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Profile and Remote Sensing Observation Datasets
North American and

This article describes the use of ground-based, upper air, and satellite-based measurement platforms for characterizing the vertical structure of the atmosphere and how information from these platforms can play a critical role in the Air Quality Model Evaluation International Initiative (AQMEII) model evaluation exercises.

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While the vast majority of operational air pollution networks across the world are designed to measure relevant metrics at the surface, the air pollution problem is a three-dimensional phenomenon. The lack of adequate observations aloft to routinely characterize the nature of air pollution throughout the air column continues to limit our understanding of pollutant transport. This is especially true in the characterization of nocturnal residual layers and the downward mixing of these layers the following day at locations far removed from the source region as the planetary boundary layer (PBL) grows during the daytime heating.

Within the AQMEII,[1,2] one of the main goals is to work across continents to develop a sustained capability to evaluate regional-scale air quality models to simulate pollutant transport and transformation processes throughout the PBL and free troposphere (FT) and identify and improve model deficiencies. An underlying objective is to promote the need for high-quality observations to adequately characterize atmospheric processes and changes

for Regional-Scale Model Evaluation under the AQMEII

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throughout the troposphere. This article is devoted to the upper air measurements fulfilling the scope of air quality model evaluation pursued by the AQMEII consortium, while a companion article[3] deals with the ground-based monitoring networks.

Upper-Air Measurement Needs

Over the past decades, the regional air quality modeling community has often stated the need for routine and systemic observations above the atmospheric surface layer to evaluate regional-scale numerical air quality models.[4,5] The deficiency of available observations above the atmospheric surface layer is echoed by the National Research Council in two recent reports,[6,7] which highlight the need for chemical and physical measurements throughout the atmosphere, with a special emphasis on the need for vertical profile measurements of atmospheric composition aloft to help address current inadequacies. A similar set of conclusions was drawn by the United Nations Task Force on Hemispheric Transport of Air Pollution (HTAP).[8]

Within the United States, Zhang and Rao[9] show how pollution trapped aloft in the nighttime residual layer is entrained downward at locations far removed from the source regions as the atmospheric boundary layer starts to grow during the day. Research has also shown that in certain regions, oxides of nitrogen emissions from lightning can contribute to significant ozone production in the FT[10] and the pollutant concentrations in the FT along the regional model's lateral boundary in the western United States may underestimate the impact of long-range transport.[11] The complexity of assessing the true impact of long-range transport from a measurement perspective is captured in a recent study[12] using numerous observations collected during CalNex,[13] a specialized field-intensive, and a high-resolution research model to help quantify the nexus between ozone produced by East Asia emissions and ground-level concentrations measured at the surface in the Western United States.

Profile Observations Selected for Use in the AQMEII

While the lack of observations above the surface layer continues, the atmospheric science and satellite research communities have made progress with sustained efforts to fill this gap. In particular, the need to validate satellite aerosol and trace gas observations on a global basis has provided part of the scientific motivation for the highly successful European-based aircraft program Measurement of Ozone, Water Vapor, Carbon Monoxide and Nitrogen Oxides Aboard Airbus In-Service Aircraft (MOZAIC; www.iagos.fr/web).[14,15]

More recently, research satellites have demonstrated a sustained operations capability for Light Detection and Ranging (LIDAR) measurements with the NASA Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) instrument[16] aboard the CALIPSO satellite; now in its sixth year of providing high spatial resolution vertical profiles of aerosols.

In addition, numerous ground-based research locations have the capabilities to provide vertical profile information or total column observations, such as the international Network for the Detection of Atmospheric Composition Change (NDACC), Global Atmosphere Watch-GAW Atmospheric

Table 1. Selected vertical profile and total column data to be used in the AQMEII.

