, and EPA should play a key role

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[1] EPAAR 1552.211.78 information: Project award amount of $99,688.00 as a result of full and open competion to Solicitation RFQ-RT-04-00038
[22] Principal authors of this section are Anne Thompson, Nelson Seaman, and Jim Szykman.
[3] $PM_{2.5}$ refers to particulate matter with diameters ≤2.5 µm, and PM_{10} diameters are ≤10 µm.

[4] INTEX-NA/NEAQS is also referred to as ICARTT (International Consortium for Atmospheric Research on Transport and Transformation (http://www.al.noaa.gov/ICARTT/ICARTTmain.shtml). Several groups in North America and Europe have independently developed plans for field experiments in the summer of 2004, aimed at developing a better understanding of the factors that shape air quality in their respective countries and the remote regions of the North Atlantic. For example, NASA and NOAA are planning experiments under the Intercontinental Chemical Transport Experiment - North America (INTEX-NA) and the New England Air Quality Study - Intercontinental Transport and Chemical Transformation (NEAQS-ITCT) 2004(http://www.al.noaa.gov/2004/) programs, respectively, while the Europeans (U.K., Germany, and France) are organizing coordinated studies under Intercontinental Transport of Pollution (ITOP). While each of these programs has regionally focused goals and deployments, they share many of the same goals and objectives and the proposed study areas overlap significantly. ICARTT was formed to take advantage of this synergy by planning and executing a series of coordinated experiments to study the emissions of aerosol and ozone precursors, their chemical transformations, and removal during transport to and over the North Atlantic. The capabilities represented by the consortium will allow an unprecedented characterization of the key atmospheric processes. The combined research conducted in the programs that make up ICARTT will focus in three main areas: regional air quality, intercontinental transport, and radiation balance in the atmosphere.

[5] This section is adapted from Dabberdt et al. (2004).
[6] Principal authors of this section are Mary Anne Carroll and Alex Guenther.
[7] Principal authors of this section are Dick McNider with Nelson Seaman, Jason Ching, and John McHenry.
[8] Principal authors of this section are Alex Guenther and Gregory Carmichael with Jack Fishman.
[9] Principal author of this section is Jason Ching with contributions from Richard McNider.
[10] Principal authors of this section are John McHenry and Alex Guenther.
[11] Principal author of this section is Sharon LeDuc with contributions by Walt Dabberdt.
[12] Principal authors of this section are Jeremy Hales, Sharon LeDuc, and Jack Fishman.
[13] The importance of a rapid-turnaround (e.g., quasi real-time) feature for the IGOS data-management system, at least for some classes of data, should be emphasized.
[14] Principal author of this section is Mary Anne Carroll with contributions from Alex Guenther.