

Table 2.1. DISCOVER-AQ Science Traceability Matrix

Science Objectives, Associated Questions, and Expected Outcomes	Scientific Measurement Requirements	Instrument Functional Requirements*	Investigation Functional Requirements	Modeling and Analysis Tools
<p>Objective 1: Relate column observations to surface conditions for aerosols and key trace gases O₃, NO₂, and CH₂O</p> <p><i>A: How well do column and surface observations correlate?</i></p> <p><i>B: What additional variables (e.g., boundary layer depth, humidity, surface type) appear to influence these correlations?</i></p> <p><i>C: On what spatial scale is information about these variables needed (e.g., 5 km, 10 km, 100 km) to interpret column measurements?</i></p> <p>Outcome: Improved understanding of the extent to which column observations (as observed from space) can be used to diagnose surface conditions</p>	<p>Concurrent, urban-scale observations of column and in situ aerosols, O₃, NO₂, and CH₂O from aircraft and ground sites</p> <p>Observations of boundary layer depth, T, winds, and water vapor (column and profiles)</p>	<p>Active remote sensing of aerosols between surface and aircraft level with horizontal and vertical resolution of 1 km and 60m (backscatter and depolarization)</p> <p>Passive remote sensing of trace gas columns between surface and aircraft level to determine column amounts with spatial resolution of a few kilometers or better</p>	<p>Level flight in the mid-to-upper troposphere with a dedicated aircraft observing trace gas columns (passive) and aerosol distribution/BL depth (active) beneath the aircraft</p> <p>Airborne profiling with a dedicated platform to observe in situ vertical distribution of key trace gases, humidity, and boundary layer depth</p> <p>Distributed surface network to provide in situ and total column observations for key trace gases and aerosols</p> <p>One or more ground-based lidars to provide aerosol profiles</p>	<p>Multivariate statistical analysis to assess overall correlation between column and surface observations as well as sensitivity to location, time of day, boundary layer depth and mixing, humidity, surface and cloud optical properties, etc.</p> <p>Retrieval models capable of reanalysis of remote sensing measurements including information at a range of spatial resolution</p>
<p>Objective 2: Characterize differences in diurnal variation of surface and column observations for key trace gases and aerosols</p> <p><i>A: How do column and surface observations differ in their diurnal variation?</i></p> <p><i>B: How do emissions, boundary layer mixing, synoptic transport, and chemistry interact to affect these differences?</i></p> <p><i>C: Do column and surface conditions tend to correlate better for certain times of day?</i></p> <p>Outcome: Improved understanding of diurnal variability as it influences the interpretation of satellite observations from both LEO and GEO perspectives and improved knowledge of the factors controlling diurnal variability for testing and improving models</p>	<p>Continuous observation of column and in situ aerosols, O₃, NO₂, and CH₂O throughout daylight hours</p> <p>Key trace gas and aerosol observations identifying the influence of source emissions and chemistry (e.g., CO, CO₂, CH₄, reactive nitrogen, aerosol inorganic and organic composition)</p>	<p>Airborne in situ observation of aerosol and trace gas profiles through the boundary layer and into the lower free troposphere at 1 hz (~5 m vert. and ~100 m hor. res. at nominal flight speeds)</p> <p>Passive remote sensing of total columns for trace gases and aerosol optical depth and in situ measurements of key trace gases and aerosols from a regional surface network with 10 minute resolution</p>	<p>All of the above plus:</p> <p>8 hours of flight per day by both aircraft to observe column and profile evolution throughout daylight hours to include morning/evening rush hour emissions</p> <p>Observation of trace gas total columns at surface locations throughout daylight hours</p> <p>24-hour observation of in situ trace gases and lidar aerosol profiles</p>	<p>All of the above plus:</p> <p>Regional chemical transport modeling to assess model capability to represent key meteorological parameters affecting column-surface correlations and interpret the role of various emissions sources (e.g., transportation, industry, power generation) and meteorological processes in affecting column and surface variability throughout the day</p>
<p>Objective 3: Examine horizontal scales of variability affecting satellites and model calculations</p> <p><i>A: How do different meteorological and chemical conditions cause variation in the spatial scales for urban plumes?</i></p> <p><i>B: What are typical gradients in key variables at scales finer than current satellite and model resolutions?</i></p> <p><i>C: How do these fine-scale gradients influence model calculations and assimilation of satellite observations?</i></p> <p>Outcome: Improved interpretation of satellite observations in regions of steep gradients, improved representation of urban plumes in models, and more effective assimilation of satellite data by models</p>	<p>Observe horizontal gradients in column and in situ aerosols, O₃, NO₂, and CH₂O as well as pollution tracers CO, CO₂, CH₄, and reactive nitrogen</p>	<p>Ground-based, vertically-pointing lidar observations with 10 m and 10 minute resolution to provide 24-hour monitoring of aerosol profiles</p> <p>*Specific instrument capabilities are listed in Tables 3.1-3.7</p>	<p>High spatial resolution observations collected along flight transects to resolve variability down to scales of 100 m.</p> <p>Extensive sampling for different locations to characterize variability due to changes in emission (e.g., day-of-week), meteorological parameters, surface optical parameters, and local topography</p>	<p>Statistical analysis of spatial variability to characterize expected sub-grid gradients for coarser resolution satellites and models</p> <p>Multi-scale modeling to assess influences of model resolution on nonlinear chemical processes</p>