Network and/or Instrument	Lead Organization	Total Number of Sites/Satellite Coverage	Potential Evaluation Approach	Initiated Measurement	Relevant Constituent/ Properties for AQMEII	URL for Information on Measurements/ Data
International Aircraft Measurements						
MOZAIC/IAGOS (Measurement of ozone [O_3], water vapor, carbon monoxide [CO], and nitrogen oxides [NO_x] aboard Airbus in-service aircraft)	CNRS/FZJ	2500 Airbus International flights/year (12 select airports in North America and 3 select airports in Europe)	Operational, Diagnostic, Dynamic, and Probabilistic	1994-2010	O_3, CO, NO, NO_x, NO_y, wind speed/ direction, temperature, relative humidity	http://www.iagos.org
Ground-Based Networks						
AERONET – Aerosol Robotic Network	NASA (federated)	~275	Operational, Diagnostic, and Dynamic	1998	Aerosol spectral optical depths, aerosol size distributions, and precipitable water	http://aeronet.gsfc.nasa.gov/index.html
MPLNET – Micro-pulse Lidar Network	NASA (federated)	35	Operational, Diagnostic	2000	Aerosols and cloud layer heights	http://mplnet.gsfc.nasa.gov/
Ozonesonde Network	NOAA/NASA	12 (5 sites within the US)	Operational, Diagnostic, Dynamic, and Probabilistic	1986	Weekly Upper Air measurements of O_3, temperature, and humidity information fromsurface to approximately 32 km	http://www.esrl.noaa.gov/gmd/dv/site/site_table.php
Instrument/Satellite						
CloudAerosol Lidar with Orthogonal Polarization (CALIOP)	NASA and CNES	Polar Orbiting with 16-day repeat pattern day/night	Operational, Diagnostic, Dynamic, and Probabilistic	2006-CALIPSO	Aerosol backscatter, aerosol optical depth, Aerosol extinction coefficient	http://www-calipso.larc.nasa.gov/about/
Clouds and Earth's Radiant Energy System (CERES)	NASA/NOAA			1999-Terra 2002-Aqua 2011-NPP	TOA/Surface Fluxes	http://ceres.larc.nasa.gov/
Measurement of Pollution in the Troposphere (MOPITT)	NASA	Polar Orbiting with 1-day repeat pattern – day/night	Operational, Diagnostic, Dynamic	1999-Terra	Tropospheric columns for CO and CH_4	http://www.eos.ucar.edu/mopitt/
Moderate Resolution Imaging Spectroradiometer (MODIS)	NASA	Polar Orbiting with 1-day repeat pattern – day only	Operational, Diagnostic, Dynamic	1999 – Terra, 2002-Aqua	Aerosol optical depth	http://modis-atmos.gsfc.nasa.gov/
Multi-angle Imaging Spectro Radiometer (MISR)	NASA	Polar Orbiting with 9-day repeat pattern day only	Operational, Diagnostic, Dynamic	1999-Terra	Aerosol optical depth	http://misr.jpl.nasa.gov/
Ozone Monitoring Instrument (OMI)	KNMI/NASA	Polar Orbiting with x-day repeat pattern	Operational, Diagnostic, Dynamic	2004-Aura	Derived-tropospheric columns for O_3, SO_2, HCHO, NO_2, and aerosol	http://aura.gsfc.nasa.gov/instruments/omi.html
Total Emission Spectrometer (TES)	NASA	Polar Orbiting with x-day repeat pattern, day/night	Operational, Diagnostic, Dynamic	2004-Aura	Tropospheric columns for O_3, NO_y, CO, SO_2, CH_4	http://tes.jpl.nasa.gov/

Lidar Observation Network (GALION), and the Aerosol Robotic Network (AERONET) program, a federated ground-based remote sensing aerosol network. Table 1 lists select profile and total column observations from various observing systems and networks to be used throughout AQMEII for operational, diagnostic, dynamic, or probabilistic model evaluation.[17]

MOZAIC

Since 1994, European scientists working with several commercial airlines have successfully led the development and operation of the MOZAIC program, resulting in the collection of tens-of-thousands of atmospheric profiles at several major airports throughout the world. The MOZAIC program demonstrated a cost-effective method for measuring air pollutants aloft through the installation of monitoring equipment on commercial airliners. Over Europe and North America the MOZAIC data are a key component of the AQMEII.[1,2] The MOZAIC profiles provide the only internally consistent measurements of ozone and carbon monoxide and, therefore, help provide a more consistent interpretation of results across the groups participating in AQMEII, even though the regional-scale numeric models are run over different continents.

Because MOZAIC measurements exist over a long period of time and also can be aggregated to provide some representation of volume concentration through the atmosphere, MOZAIC data are more useful for performing different types of model evaluation, namely, operational, diagnostic, dynamic, and probabilistic. Under Phase 1 of AQMEII, MOZAIC measurements were used for operational model evaluation, as illustrated in Figure 1, where the monthly averaged ozone concentrations are extracted at two airport locations on the West Coast of North America (Portland and Vancouver), in the proximity of the borders of the AQMEII simulation domain. This analysis is useful for comparing the effectiveness of boundary conditions for ozone, and possible biases introduced by these into the domain.[18]

