Executive Summary

DISCOVER-AQ (Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality)

DISCOVER-AQ provides an opportunity to bridge the existing knowledge gap severely limiting the relevance of satellite observations to air quality. Although great strides improving air quality have resulted from measures taken since the inception of the Clean Air Act, regions of non-attainment for air quality standards are increasing. This is driven in part by the tightening of air quality standards in light of improved understanding of what constitutes harmful pollutant levels. It is also related to increasing difficulty in attaining incremental reductions in the face of increasing background levels. As a result, progress in reaching air quality goals has begun to plateau for many locations.

Near-surface pollution is one of the most challenging problems for Earth observations from space. Nevertheless, the potential benefits of satellite observations to air quality are myriad. These include improved forecasting ability for current air quality conditions, assessment of air quality for purposes of attribution to specific causes, and improved estimation of emissions which undergo constant change.

To date, many millions of dollars have been spent on satellite measurements to address air quality issues. Through the Decadal Survey implementation and international efforts, billions more will be spent. By comparison, the $30M proposed for DISCOVER-AQ represents a modest investment with the potential for dramatic improvement in the applicability of satellite observations for this important problem.

DISCOVER-AQ will focus squarely on NASA's goals to study the Earth from space to increase fundamental understanding and to enable the application of satellite data for societal benefit. The overarching objective of the mission is to improve the interpretation of satellite observations to diagnose near-surface conditions relating to air quality. This will be achieved through concurrent, integrated observations of column abundances and surface concentrations for key trace gases and aerosols throughout the day. These observations will be used to:

1) Relate column observations to surface conditions for aerosols and key trace gases O_3, NO_2, and CH_2O
2) Characterize differences in diurnal variation of surface and column observations for key trace gases and aerosols
3) Examine horizontal scales of variability affecting satellites and model calculations

The DISCOVER-AQ observation strategy will employ two aircraft, NASA's P-3B and B200, and a network of ground sites to monitor key trace gases and aerosols throughout the day from multiple perspectives. Flights will be integrated with existing surface sites for research as well as operational monitoring sites that report data to EPA's Air Quality System (AQS) national repository. Remote sensing of the atmospheric column will be accomplished from the NASA B200 with nadir observations of aerosol profiles and trace gas columns using the High Spectral Resolution Lidar (HSRL) and the Airborne Compact Atmospheric Mapper (ACAM), respectively.

Concurrently, trace gas and aerosol columns will be monitored from below with one dozen Pandora sun-tracking spectrometers, five AERONET sun-photometers, and two aerosol lidars integrated with existing AQS sites. The P-3B will be used to provide in situ profiling of trace gases and aerosols beneath the B200 and above selected ground sites throughout the day. The P-3B instrument suite includes seven instrument teams providing in situ trace gas and aerosol observations. Additional research-grade surface measurements and ozonesondes will be provided by the NATIVE research trailer as well as research-grade NO_2 measurements at three sites to be furnished by EPA collaborators.

After an initial year of preparation, annual deployments of 30 days are planned for a different location each year. The nominal deployment schedule includes Baltimore-Washington (July 2011), Houston (Sept. 2012), Sacramento (Feb. 2013), and a final site (June 2014) to be determined based on experience gained in the first three deployments. Analysis of observations will occur in parallel with the annual deployments and it is anticipated that subsequent deployments will benefit from lessons learned in previous outings.

The science team will employ multivariate statistical techniques, retrieval algorithms, and regional chemical transport models to assess the factors influencing the spatial and temporal variability in surface concentrations and column abundances and their correlation.

Expected outcomes include fundamental improvement in our understanding of the factors governing surface versus column variability, improved understanding of diurnal variability, and improved characterization of variability at scales finer than current models and satellites can resolve. **This knowledge will be invaluable in leading to more effective use of current satellite observations, more effective design and observing strategies for future satellites, and improved air quality models.**

Dr. James Crawford (NASA Langley) will lead the DISCOVER-AQ team as the Principal Investigator. He will be assisted by a Project Manager (Dr. Mary Kleb, NASA Langley), a Project Scientist (Dr. Kenneth Pickering, NASA Goddard), and a Science Data Manager (Dr. Gao Chen, NASA Langley). The DISCOVER-AQ team is composed of 21 investigators and 63 total participants representing three NASA Centers, four universities, and one foreign institution. The team includes four post-docs and six graduate students. Additional educational opportunities will be pursued through externally sponsored NPP, GSRP, and NASA summer student programs.

The success of DISCOVER-AQ will rely heavily on local partners and EPA as deployment strategies will require their expert knowledge and input concerning the factors governing air quality in each specific deployment site. Great interest on the part of collaborators has also been expressed concerning the DISCOVER-AQ observations, so it is anticipated that analysis and use of observations will extend well beyond the DISCOVER-AQ investigators from the start.

Table of Contents

1. Science Investigation..... 1
    1.1. Background..... 1
    1.2. Science Goals and Objectives..... 1
    1.3. Relevance to NASA's science goals..... 6
    1.4. Investigative Approach..... 7
2. Science Implementation..... 10
    2.1. Science Investigation Concept..... 10
    2.2. Science Data..... 12
        2.2.1. Data analysis approaches..... 14
        2.2.2. Data Management..... 17
    2.3. Science Team..... 17
3. Investigation Implementation..... 18
    3.1. Measurement Platform System Capabilities..... 18
    3.2. Instrumentation..... 19
        3.2.1. P-3B Instrumentation..... 19
        3.2.2. B200 Instrumentation..... 21
        3.2.3. Ground Instrumentation..... 23
    3.3. Assembly, Integration, Test..... 24
4. Management..... 25
    4.1. Management Approach..... 25
    4.2. Risk Management..... 27
    4.3. Schedule..... 28
    4.4. Descope Options..... 29
5. Cost and Cost Estimating Methodology..... 29
6. Additional Documentation..... 33
    6.1. Work Breakdown Structure (WBS)..... 33
    6.2. WBS Dictionary..... 34
    6.3. Detailed Costs..... 39
    6.3.1. Cost Tables, Budget Justifications, and Statements of Work..... 40
    6.3.2. GSFC Omnibus Budget Justification..... 221
    6.4. Curriculum Vitae..... 226
    6.5. Letters of Commitment..... 265
    6.6. Letters of Support and Collaboration..... 277
    6.7. Current and Pending Support..... 291
    6.8. Discussion on Compliance with US Export Laws and Regulations..... 314
    6.9. Abbreviations and Acronyms..... 314
    6.10. References..... 316

1. Science Investigation

1.1. Background

Near-surface pollution is one of the most challenging problems for Earth observations from space [*Fishman et al.*, 2008; *Martin*, 2008; *Hoff and Christopher*, 2009]. Currently, active remote sensing of aerosols by CALIPSO provides the only direct observation of near-surface pollution, albeit for a very small nadir footprint. Otherwise, near-surface information must be inferred from column-integrated quantities obtained by passive remote sensing from nadir-looking satellite instruments. While these broad swath sensors have the advantage of providing global coverage, the interpretation of column-integrated observations is complicated by several factors. The most significant challenge exists for constituents with large relative concentrations in the stratosphere and/or free troposphere (e.g., ozone and NO_2), making it difficult to distinguish the near-surface contribution to the total column. This is mitigated for NO_2 since its stratospheric variability can be compensated and removed. Diminished sensitivity near the Earth's surface is another fundamental problem. In the case of NO_2 and aerosols, this problem is partially alleviated by the fact that their near-surface abundance can dominate the total column amount, particularly in polluted areas. Additional challenges exist in the horizontal dimension as the resolution of current satellites and models cannot account for important sub-grid variability in ozone precursors (e.g., NOx) and their associated nonlinear chemical impacts.