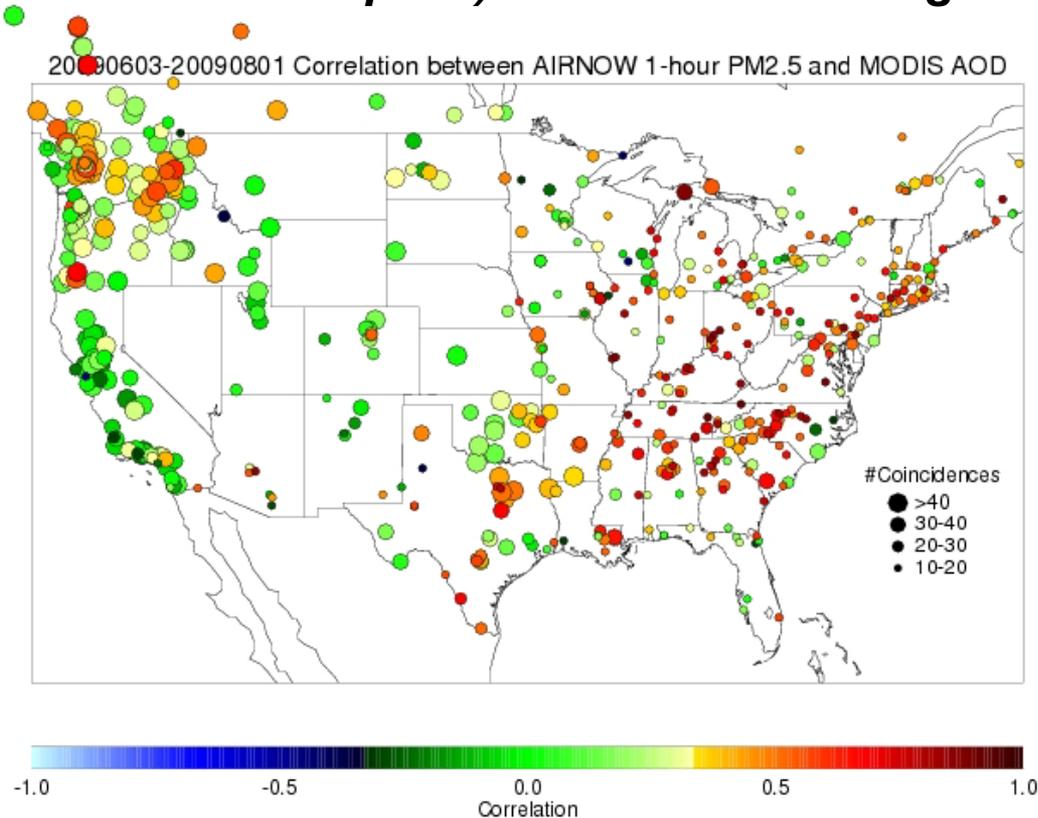
Science Objective 1: Relate column observations to surface conditions for aerosols and key trace gases O_3 , NO_2 , and CH_2O

A. How well do column and surface observations correlate?

B. What additional variables (e.g., boundary layer depth, humidity, surface type) appear to influence these correlations?