WMO Ozonesondes

Ozonesonde data for AQMEII Phase 1 were extracted from the World Meteorological Organization's

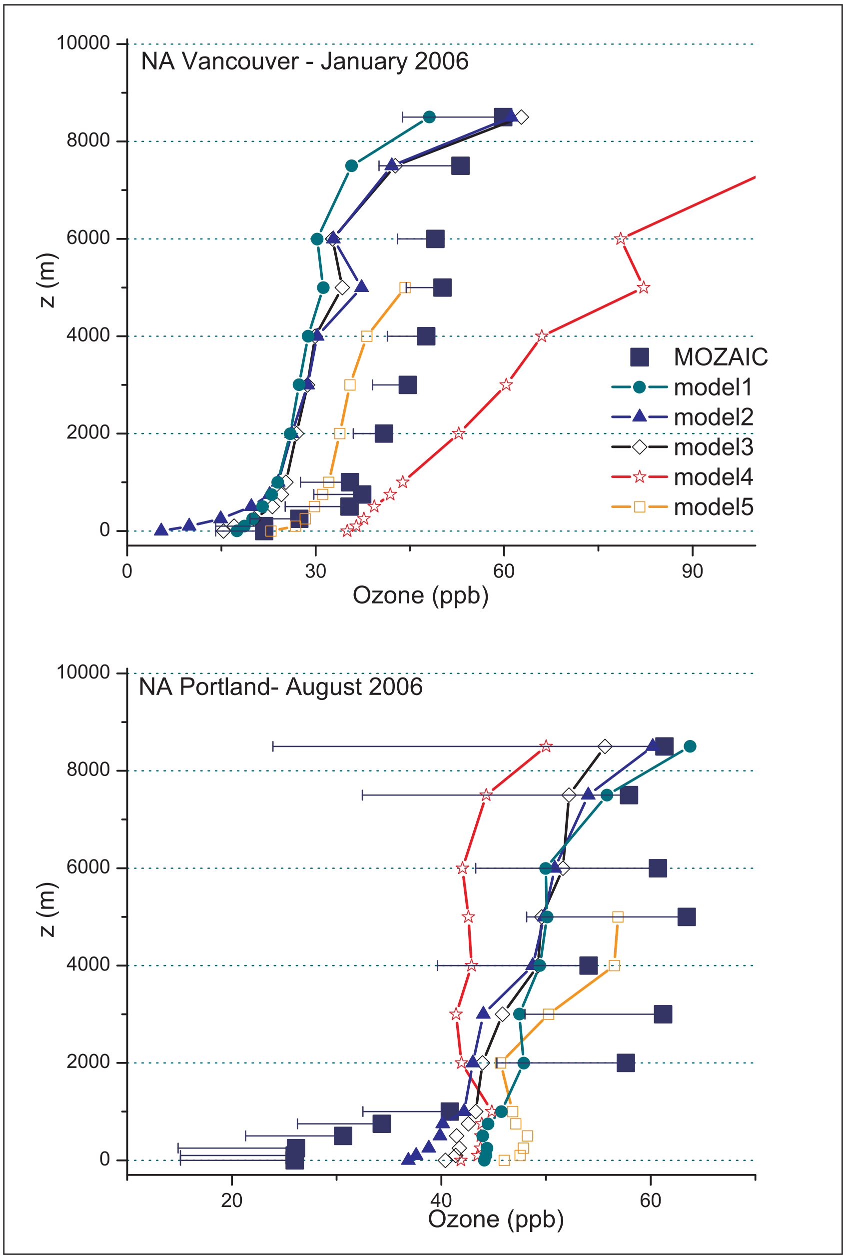


Figure 1. Modeled and measured ozone profiles at (top) Vancouver and (bottom) Portland airports for the months of January and August 2006. The blue squares are the mean of the MOZAIC data with the bars one standard deviation (only the minus half) at each height.

(WMO) World Ozone and Ultraviolet Radiation Data Centre in Toronto. These measurements report vertical profiles of ozone partial pressure at several vertical pressure levels. Since the AQMEII model vertical levels are expressed in meters above ground, only soundings datasets with reported geopotential height were used. Of the 65 reported launch sites within the North American AQMEII domain, a total of 19 were used in Phase 1.[19] The European domain included 45 launch sites, but only 9 reported geopotential height.