The desire to improve interpretation of satellite observations to diagnose near-surface conditions is in strong alignment with NASA's Science Strategy and Applied Science Goals aiming to "Study planet Earth from space to advance scientific understanding and meet societal needs" with the expectation of "Progress in understanding and improving predictive capability for changes in the ozone layer, climate forcing and **air quality** associated with changes in atmospheric composition." Success in achieving these goals relies heavily on fundamental understanding of how satellite data can be used to infer surface conditions more quantitatively, not just for prediction, but also for assessment studies and top-down emissions estimation in a changing environment. Developing these capabilities not only strengthens the interpretation of current satellite observations (e.g., OMI and MODIS) but will be required to ensure the success of several future Decadal Survey missions (GEO-CAPE, ACE, and GACM) that have air quality as an important focus.

Concurrent, integrated observations from suborbital platforms and surface sites of column abundances, surface concentrations, and in situ profiles for relevant trace gases and aerosols will allow for a detailed examination of the relation between column-integrated and surface quantities throughout the day across urban areas due to the influences of varying emissions, chemistry, and meteorology. This information will lead to improved interpretation of satellite observations, more effective strategies for data assimilation, and improved air quality models.

1.2. Science Goals and Objectives

To diagnose air quality conditions from space, reliable satellite information on aerosols and ozone precursors is needed for specific, highly-correlated times and locations. A significant science question is how satellite observations of column-integrated quantities can be effectively used to interpret concurrent near-surface conditions. DISCOVER-AQ will provide an integrated dataset of airborne and surface observations relevant to the diagnosis of surface air

quality conditions from space. The following discussion details the specific science objectives, associated questions, and expected outcomes that drive the suite of measurements and experimental design for the proposed deployments.

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

Simple correlations between satellite observations of column aerosol optical depth (AOD) and surface PM2.5 exhibit highly inconsistent behavior [*Hoff and Christopher*, 2009]. As highlighted in Figure 1, there can be geographical tendencies such as correlations tending to be worse in the western United States [*Engel-Cox et al.*, 2004] that could be related to variations in several factors such as vertical distribution, humidity, surface albedo, aerosol source and type. The use of lidar observations to assess boundary layer depth and the vertical distribution of aerosols has been demonstrated to be an invaluable tool for improving correlations between satellite AOD and surface PM2.5 observations [*Engel-Cox et al.*, 2006]. Recent field work in California [*Al-Saadi et al.*, 2008] and a 3-year analysis in Taiwan [*Tsai et al.*, 2009] using airborne (HSRL) and ground-based measurements (MPLnet/AERONET), respectively, suggest that lidar estimates of boundary layer depth can be used to normalize satellite observations of column AOD to dramatically improve correlation with surface PM2.5 observations. Additional data are needed to determine the degree to which this approach is successful in other regions as well as to determine the horizontal scales over which a given observation of boundary layer depth can be usefully applied, and whether we can use model predictions for this parameter if lidar data are not available. This calls for short-term oversampling of a region to determine the spatial resolution required for sustained observations of boundary layer depth (and/or model-derived estimates) to be effective in relating surface PM2.5 to column AOD observations. Another variable in need of attention is water vapor. The measurements of PM2.5 used for regulatory purposes

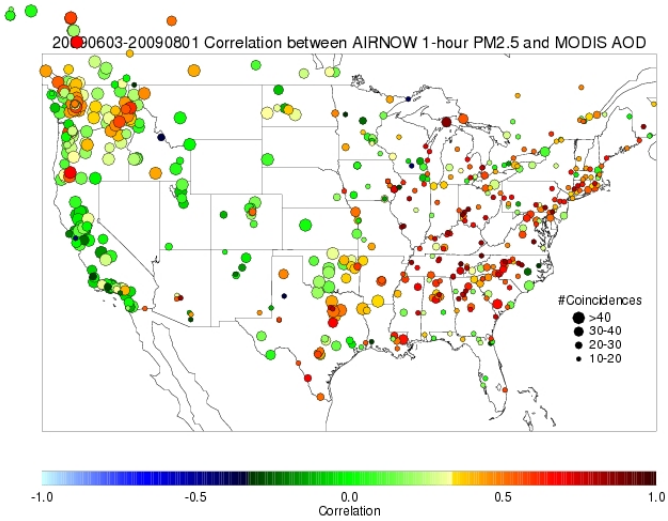


Figure 1. Correlation between MODIS AOD and surface PM2.5 for 3 June - 1 August 2009. (http://www.star.nesdis.noaa.gov/smcd/spb/aq/)

are based on dry aerosol mass, while satellite AOD measurements are based on ambient, humidified aerosol. Correction for this important difference requires knowledge of the water vapor column amount and profile.

For trace gas observations, NO_2 stands out as the key satellite-observed quantity related to air quality due to several factors. First is its importance as a precursor of ozone. Most urban regions are NO_x-limited for ozone production. The short lifetime of NO_2 also makes its distribution useful for combustion source mapping. Finally, the distribution of atmospheric NO_2 is weighted toward the surface, due to the temperature dependent partitioning of NO_x ($NO+NO_2$), such that in polluted regions, the total column variability is dominated by the near-surface distribution. All of that aside, satellite observations of NO_2 often exhibit little direct correlation to daily surface observations without significant application of local scaling factors from a model [*Lamsal et al.*, 2008], although long-term averages are useful in providing qualitative information on the distribution and magnitude of emissions. An important problem limiting the effective use of satellite NO_2 observations is the lack of a network of validating surface observations. Current instruments in use by the EPA's Air Quality System (AQS) network measure NO_2 via catalytic conversion to NO and subsequent detection by chemiluminescence [*Demerjian*, 2000]. The catalytic conversion step uses a molybdenum converter heated to 400°C which is non-specific to NO_2 and results in additional production of NO from thermally labile reactive nitrogen species (e.g., PAN, alkyl nitrates) and even evidence for conversion of some HNO_3. Discrepancies in NO_2 have been documented to be as high as 50% [*Dunlea et al.*, 2007] in Mexico City; however, *Lamsal et al.* [2008] estimate a more conservative but significant bias of 11-36% across the AQS and Canadian NAPS networks. More observations of NO_2 are needed based on photolytic conversion which is specific to NO_2 as well as direct methods (e.g., laser-induced fluorescence and cavity ring-down spectroscopy).