C. On what spatial scale is information about these variables needed (e.g., 5 km, 10 km, 100 km) to interpret column measurements?

Expected outcome: Improved understanding of the extent to which column observations (as observed from space) can be used to diagnose surface conditions



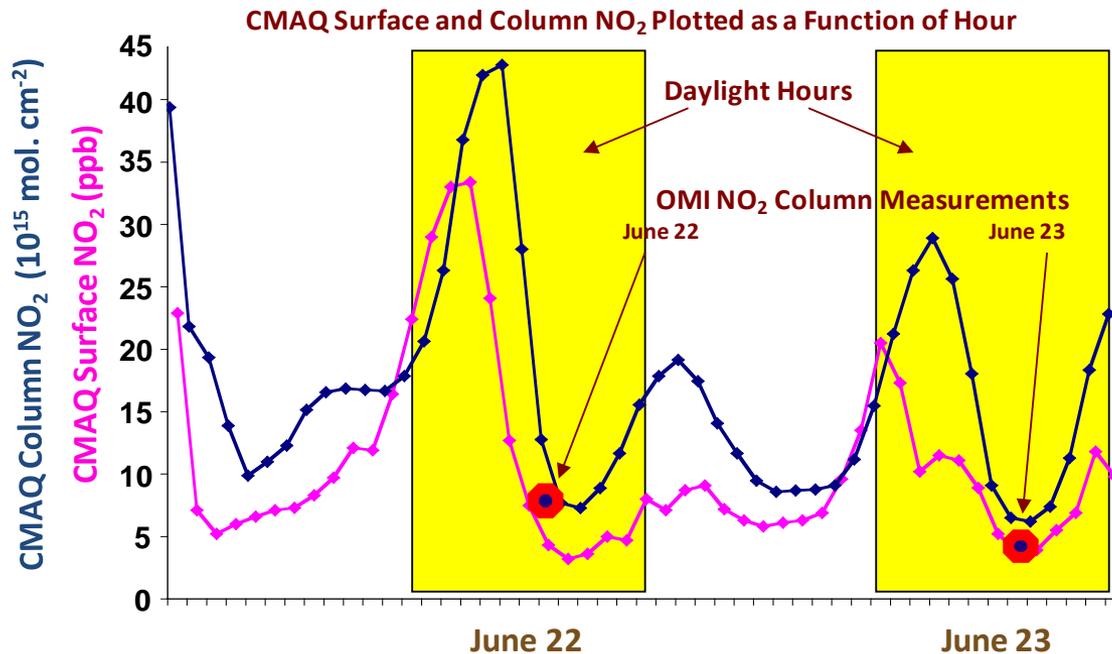
Science Objective 2: Characterize differences in diurnal variation of surface and column observations for key trace gases and aerosols

A. How do column and surface observations differ in their diurnal variation?

B. How do emissions, boundary layer mixing, synoptic transport, and chemistry interact to affect these differences?

C. Do column and surface conditions tend to correlate better for certain times of day?

Expected Outcome: Improved understanding of diurnal variability as it influences the interpretation of satellite observations from both LEO and GEO perspectives and improved knowledge of the factors controlling diurnal variability for testing and improving models