Space-Based LIDAR Measurements

The CALIPSO satellite (http://eosweb.larc.nasa.gov/PRODOCS/calipso/table_calipso.html) is part of the "A-Train," a constellation of five Earth-observing satellites. CALIPSO's CALIOP instrument uses LIDAR to profile aerosols through the atmosphere from 40 km to the Earth's surface. Since the launch of CALIPSO in 2006, CALIOP continues to circle the Earth sending laser pulses to measure the thickness and composition of clouds and aerosol layers at a vertical resolution of 30 m. This unprecedented data set is comprised of day and night profiles of aerosol extinction with 3 descending daytime and 3 ascending nighttime transects per day across the North American AQMEII model domain and 2 descending daytime and 2 ascending nighttime transects per-day across the European AQMEII model domain.

Figure 2 shows the CALIOP extinction coefficient projected onto the model grid from the Chemistry-Transport Model, Community Multi-scale Air Quality (CMAQ), along with the CMAQ reconstructed extinction along CALIPSO track and the CMAQ aerosol optical depth over a wider domain. For AQMEII Phase 2, CALIOP data will be used in both operational and diagnostic model evaluation studies, including aerosol direct and indirect effects on meteorology.

Although only MOZAIC, ozonesonde, and CALIOP profile data are highlighted here, it is critical to acknowledge the contributions of other relevant (ground-based and satellite) observing networks and systems routinely collecting data relevant to AQMEII Phases 1 and 2, as listed in Table 1. Taken as a whole, the observations listed in Table 1 only begin to adequately characterize processes and changes throughout the troposphere and the three-dimensional nature of air pollution.

Data Systems

A critical aspect of the AQMEII is the ability to efficiently match model output with available measurements. Under the AQMEII, the European Commission Joint Research Centre's ENSEMBLE system, a Web-based platform (http://ensemble2.jrc.ec.europa.eu/public/), is being used to facilitate the intercomparison of multiple models and measurements.[20] An additional challenge in Phase 2 will be the inclusion of satellite data such as CALIOP into the ENSEMBLE system. To accomplish this task, the U.S. Environmental Protection Agency's

(EPA) Remote Sensing Information Gateway (RSIG; http://badger.epa.gov/rsig/)[21] will be used to directly access CALIOP data products at the NASA Langley Atmospheric Science Data Center, extract relevant parameters for the AQMEII model domains, and provide only the necessary data for inclusion into ENSEMBLE. Through the use of Web server scripts, the RSIG system provides an efficient and effective means to access and process satellite data either at native resolution or to re-project data onto a custom-Lambert regional model domain for a specified time-range, variable, and longitude-latitude-layer domain without first writing original data files to disk.

Ongoing Efforts to Increase Chemical Profile Observations

MOZAIC and IAGOS

The MOZAIC program (1994–2010) will continue routine profiling of the atmosphere through the newly initiated In-Service Aircraft for the Global Observing System (IAGOS) program, a partnership between European research institutions, universities, aviation industry, and commercial airlines around the world. Under IAGOS, new instruments designed to fly on Airbus A340 and A330 aircraft will be contained in the standard instrument package (Package I) to measure ozone, carbon monoxide, relative humidity, and cloud droplet backscatter. Optional instrument packages can be deployed (in addition to Package 1) to measure nitrogen oxides, reactive nitrogen, carbon dioxide and methane, or particulate matter size distribution. The measurement time for each species varies, but all data will be reported at 4-second intervals, corresponding to a horizontal (vertical) resolution of approximately 1 km (20–30 m).

To bring IAGOS to fruition in the United States, an ad-hoc IAGOS working group was formed in 2010. Given that the IAGOS data are relevant to the research and monitoring needs of many U.S. agencies and research institutions, U.S.-based IAGOS aircraft could be funded by a consortium of agencies and institutions. Bringing the IAGOS program to the United States will require the cooperation and enthusiasm of research institutions, partner airlines, and the Federal Aviation Administration (FAA). In addition to developing the infrastructure for the program and certifying that the instrumentation will function reliably and in accordance with U.S. safety standards, funding must be secured to sustain the program over several years. But these challenges are surmountable as they have been overcome before. From 1975–1979, NASA partnered with United Airlines, Pan Am, and Qantas to operate Global Atmosphere Sampling Program (GASP), the world's first initiative to sample trace gases from commercial airlines.[22-24]

U.S. Ozone Air Quality Lidar Working Group

Recently, NASA formed an interagency research initiative with EPA and NOAA for ground-based LIDAR profiling of tropospheric ozone and aerosols. This group focuses on the development of robust measurements of PBL and FT ozone structure for science studies in advance of future air quality satellite missions such as Geostationary Coastal and Air Pollution Events (GEO-CAPE; more later). Although advances in ground-based aerosol profiling capability are also needed, the near-term efforts are focused on operational and near-surface ozone measurements where ozone LIDAR capability significantly lags aerosol LIDAR capability. The primary long-term scientific objective of the group is to provide time/height measurements of ozone and aerosols, from near the surface to the tropopause. These high-fidelity measurements will provide the GEO-CAPE science team with accurate representations of the PBL and FT ozone and aerosol structure as benchmarks for the high temporal resolution observations from a geostationary satellite.