Formaldehyde (CH_2O) represents the class of other essential ozone precursors, volatile organic carbon (VOCs), in that it is a common oxidation product of the photochemical degradation of the diverse mix of atmospheric hydrocarbons. Thus, it provides an integrated measure of VOC oxidation. It is also short-lived (2-6 hours) with a distribution weighted heavily towards the surface and no stratospheric burden. While anthropogenic hydrocarbons are not unimportant (especially in urban areas), satellite observations clearly demonstrate the dominance of biogenic emissions (i.e., isoprene) as the dominant source [*Millet et al.*, 2008] for the preponderance of the globe. Validating observations are practically nonexistent except for sporadic observations from airborne field campaigns (e.g., INTEX-B and ARCTAS). Any focused sampling of atmospheric CH_2O would be of immeasurable value to improving the quantitative value of satellite observations for this important constituent.

As the criteria trace gas pollutant, ozone (O_3) is the ultimate focus of satellite observations of air quality. However, its near-surface distribution is the least likely to be directly observed from space due to its dominant stratospheric burden. Even large changes in boundary layer ozone during pollution events are small compared to the total column (e.g., an O_3 increase of 50 ppbv in the lowest 2 km would be equivalent to ~7.5 DU compared to a typical total column amount of ~300 DU over summertime North America). This presents a daunting challenge for direct observation of O_3 exceedances. Nevertheless, detailed in situ and column observations of O_3 are critical for any air quality study for several important reasons. First, total O_3 controls

photolysis frequencies and the photochemical oxidation chemistry responsible for its catalytic production. O_3 also controls the partitioning of NO_x ($NO+NO_2$) making it critical to deriving total NO_x emissions from space-based observations of NO_2. Finally, O_3 observations also provide a critical test of air quality model predictions, particularly those attempting to benefit from assimilation of satellite data for precursors.

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

Current polar-orbiting satellites provide information once or twice per day on air quality constituents. The call for geostationary observations in the Decadal Survey by the GEO-CAPE satellite promises to address the critical need to observe aerosols and trace gases as they change throughout the day. NOAA, South Korea, and ESA, too, are planning for geostationary air quality missions. Interpretation of such observations, however, will rely on a clear understanding of the various factors controlling near- surface versus column variability. This is illustrated by results for NO_2 diurnal variation shown in Figure 2 from a simulation by the EPA CMAQ model for Houston Texas (results provided courtesy of Drs. Jack Fishman and Daewon Byun). For instance, emissions will influence both surface and column quantities similarly while changes in boundary layer depth will have much greater influence on surface concentrations as compared to the total column. This is seen in the figure as both column and surface NO_2 increase in the morning due to rush hour traffic emissions; however, the onset of growth in the boundary layer serves to dilute surface NO_2 while column NO_2 continues to increase. The impacts of horizontal dispersion and chemistry lead to dramatic decreases in both quantities by early afternoon coincident with the overpass of the OMI instrument onboard NASA's Aura satellite. An analysis by *Lamsal et al.* [2008] suggests that "annual mean 24-hour average concentrations are 36% higher than those at the OMI overpass time of ~13:00 over North America." While observations are needed to validate these modeled behaviors, current satellites do not

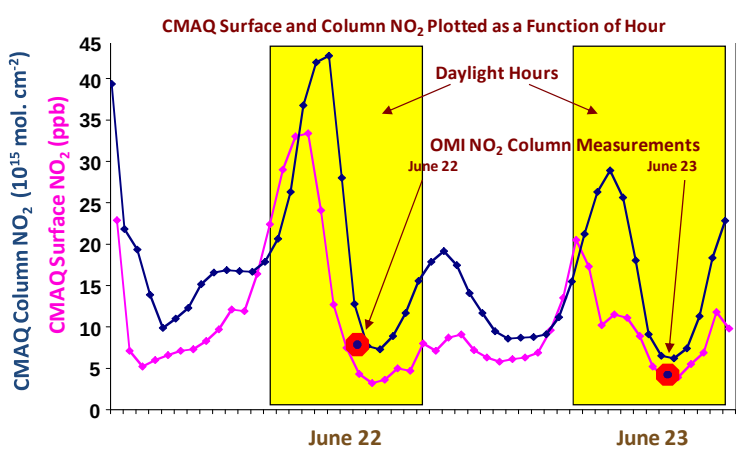


Figure 2. Diurnal variation in column integrated and surface NO_2 as simulated by EPA's CMAQ model for Houston, Texas

offer diurnally resolved observations of trace gases or aerosols. Analysis of morning and afternoon overpasses (e.g., SCIAMACHY and OMI for NO_2; Terra and Aqua for MODIS AOD) have been evaluated for evidence of differences associated with diurnal variation [*Boersma et al.*, 2008; *Ichoku et al.*, 2005], but two observations are insufficient for evaluating diurnal variability. Surface lidar measurements have shown that there can be considerable diurnal variability in the vertical distribution of aerosols and water vapor within the lowest few kilometers [*Ferrare et al.*, 2002]. Understanding the interplay between emissions, mixing, and chemistry will require continuous and concurrent monitoring of trace gas and aerosol columns, profiles, and surface abundances throughout the day. This problem also calls for additional measurements to help diagnose emission sources. Such measurements include CO_2, CO, CH_4, reactive nitrogen, and aerosol inorganic and organic composition. Ultimately, untangling these competing processes must be accomplished with models that are adequately constrained by observations. Results of such analyses hold the promise of improving both retrievals and interpretation of current satellite observations as well as future observations from geostationary orbit. Additionally, observations of the diurnal behavior of column quantities are important for developing the design criteria of geostationary observational platforms since the measurement precision may also have a diurnal criterion as early morning boundary layers are lower while at the same time, sun angles are lower. DISCOVER-AQ can lead to reduced risk in the design phase of GEO-CAPE. Results may also reveal optimal overpass times for future satellites in low earth orbit (e.g., GACM) focused on air quality and pollution.

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

Ozone photochemistry is highly nonlinear with respect to NO_x levels which can vary by several orders of magnitude across urban regions experiencing poor air quality. This is demonstrated by the calculations in Figure 3. Even at spatial resolutions of a few kilometers, it is likely that nonlinear chemistry associated with sub-grid variability (particularly for NO_x) often impacts model predictions of ozone and free radicals for polluted regions. This again calls for intense short-term oversampling to understand the expected variability in aerosols and trace gases at scales much finer than that of current and future models and satellite observations. For aircraft in situ observations, collecting data at 1 hz provides information roughly every 100 meters. In combination with airborne remote sensors mapping column variability at resolutions approaching 1 km, the impact of sub-grid variability on satellite observations and model calculations could be evaluated. Sampling would need to target a variety of phenomena that

provide a challenge to model and satellite resolution such as plume dispersion under various meteorological conditions; the range of expected atmospheric concentrations under weekend versus weekday emissions or over locations dominated by point versus area sources; and locations with variable surface conditions or topography expected to affect retrievals. Multi-scale modeling to represent these variations at differing resolutions would be useful to assess the impact of resolution on satellite observations and model predictions. Statistical analysis of these variations (e.g., variogram analyses) would also provide a framework for evaluating expected sub-grid gradients for a given satellite resolution. Should results provide some level of predictability for sub-grid variability, variograms could provide the basis for sub-grid parameterizations of nonlinear chemical effects. Ultimately, these data are critical to geostationary instrument design as the spatial and temporal scale tradeoff costs can be large for such a mission.