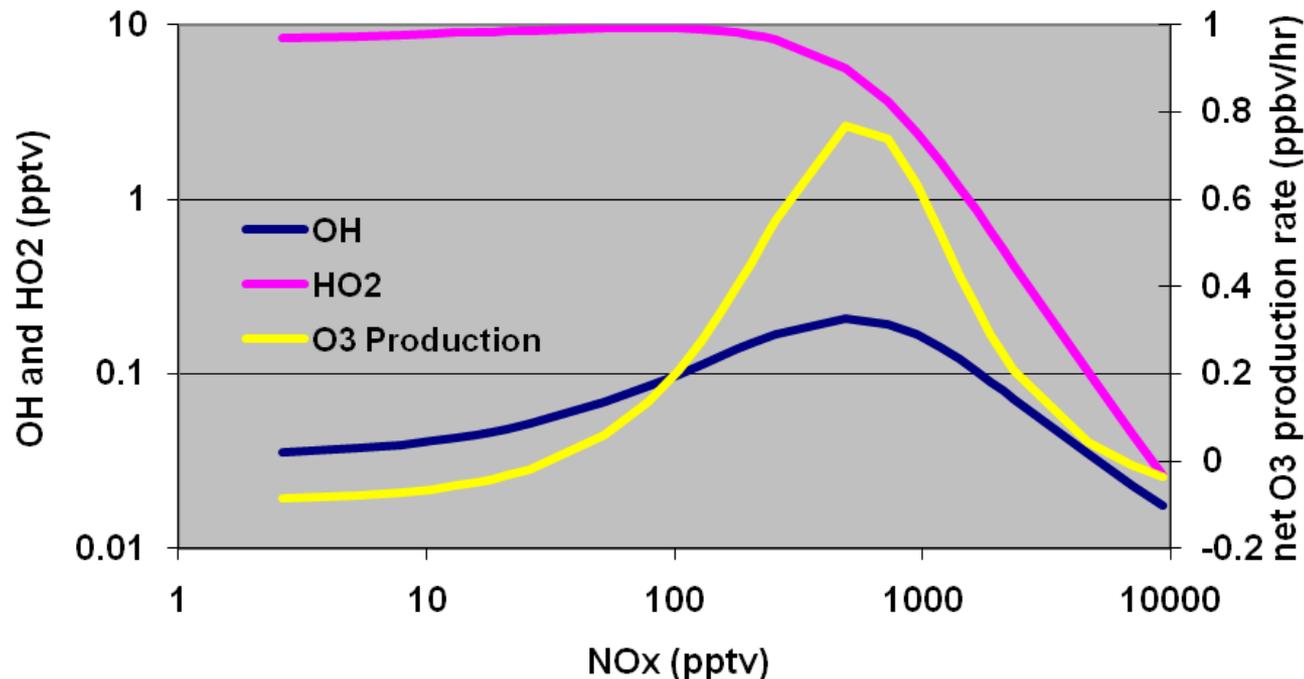
Science Objective 3: Examine horizontal scales of variability affecting satellites and model calculations

A. How do different meteorological and chemical conditions cause variation in the spatial scales for urban plumes?

B. What are typical gradients in key variables at scales finer than current satellite and model resolutions?

C. How do these fine-scale gradients influence model calculations and assimilation of satellite observations?

Expected outcome: Improved interpretation of satellite observations in regions of steep gradients, improved representation of urban plumes in models, and more effective assimilation of satellite data by models



Relevance

DISCOVER-AQ aligns with priorities for both the Atmospheric Composition Focus Area and the Applied Sciences Air Quality Program at NASA.

- NASA Strategic Goal 3.1: “Study planet Earth from space to advance scientific understanding and meet societal needs”
- Outcome 3.1.1 calling for “Progress in understanding and improving predictive capability for changes in the ozone layer, climate forcing, and **air quality** associated with changes in atmospheric composition.”

Benefits to current satellites include improved understanding of:

- surface PM_{2.5} and MODIS AOD observations
- surface NO₂ and OMI column NO₂ observations.

Benefits to future satellites having air quality relevance (GEO-CAPE, ACE, GACM):

- Possible observing strategies (e.g., optimum overpass times for LEO observations)
- Interpretation of observations (e.g., better understanding of column versus surface response to emissions, chemistry, and boundary layer dynamics).
- Optimization of surface observation networks supporting satellites

Benefits to air quality models:

- Better understanding of fine scale variability in NO_x and the associated nonlinearities in ozone chemistry at sub-grid resolutions
- Ability to assess the impact of fine scale variability on assimilation of satellite observations.

Investigative Approach: *Systematic* and *concurrent* observation of *column-integrated*, *surface*, and *vertically-resolved* distributions of aerosols and trace gases relevant to air quality as they evolve throughout the day.