Figure 2. Top two panels: CALIOP 532 nm extinction coefficient regridded to CMAQ 12 km and CMAQ reconstructed extinction along CALIPSO track. Bottom image: CMAQ calculated aerosol optical depth with CALIPSO track over-plotted in Northwest United States.

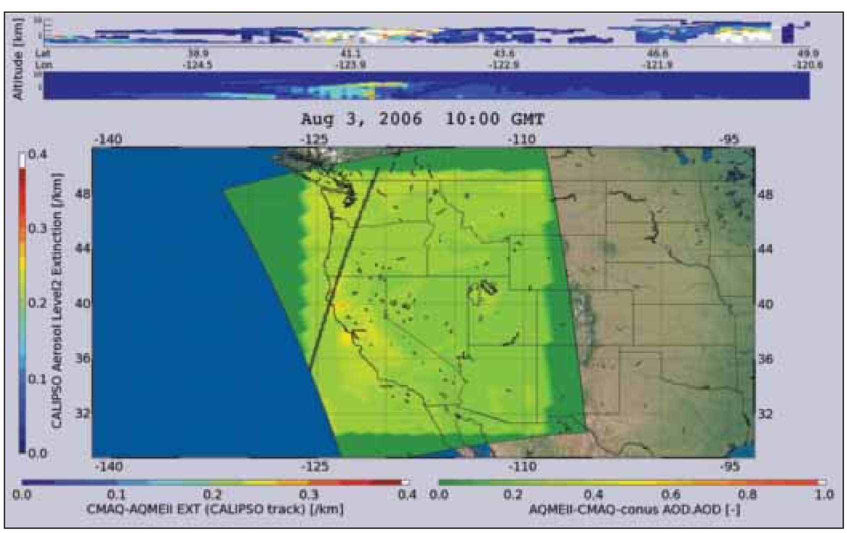


Image courtesy of Matt Freeman, U.S. EPA Environmental Modeling and Visualization Laboratory.

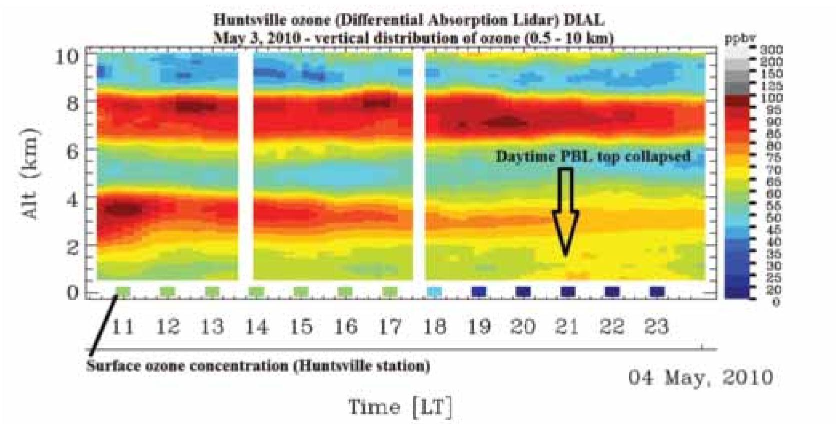
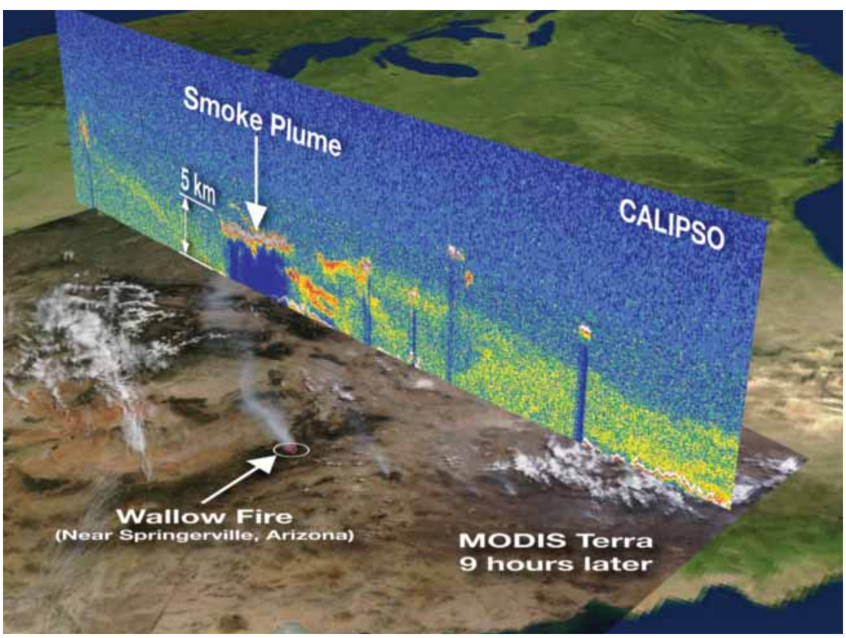