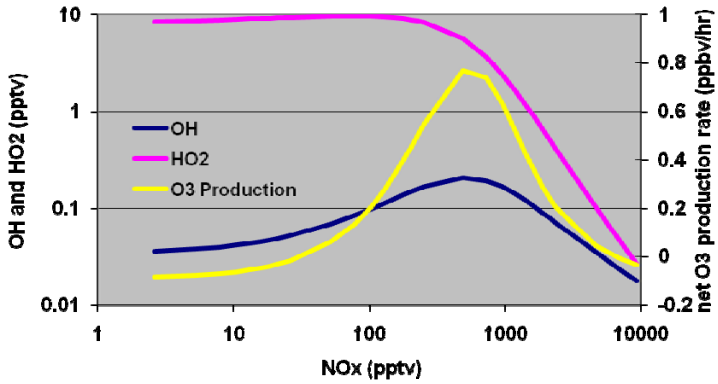


Figure 3. Example calculations of HO_x radicals and O_3 production for a range of NO_x abundances. Precise location of peak and general behavior vary with radical source strength. (J. Crawford, NASA Langley Photochemical Box Model)

1.3. Relevance to NASA's science goals

DISCOVER-AQ aligns with priorities for both the Atmospheric Composition Focus Area and the Applied Sciences Air Quality Program at NASA. Fundamentally, DISCOVER-AQ will provide data needed to critically examine the ability to determine surface air quality conditions from space. The results of this evaluation will support NASA Strategic Goal 3.1: "Study planet Earth from space to advance scientific understanding and meet societal needs" and directly contribute to 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." Findings will enable both short and long-term benefits as they will contribute to improving interpretation of both current and future satellite observations to diagnose, assess, and predict air quality conditions. Potential improvements in the use of current satellite data include improved understanding of the relationships between surface PM2.5 and satellite-derived AOD (e.g. from MODIS, MISR, and GOES-observations) and between surface NO_2 and OMI column NO_2 observations. These results will further translate to several NRC Decadal Survey missions having air quality relevance (GEO-CAPE, ACE, GACM). This includes possible observing strategies (e.g., optimum overpass times for LEO observations) as well as interpretation of observations (e.g., better understanding of column versus surface response to emissions, chemistry, and boundary layer dynamics). Benefits to air quality models will accrue from a better understanding of fine scale variability in NO_x and the associated nonlinearities in ozone chemistry at sub-grid resolutions as well as the ability to assess the impact of fine scale variability on assimilation of satellite observations.

1.4. Investigative Approach

The success of DISCOVER-AQ relies on the 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. This will be accomplished with a combination of two airborne platforms sampling in coordination with relocatable and fixed surface networks. One aircraft would be used for extensive in situ profiling of the atmosphere while the other would conduct both passive and active remote sensing of the atmospheric column extending below the aircraft to the surface. These aircraft would repeatedly overfly instrumented surface locations continuously monitoring both column and surface conditions for select variables throughout the day. Specific platforms and instruments are outlined below.

Airborne in situ profiling: This component of the DISCOVER-AQ observing strategy would employ the NASA P-3B. Measurements directly related to satellite observations of air quality will include O_3, NO_2, CH_2O, and aerosol optical and microphysical properties. Additional critical variables needed for retrievals and data interpretation include atmospheric state (T, P, winds), H_2O, CO, CH_4, CO_2, NO, the components of reactive nitrogen, and aerosol inorganic and organic composition. The proposed P-3B instruments are well characterized having been deployed previously on multiple airborne campaigns and used in published research findings.

Airborne remote sensing: This component of the DISCOVER-AQ observing strategy would employ the NASA B-200 with two instruments onboard. Aerosol observations would be accomplished with the High Spectral Resolution Lidar (HSRL) (http://science.larc.nasa.gov/hsrl/) [*Hair et al.*, 2008] which would provide both column-integrated and vertically-resolved information on aerosols below the aircraft. Observations from HSRL will also be useful for diagnosing boundary layer depth. Trace gas column observations below the aircraft will be conducted with the Airborne Compact Atmospheric Mapper (ACAM). HSRL produces science quality data and has been deployed extensively onboard the NASA B-200 in support of CALIPSO validation as well as science campaigns for NASA, DOE, and EPA. ACAM has been fielded on NASA WB-57 aircraft and has demonstrated the ability to collect trace gas observations of O_3, NO_2, and SO_2 over the Houston area. Only minor improvements are needed for ACAM to produce science quality data.

Surface observations: The primary component of the surface network will be the Pandora instrument [*Herman et al.*, 2009], a sun-tracking UV-visible spectrometer capable of continuous monitoring of trace gas columns for O_3, NO_2, and CH_2O throughout the day. Pandora has demonstrated capability, is relatively low-cost, and can be left unattended making it ideal for use in a distributed network. However, the current number of operating instruments (four) is inadequate and fabrication of additional units is required to satisfy the need to broadly sample trace gas columns over selected urban areas and under aircraft flights. To the greatest extent possible, it is intended that these instruments would be located alongside O_3, NO_2, and PM2.5 monitors within EPA's AQS network (http://www.epa.gov/ttn/airs/airsaqs/) providing in situ information on surface conditions. Five AERONET sun-photometers will be procured by the project to ensure adequate coverage in each study region. Other existing ground assets (e.g., local research sites) will also be considered in the placement of Pandora instruments. Detailed

observations at an anchor site will provide important context for the more limited observations throughout the surface network. This support will come from the Nittany Atmospheric Trailer and Integrated Validation Experiment (NATIVE) which will include in situ observations of trace gases (O_3, CO, NO, NO_y, SO_2), aerosol lidar observations, and balloon soundings of ozone and water vapor. Additionally, UMBC will relocate an MPL and Leosphere scanning lidar in support of field observations, while the full suite of observations at the UMAP site will support flights in the Baltimore area (to be discussed in section 2).