NASA P-3B: Suite of in situ trace gas and aerosol measurements

NASA B200: Remote Sensing of aerosol profiles (HSRL) and trace gases (ACAM)

Surface Network: Continuous monitoring of surface aerosols and trace gases using existing AQS network augmented with column remote sensing of trace gases (Pandora) and aerosols (Aeronet); some profiling capability (lidar and ozone sondes) at temporary (NATIVE) and existing sites (e.g., Beltsville, UMBC, Moody Tower).

Modeling and Analysis:

- Basic correlative studies of column versus surface observations.
- Simple conceptual models relating column and surface quantities using other key variables such as boundary layer depth, humidity, time of day, etc.
- Improved retrieval methods through examination of vertical profile and column observations.
- Regional model interpretation and testing.
- Auto-covariance and variogram techniques to assess fine scale variability in near-surface observations.
- Effects of fine scale variability on model predictions of ozone.

DISCOVER-AQ Deployment Strategy

Systematic and concurrent observation of column-integrated, surface, and vertically-resolved distributions of aerosols and trace gases relevant to air quality as they evolve throughout the day.

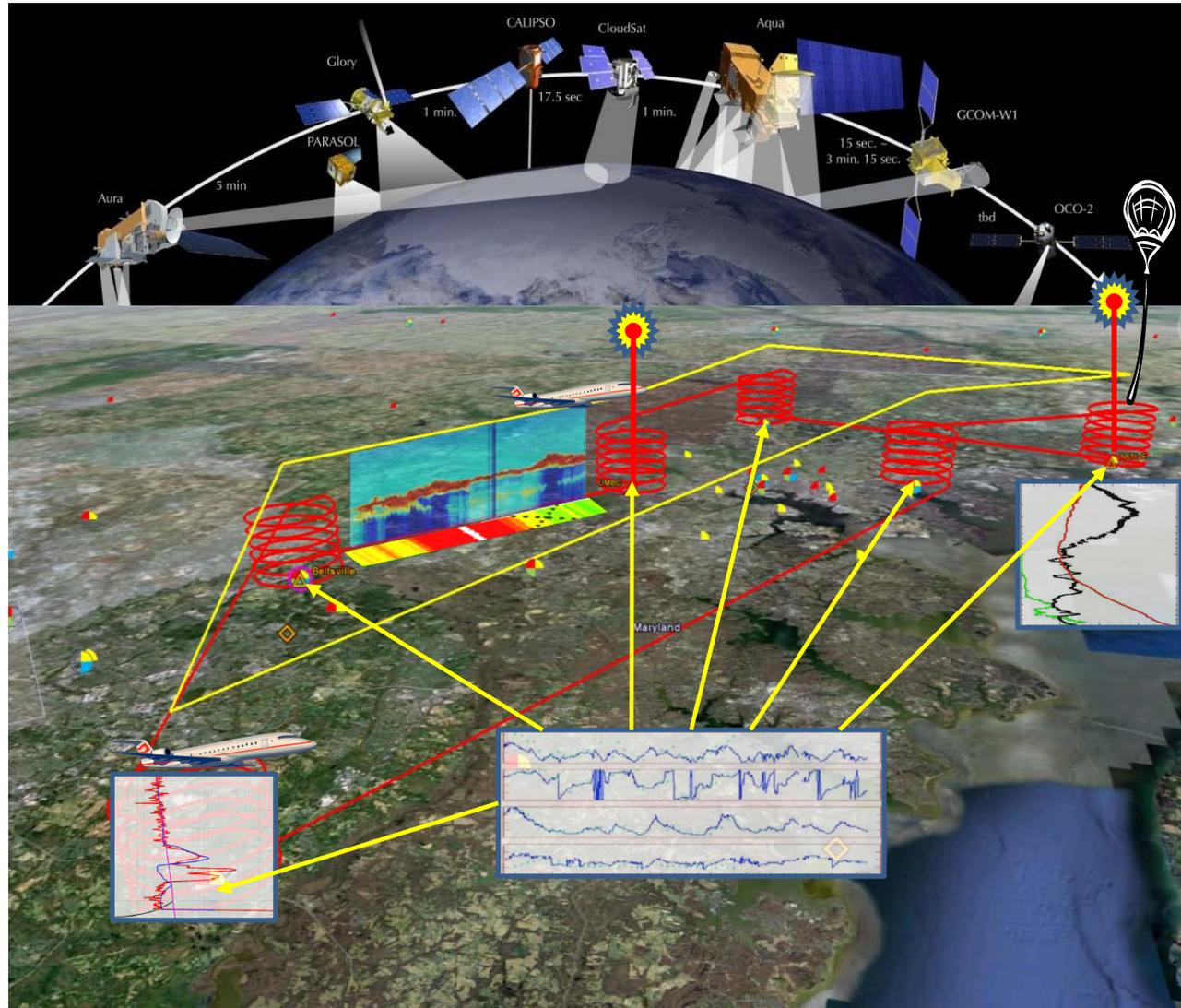
Continuous lidar mapping of aerosols with HSRL on board B-200