Figure 3. Example of the time (CDT)/height distribution of ozone over Huntsville, AL, measured by lidar and surface ozone from local SLAM site.

A second objective of this initiative is to develop an ozone LIDAR instrument suitable to populate a network and address the needs of NASA/EPA/NOAA air quality scientists and managers who increasingly express a desire for ozone profiles. It is the hope that near-term technology advances could provide the United States with an operational ozone LIDAR network and observations of the detailed ozone structure at multiple locations across the US. Figure 3 provides an example data product from one of the five ozone LIDAR stations,[25] which shows the observed laminar ozone structure and the associated decay of the PBL, one of the processes critical to model development.



A CALIPSO vertical profile from space shows the smoke plume on June 3, 2011, from the wildfires in Arizona. It is overlaid on an image captured by the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument on the Terra satellite nine hours later. The data show that the smoke plume reached heights of 5 km (3 miles). CALIPSO and Terra are part of the 'A-Train' constellation of five Earth-observing satellites. *Image courtesy of NASA/Kurt Severance, Jason Tackett, and CALIPSO Team.*

Future Space-Based Observations

In the United States, NASA and NOAA continue their efforts to move to new research and operational satellite instruments as directed in the National Research Council's (NRC) *Earth Science Decadal Survey* report.[26] Two missions in the NRC report most relevant to future AQMEII efforts include Geostationary Coastal and Air Pollution Events (GEO-CAPE)[27] and Aerosol-Cloud-Ecosystem (ACE).

The GEO-CAPE satellite is a geostationary satellite with instruments to measure troposheric trace gas and aerosols with increased temporal frequency. The European Space Agency (ESA) and the Korea Aerospace Research Institute (KARI) are planning missions similar to GEO-CAPE, resulting in a global constellation of geostationary atmospheric chemistry satellites by the end of the decade.[28] The ACE mission is a satellite with a series of instruments that include the next generation of lidar measurements with the potential to provide profiles of measured aerosol extinction along with a polarimeter for information on aerosol optical properties and aerosol types.

Prior to these missions, the NOAA-NASA GOES-R program will launch the next generation of U.S. geostationary weather satellites over North America in 2015 with the Advanced Baseline Imager (ABI) providing high spatial and temporal resolution of MODIS-like Aerosol Optical Depth (AOD). An additional GOES-R instrument, the Geostationary Lightning Mapping (GLM) will detect up to 90% of all lightning flashes, continuously, leading to improved parameterizations of FT nitrogen oxides budgets calculations over North America. Over the next decade, it will be important to continue to develop model evaluation techniques for regional-scale numerical air-quality models through efforts like AQMEII to exploit the scientific value of future satellite measurements.

Summary

The ability to directly compare the performance of different regional-scale numerical air quality model simulations over different continents has been limited because of the lack of continuous measurements. The progress made in surface, aircraft, and satellite profile observations over the past decade provides the beginning of the visions expressed in the Integrated Global Atmospheric Chemistry Observations (IGACO) Theme report[29] and the Global Earth Observing System of Systems. In contrast to country-specific monitoring networks, global networks and observations provide consistent measurements for inter-comparison of model results, and ensure a level of confidence in the measurements through standard operating protocols.

Continued advancements in routine and systemic observations capable of characterizing key tropospheric constituents will facilitate collaboration between regional modeling communities on different continents. Such advancements will help evaluate inadequacies in both the model input data and the model's representations of the relevant atmospheric processes, thereby enhancing the scientific credibility of regional air quality models in regulatory-policy assessments and forecasting. **em**

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