Modeling and Analysis: Interpretation of the DISCOVER-AQ observations will involve statistical analyses as well as a hierarchy of models. Statistical analysis of observations will include basic correlative studies of column versus surface observations. These correlations will be evaluated in terms of other key variables such as boundary layer depth, humidity, location, time of day, day of the week, etc. Vertical profiles of constituents at various locations and under various meteorological regimes will be examined for patterns that may allow for simple conceptual models useful for deriving surface information from column observations. Vertical profile and column observations will be evaluated in the context of current retrieval methods and the potential for improvements. The use of regional models will play an important role in helping to capture how the interplay of emissions, chemistry, and dynamics are expected to affect column versus surface quantities. In turn, observations will be used to evaluate model success at capturing observed variations. Fine scale variability in near-surface observations will be evaluated using auto-covariance and variogram techniques. Effects of fine scale variability on model predictions of ozone will also be assessed. Finally, lessons learned from the analysis of DISCOVER-AQ observations will be applied to current satellite overpasses (e.g., Terra, A-Train, as well as non-NASA satellites) to assess their impact on satellite retrievals and interpretation.

Overlapping measurements: For DISCOVER-AQ to succeed in addressing stated science objectives, concurrent observations of column and in situ aerosols and key trace gases must be accomplished along with supporting measurements to aid retrievals, interpret emission sources, and diagnose mixing. The suite of specific variables and overlapping measurements to be conducted within the DISCOVER-AQ sampling strategy are listed in Table 1.

Opportunity for Interdisciplinary Science: During the recent GEO-CAPE Science Working Group meeting (22-24 Sept. 2009), better definition of the atmospheric correction for ocean color measurements was identified as a critical need. Atmospheric aerosols present an interfering signal larger than that associated with ocean color itself [*Gordon*, 1997]. Another often neglected source of interference is associated with high levels of NO_2 in the outflow of urban plumes over coastal waters [*Ahmad et al.*, 2007; *Crawford et al.*, 2008]. The DISCOVER-AQ airborne observations are ideally suited to characterize the small-scale variability in aerosols and NO_2 relevant to the atmospheric correction requirements for the planned GEO-CAPE ocean color observations. Discussed in section 2, DISCOVER-AQ deployment sites allow for observations over the Chesapeake Bay and to a limited degree over the Gulf Coast. These observations can be accomplished with minimal impact to primary DISCOVER-AQ science objectives. While the over water data would not be the primary focus of DISCOVER-AQ analysis, the data would be archived and freely available to the GEO-CAPE Science Working Group and any other interested parties. It should be noted that the DISCOVER-AQ PI and

several Co-I's are members of the GEO-CAPE Science Working Group, and they are committed to ensuring that these data are not overlooked in the analyses of GEO-CAPE ocean color science requirements. Significant additional value will be provided by ocean subsurface beam attenuation and particulate backscatter products retrieved from the HSRL data. The beam attenuation parameter has been validated with in situ measurements on an ODU research vessel during overflight by the B200 (Yongxiang Hu, LaRC, pers. comm.). EPA has also expressed interests in joint flights to test a set of hyperspectral ocean color radiometers onboard NASA's Cessna 206 (see EPA support letter).

Table 1. DISCOVER-AQ Trace Gas and Aerosol Observations

Trace Gas Observations	O_3	NO_2	CH_2O	NO	NO_y	CO	CO_2	CH_4	H_2O	VOC
Pandora, total column[1]	X	X	X						X	
ACAM, nadir column (B200)[2]	X	X	X							
In situ airborne profiles (P-3B)[3]	X	X	X	X	X	X	X	X	X	X
In situ surface observations (AQS)[4]	X	X			X	X			X	X
NATIVE in situ surface observations[5]	X			X	X	X			X	
NATIVE sondes[6]	X								X	
Aeronet[7]									X	

Aerosol Observations (X) = dry aerosol measurement	AOD	PM2.5	Scattering	Absorption	Extinction	Non-Sphericity	f(RH)	Black Carbon	Soluble Ions	Size Distribution	PBL Height
HSRL, nadir aerosol profiles (B200)[2]	X		X[10]		X	X					X
In situ airborne profiles (P-3B)[3]	(X)[9]		(X)	(X)	(X)		X	X	X	(X)	X
In situ surface observations (AQS)		(X)									
NATIVE lidar[5]			X[10]								X
UMBC UMAP site with AERI	X	X	X[10]		X[11]		X[12]			X	X
AERONET[7]	X			X						X	
Pandora[8]	X		X	X							

1 - Surface network of 12 Pandora instruments to be integrated with existing sites (e.g., AQS)
2 - B200 will fly a repetitive track over the surface sites throughout the morning and afternoon (midday refuel required)
3 - P-3B will profile the boundary layer over 6 sites 3-4 times daily. Profiles may extend up to 5 km, but will rely on guidance from HSRL regarding the presence of plumes aloft.
4 - Individual AQS sites may not have all measurements listed, and NO_2 measurements do not discriminate against thermally labile reactive nitrogen species. At least one EPA NCORE site is located in each deployment region and will be instrumented with high-quality, research-grade instrumentation. EPA is also planning to field three research-grade NO_2 instruments in support of DISCOVER-AQ (see support letter).
5 - NATIVE will be located to best augment the existing network.
6 - Daily ozonesondes to be launched providing profiles of O_3, RH, and T through the troposphere into the stratosphere
7- Five AERONET instruments will be procured for this project.
8 - UV wavelengths (265-500 nm)
9 - AOD derived from integrated in situ measurements
10 - Aerosol backscatter is a more accurate description for lidar observations
11 - Assumes co-location with AERONET
12 - AERI and Raman H_2O lidar

2. Science Implementation

2.1. Science Investigation Concept

DISCOVER-AQ will proceed as a 5-year experiment consisting of an initial year of planning and preparation followed by four years with a 30-day deployment each year to various urban areas with histories of experiencing violations of air quality standards for ozone and/or PM2.5. Analysis and modeling activities will be an ongoing effort taking advantage of the full body of observations as each deployment adds new information. While a detailed schedule is offered in section 4.3, a general outline of activities and example flight plans to accomplish science objectives are outlined below.

First Year Preparations: Critical activities for the first year preparations and planning activities include the fabrication of one dozen Pandora instruments, upgrades to airborne instrumentation, drafting aircraft payload integration plans, and arrangements for integration of ground equipment with existing AQS and permanent research sites for the first deployment. Depending on the acquisition schedule of Pandora instruments, early positioning and data collection prior to the aircraft deployment will be considered.