Continuous mapping of trace gas columns with ACAM on board B-200

In situ profiling over surface measurement sites with P-3B

Continuous monitoring of trace gases and aerosols at surface sites to include both in situ and column-integrated quantities

Surface lidar and balloon soundings



DISCOVER-AQ Science Team

Leadership	
Jim Crawford, NASA LaRC	Principal Investigator
Mary Kleb, NASA LaRC	Project Manager
Ken Pickering, NASA GSFC	Project Scientist
Gao Chen, NASA LaRC	Science Data Manager
P-3B In Situ Airborne Measurements	
Ronald Cohen, UC Berkeley	NO ₂ , ANs, PNs, HNO ₃
Andrew Weinheimer, NCAR	O ₃ , NO ₂ , NO, NO _y
Alan Fried, NCAR	CH ₂ O
Armin Wisthaler, Innsbruck	Non-methane hydrocarbons
Glenn Diskin, NASA LaRC	H ₂ O, CO, CH ₄
Stephanie Vay, NASA LaRC	CO ₂
Bruce Anderson, NASA LaRC	aerosol optical, microphysical, and chemical properties
B-200 Remote Sensing Airborne Measurements	
Chris Hostetler, NASA LaRC	High Spectral Resolution Lidar (HSRL) aerosol profiles
Scott Janz, NASA GSFC	Airborne Compact Atmospheric Mapper (ACAM) nadir trace gas columns for O ₃ , NO ₂ , and CH ₂ O
Ground-based Measurements	
Jay Herman, UMBC	Pandora network for total trace gas columns of O ₃ , NO ₂ , and CH ₂ O
Anne Thompson, Penn State	Nittany Atmospheric Trailer and Integrated Validation Experiment (NATIVE) in situ O ₃ , CO, NO, NO _y ; aerosol lidar; ozonesondes.
Ray Hoff, UMBC	Lidar aerosol profiles, AERI, Raman H ₂ O, ground data
Brent Holben, NASA GSFC	Aeronet
Data Analysis and Modeling (PI, Project Scientist, and Science Data Manager will also participate)	
P.K. Bhartia, NASA GSFC	trace gas retrievals and interpretation
Allen Chu, UMBC	aerosol retrievals and interpretation
Robert Chatfield, NASA ARC	statistical data analysis and interpretation
Rich Ferrare, NASA LaRC	aerosol analysis and interpretation of HSRL observations

Participation

LaRC	8
GSFC	6
Univ	5
ARC	1
Foreign	1

Science Implementation

First Year Preparations:

- Fabrication of one dozen Pandora instruments
- B200 modifications to accommodate ACAM
- Minor upgrades and maintenance of in situ airborne instrumentation
- Drafting aircraft payload integration plans
- Arrangements for integration of ground equipment with existing AQS and permanent research sites for the location of the initial deployment
- Depending on the acquisition of Pandora instruments, early positioning and data collection in advance of the aircraft deployment will be considered.