Annual deployments in years 2-5: Each year, a 30-day deployment is planned to focus on an urban area known for exceeding air quality standards. At this time, candidate locations include the Baltimore-DC area, Houston, Sacramento (not necessarily in that order), and a final location (possibly Los Angeles, Birmingham, or Atlanta) based on information gained in the first three deployments. These locations are chosen for the variety in the factors contributing to their local air quality problems (e.g., upwind emissions, transportation, industrial emissions, agriculture), diversity in meteorology and surface conditions, and proximity to NASA installations, thus enabling the efficient and cost-effective deployment of aircraft. **While each of these locations have been the focus of previous air quality airborne field campaigns, the sampling strategy proposed here is unique and specifically tailored to the goal of improving satellite capability to interpret near-surface air quality conditions.**

Baltimore-Washington, DC: The Baltimore-Washington corridor experiences poor air quality throughout the year for PM2.5 while high ozone tends to be limited to the April-September time frame (Maryland Dept. of the Environment, Air Quality Seasonal Reports, 2008). However, both pollutants historically peak in the June-August timeframe, making a summer deployment desirable for this location. Emissions associated with transportation, biogenic emissions, and transport of background pollution from upwind locations all play an important role in generating poor air quality over this region. Alongside the existing AQS sites, this region also has two permanent research sites (Beltsville and UMBC) focused on air quality. For this deployment, each aircraft would conduct science flights from their home location (see Figure 4). As noted earlier, this would allow for sampling over the Chesapeake Bay on the way to and from the focus region. As shown in figure 4, both aircraft would follow the same ground track over selected AQS and research ground sites with an option to fly further east to observe conditions over the Chesapeake Bay (yellow track). From 7 km, the B200 would fly throughout the day, with a refueling break at midday, providing a continuous view of the evolution of aerosol profiles and trace gas columns along the track. The P-3B would fly more deliberately,

stopping to profile over six of the ground sites on each pass. While profiles will nominally cover the 0.3-5 km altitude range, the upper altitude of profiles may be adjusted based on HSRL observations of PBL depth and the presence of any pollution plumes aloft. While the flight strategy presented in Figure 4 is accurate, ultimate flight plans for this and other candidate locations will result from an assessment of the current status of AQS sites at the time of deployment, consultation with local air quality authorities and research experts, as well as carefully negotiated air traffic considerations (addressed specifically under section 4.2. Risk Management). Letters of support and cooperation have been secured from the Maryland Department of the Environment and Howard University (Beltsville site).

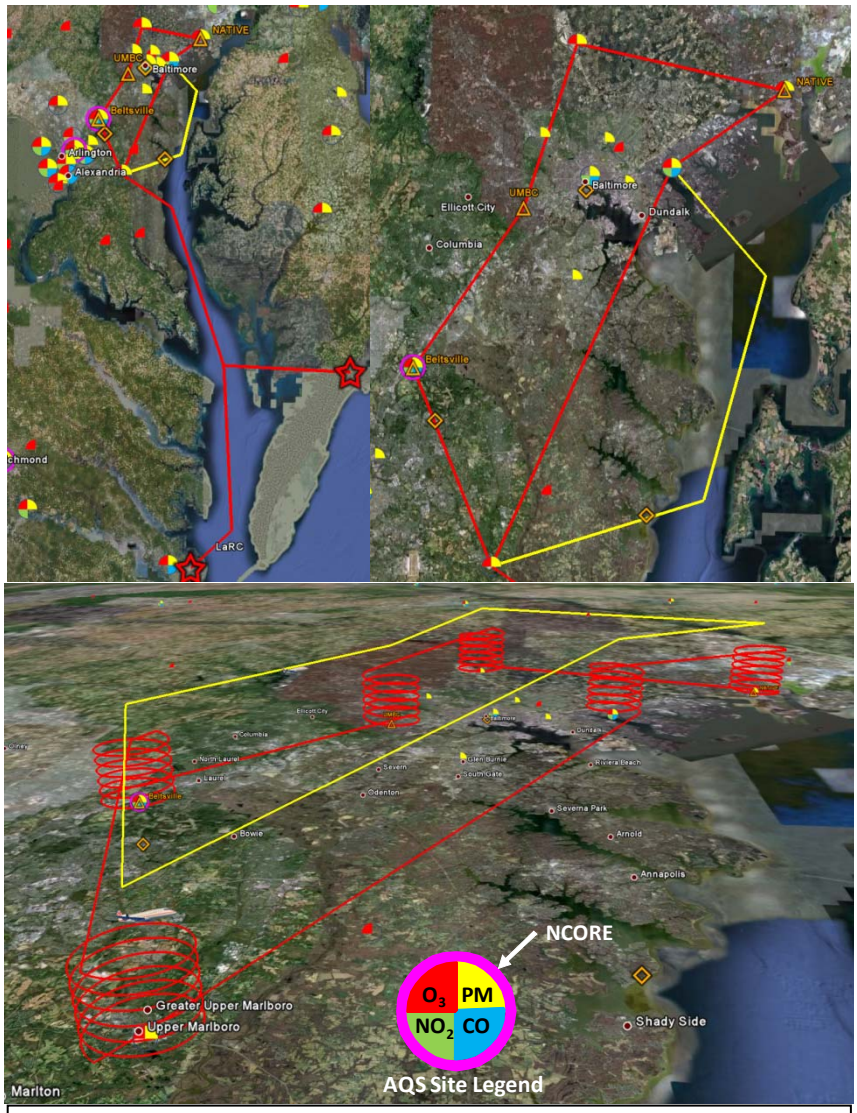


Figure 4. Nominal flight observation strategy for Baltimore-Washington. Upper left panel shows flight tracks for the B200 (LaRC) and P-3B (WFF) between their home base and the focus area. Upper right panel shows the basic ground track (red) over the focus area as well as an optional leg (yellow) to sample over the Chesapeake Bay. Bottom panel offers a 3-D perspective on how the P-3B (red) and B200 (yellow) will fly over the focus area. AQS sites are marked with pie charts denoting the species measured. Orange triangles denote permanent science sites and NATIVE. Orange diamonds denote currently existing Pandora sites.

Houston: For the Houston area, ground level ozone concentrations tend to maximize in the fall with September as the optimal month for deployment [*Nielsen-Gammon et al.*, 2005]. Transportation emissions are again important, however it is the complex, highly reactive chemical mixtures associated with petrochemical emissions that distinguish this location from others. The dominance of land-sea breeze dynamics is another important driver for air quality in this region. For this deployment, flights would be conducted from Ellington Field at NASA

JSC. Letters of support and cooperation for operational partners in this location have been secured from the Texas Commission on Environmental Quality, the City of Houston, and the University of Houston.