Annual deployments in years 2-5: 30-day deployments during each year are planned to focus on a specific location known for exceeding air quality standards. While there is **great flexibility in changing the location or order**, current plans are to visit:

Year-2: Baltimore-DC area

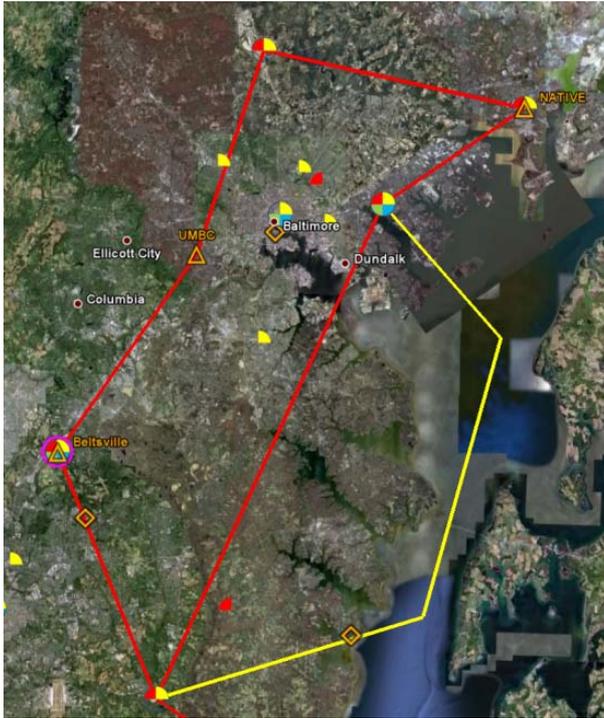
Year-3: Houston (**postponement to 2013**)

Year-4: Sacramento (**suitability of site to be discussed**)

Year-5: possibly Los Angeles, Birmingham, or Atlanta with choice based on information gained in the first three deployments (**other more recent candidates include St. Louis and Chicago**)

These locations span a variety of factors contributing to local air quality problems (e.g., upwind emissions, industrial emissions, agriculture), diversity in meteorology and surface conditions, and their proximity to NASA installations, thus enabling the deployment of aircraft to be conducted in an efficient and cost-effective manner.

Interdisciplinary Science: DISCOVER-AQ and Atmosphere-Ocean Coupling



Flight segments over water allow for evaluation of atmospheric interference on remote sensing of ocean color as well as nitrogen deposition to coastal waters

HSRL and ACAM observations will allow for simultaneous measurement of primary atmospheric interferences from aerosols and NO₂ concurrent with subsurface lidar return correlated to ocean color

Maria Tzortziou, University of Maryland, New Investigator Program, Spatial and temporal variability of NO₂ and other trace gases over Eastern US coastal regions: Applications to remote sensing observations and studies of nitrogen deposition

Yong Hu, NASA LaRC, Exploratory studies using CALIPSO and HSRL observations to diagnose ocean color (proposal pending)

HSRL Ocean Measurements

What can be measured:

beam attenuation coefficient,
particulate backscatter, profiling
capability

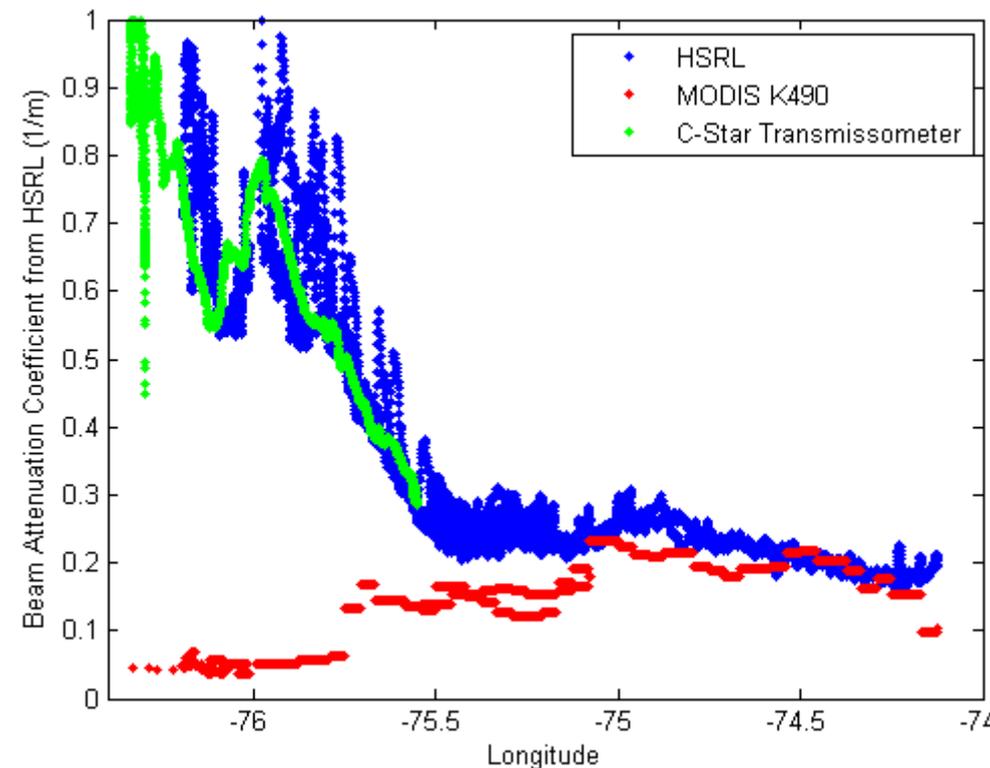
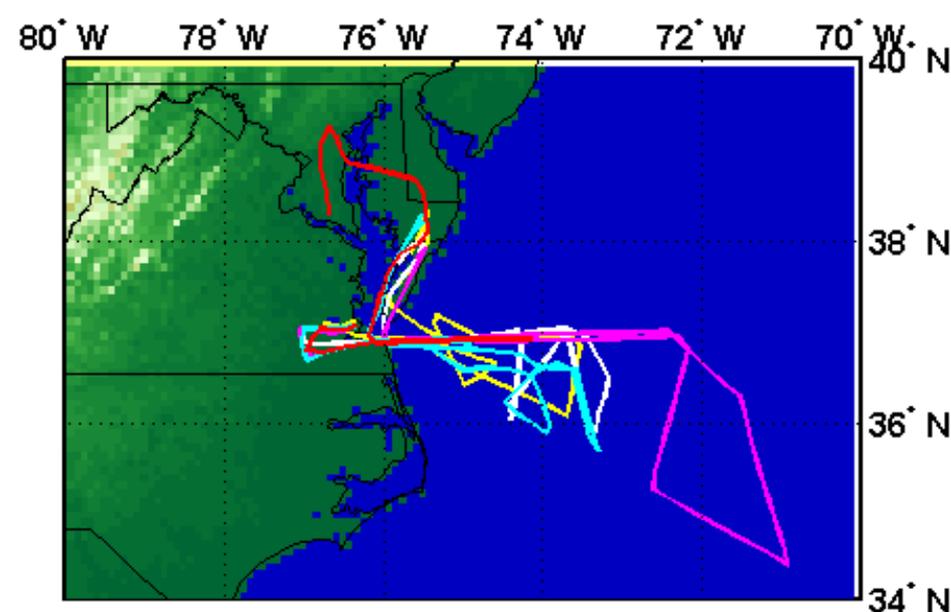
Potential applications:

1. Validation of ocean color retrievals
2. Assisting new retrieval algorithm development
3. Reducing uncertainty of net primary productivity

Recent aircraft/boat measurements:

Aircraft: HSRL (LaRC), RSP (Cairns)

Boat: Vertical profiling of optical properties in water (Zimmerman of ODU, Gilerson of CCNY); multi-angle polarization probe (in water and above water) (Gilerson of CCNY)



DISCOVER-AQ Science Reviews: Points to Consider

Two major weaknesses (summarized below) relate to the depth of the theory team and the lack of flight time devoted to process studies.

“Recommend additional science team members to broaden the 3D modeling component...”

“Recommend extending the length of the first three deployments and dropping the fourth deployment. This would improve statistical sampling and allow additional process oriented flights focusing on urban plume chemistry and aerosol formation needed for regional 3D modeling activities.”

No weaknesses identified for TMLC (Technical and Management approach, Logistics, and Cost)

If we live up to TMLC rating, then reserves may be available to address weaknesses.