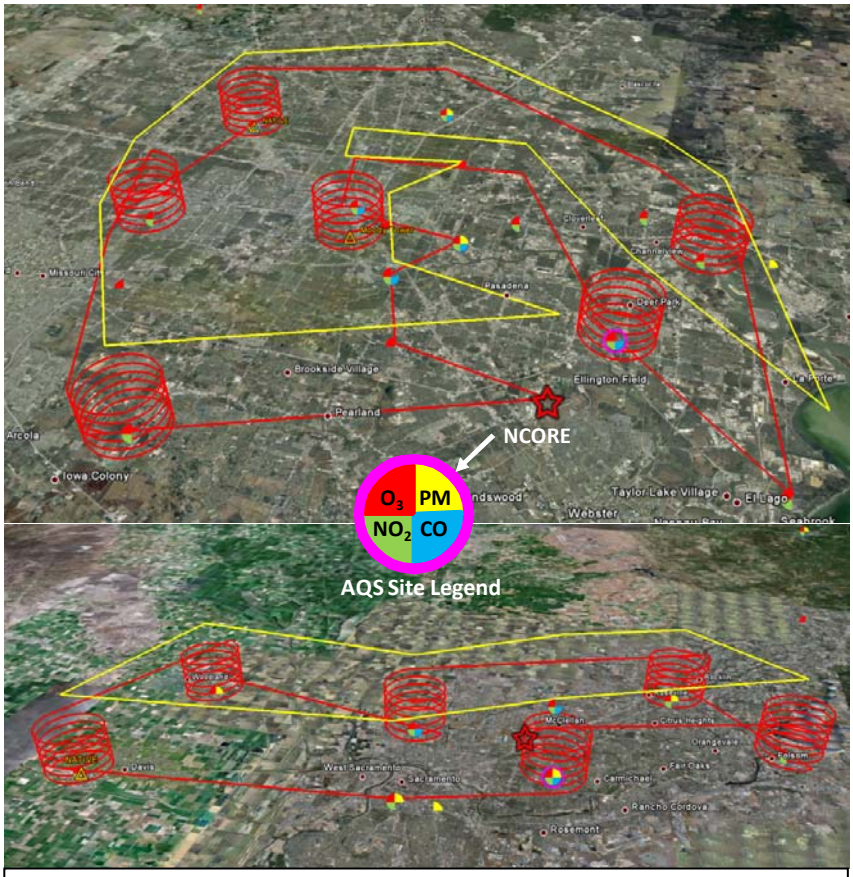


Figure 5. Same as for figure 4 except flights are over Houston (top) and Sacramento (bottom).

Sacramento: In Sacramento, high PM2.5 levels are a concern during October-April, maximizing in the November-February timeframe [*Anderson et al.*, 2007]. Residential wood burning is a dominant influence, however, other large area sources (e.g., transportation, agriculture, road dust, construction) contribute to what is a complex aerosol mixture. Although air quality issues surrounding ozone are not of concern, this location provides an opportunity to assess NO_x emissions during winter months when partitioning favors NO_2 and column amounts are greatest. This deployment site is also unique in the topography of the Sacramento Air Basin, meteorology, and generally higher surface albedo as compared to other deployment sites. For this deployment, flights would be conducted from McClellan Airfield. The prime operational partner in this location would be the California Air Resources Board, CARB (see support letter for details). Previous experience cooperating with them proved critical to the success of DC-8 flights over LA and the Central Valley as part of NASA's ARCTAS campaign.

Los Angeles, Birmingham, Atlanta: Flights to any of these locations in the fourth year would be planned for the June timeframe. While LA boasts the highest density of AQS sites and a strong research partner (CARB), the Southeastern U.S. deployment sites offer the best location for assessing biogenic influences and CH_2O measurements.

2.2. Science Data

The Science Traceability Matrix in Table 2.1 summarizes the DISCOVER-AQ measurement requirements and their relevance to achieving the stated science objectives. Success, however, also involves a subjective judgment regarding the volume of observations required to provide an adequate test of atmospheric models and to support statistically robust analyses of variability in column and surface quantities and the conditions influencing their relationship.

Table 2.1. DISCOVER-AQ Science Traceability Matrix

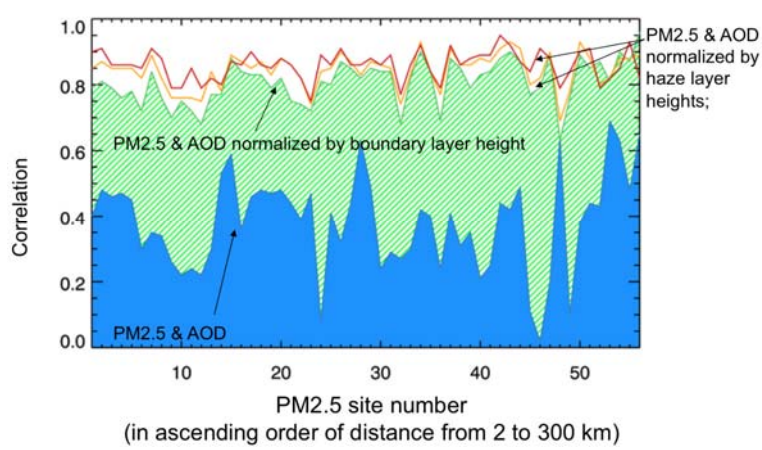
Science Objectives, Associated Questions, and Expected Outcomes	Scientific Measurement Requirements	Instrument Functional Requirements*	Investigation Functional Requirements	Modeling and Analysis Tools
Objective 1: Relate column observations to surface conditions for aerosols and key trace gases O_3, 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?* **Outcome:** Improved understanding of the extent to which column observations (as observed from space) can be used to diagnose surface conditions	Concurrent, urban-scale observations of column and in situ aerosols, O_3, NO_2, and CH_2O from aircraft and ground sites Observations of boundary layer depth, T, winds, and water vapor (column and profiles)	Active remote sensing of aerosols between surface and aircraft level with horizontal and vertical resolution of 1 km and 60m (backscatter and depolarization) 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 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) 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 Ground-based, vertically-pointing lidar observations with 10 m and 10 minute resolution to provide 24-hour monitoring of aerosol profiles *Specific instrument capabilities are listed in Tables 3.1-3.7	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 Airborne profiling with a dedicated platform to observe in situ vertical distribution of key trace gases, humidity, and boundary layer depth Distributed surface network to provide in situ and total column observations for key trace gases and aerosols One or more ground-based lidars to provide aerosol profiles	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. Retrieval models capable of reanalysis of remote sensing measurements including information at a range of spatial resolution
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?* **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	Continuous observation of column and in situ aerosols, O_3, NO_2, and CH_2O throughout daylight hours Key trace gas and aerosol observations identifying the influence of source emissions and chemistry (e.g., CO, CO_2, CH_4, reactive nitrogen, aerosol inorganic and organic composition)		All of the above plus: 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 Observation of trace gas total columns at surface locations throughout daylight hours 24-hour observation of in situ trace gases and lidar aerosol profiles	All of the above plus: 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
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?* **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	Observe horizontal gradients in column and in situ aerosols, O_3, NO_2, and CH_2O as well as pollution tracers CO, CO_2, CH_4, and reactive nitrogen		High spatial resolution observations collected along flight transects to resolve variability down to scales of 100 m. 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	Statistical analysis of spatial variability to characterize expected sub-grid gradients for coarser resolution satellites and models Multi-scale modeling to assess influences of model resolution on nonlinear chemical processes

For purposes of this project, 100 flight hours per aircraft per deployment is recommended. After accounting for test and transit hours, each deployment will have 80 to 90 hours available for science flights. This allows for at least ten days of detailed airborne sampling during the 30-day deployment period. During each 8-hour flight, the P-3B should be able to accomplish a minimum of three profiles over each of six surface sites (assumes 30 minute circuit and 15 minutes per profile). Likewise, the B200 should be able to complete a minimum of six circuits in the morning and another six in the afternoon. (These are conservative estimates based on use of the Langley flight planning tool used on previous field campaigns.) Over ten flights, this would result in 180 profiles from the P-3B and 120 data curtains from the B200 available for use with the continuous surface observations. These numbers could be reduced due to uncooperative weather conditions or temporary malfunction of a given instrument; however, vigilant monitoring of instrument performance and use of operational (e.g., NCEP WRF/CMAQ) weather and air quality forecasts to plan flights should minimize unproductive use of flight hours. While clear skies will be targeted most often for this work, sampling under conditions of fair weather cumulus is likely to be common and will be useful in improving the handling of cloud issues affecting satellite retrievals. As noted earlier, collection of data during transits and circuits over the Chesapeake Bay to assess atmospheric correction statistics for ocean color will not have a significant impact on meeting these goals. More limited opportunities for such observations over the Gulf coast and Mississippi Delta region will also be possible during transits to and from Houston. Flights will also target a mix of weekend and weekdays periods to characterize temporal variability in emissions. Finally, it should be mentioned that for a few flights, each aircraft may take off early enough to perform an initial circuit before sunrise. While profiling will not be possible in darkness, in situ measurements in the lower free troposphere and lidar observations of boundary layer depth just prior to sunrise will be of critical value for testing air quality models which struggle to represent the shallow nocturnal boundary layer and its morning evolution as air from above is mixed down to the surface.

2.2.1. Data Analysis Approaches

As noted in the Science Traceability Matrix, a variety of modeling and analysis tools will be applied to the DISCOVER-AQ observations. The following discussion briefly highlights the general approaches to be employed and their relevance to DISCOVER-AQ objectives.

Multivariate Statistical Analyses: The figure on the right (D. A. Chu, unpublished data) demonstrates a dramatic improvement in the correlation between PM2.5 measurements and MODIS AOD when satellite observations are normalized by boundary layer height. Additional incremental improvement results when haze layer heights are considered. Even more remarkable is that the MODIS



observations have been normalized by profiles from a single lidar applied over distances of 2 to 300 km corresponding to PM2.5 measurement sites across Taiwan. While the statistics here are based on 3 years of data, observations are limited to the time of the satellite overpass. During DISCOVER-AQ, data will be gathered throughout the day under changing conditions (e.g., boundary layer depth and mixing, humidity, emissions, chemistry, etc.) that will allow for statistical assessment of the extent to which these variables influence the correlation between column and surface conditions for both trace gases and aerosols. The high density of DISCOVER-AQ observations will also enable assessment of the spatial scales over which these variables are needed, thus enabling the effective design of surface networks to provide information on the most critical variables at appropriate scales, both of which may vary depending on the region of study.

Retrieval Algorithms: While the DISCOVER-AQ column observations from the B200 and surface sites represent distinct viewing geometries compared to satellite observations from LEO or GEO, the density of supporting information on the spatial distribution of trace gases and aerosols provides an ideal environment for studying retrieval sensitivity and assumptions. For instance, ACAM retrievals can be accomplished with the traditional DOAS method as well as with an optimal estimation-based algorithm developed originally to retrieve the ozone profile and tropospheric ozone from GOME [*Liu et al.*, 2005, 2006] which can also be applied to retrieval of NO_2 and CH_2O with slight modification. Furthermore, retrievals based on climatological data (e.g., monthly mean trace gas profiles from NASA's GMI-CTM) can be compared with retrievals based on more complete information on actual profiles from in situ and Pandora observations. These retrievals will be validated against airborne in-situ profiles and/or sonde measurments and compared with satellite observations at the time of overpasses to assess how satellite retrievals are affected by the existence of aerosls and clouds and the extent to which they are influenced by sub-grid variability. Assessing how different retrieval assumptions influence column-surface correlations will also provide insight into the factors limiting current satellite observations in the diagnosis of surface conditions.

Regional Chemical Transport Models: While data analysis may provide strong evidence for the primary factors controlling column-surface correlations, unraveling the details of their combined influence is only achievable through the use of models. For air quality, two models in particular are widely used: the Community Multiscale Air Quality (CMAQ) model developed by EPA and the Weather Research and Forecasting model with online chemistry (WRF-Chem) developed at the NOAA Forecast Systems Lab with substantial community input. CMAQ [*Ching and Byun*, 1999; plus updates] is the primary regulatory tool used for air quality assessment and management and is also used in the operational air quality forecasting performed by NOAA. WRF-Chem [*Grell et al.*, 2005] is primarily being used for air quality applications within the research community. While it is not possible to provide detailed descriptions here, both of these models offer capability to choose among several chemical mechanisms and meteorological fields/boundary conditions. The Project Scientist, Ken Pickering, is an active user of both models. He is currently involved in directing a NASA applications project to include lightning NO_x emissions in CMAQ, and he is also engaged in work to take initial and boundary conditions for WRF-Chem from NASA's GMI-CTM.

Some specific modeling tasks for DISCOVER-AQ are described below:

- Run the WRF-Chem model with 4-km resolution over the field mission regions (nested in 12-km and 36-km resolution domains). Simulations will be based on the best possible source emission data to derive the model distribution of trace gas and aerosol amounts. Use comparisons with ground-based data (Pandora spectrometer and in-situ) and aircraft data (ACAM and in-situ) to evaluate various model configurations (e.g., photolysis scheme, chemical mechanism, aerosol module etc.) of WRF-Chem. Perform sensitivity simulations to bring the model calculation in close conformity to the measurements spatially and temporally.
- Use the regional meteorology from WRF to drive the CMAQ model. Compare model output with the ground-based and airborne data sets and run sensitivity calculations to reach good agreement with observations in a manner similar to the above.
- Evaluate boundary layer depths in the WRF model using aerosol lidar and aircraft observations.
- Use the model output to interpret the observations. For example, examine the spatial and temporal variation of observed trace gases at the surface and in the tropospheric column in both the models and observations. Compute local (grid-cell) scaling factors between tropospheric column NO_2 and surface NO_2 from the model. Compare these factors with those derived from observations and determine if the scaling factors can be related to meteorology (e.g., boundary layer depth), transport, proximity to major emission sources, time of day, etc. Employ transport feature information from the model to explain inconsistencies between surface and column observations. Examine the horizontal and temporal variability of trace gases and aerosols in the observations to determine how much of this variability is captured by the model at 4 km resolution.

While it is clear that DISCOVER-AQ observations will provide a rigorous test of current model capabilities, it will also determine the adequacy of models to substitute for surface networks in providing information on critical variables influencing column-surface correlations.

Assessing Spatial Variability and Its Impacts: Understanding spatial variability is critical to addressing the limitations of satellite observations and models relating to resolution. At nominal P-3B flight speeds, in situ data reported at 1 hz will provide information every 100 m. Observations from the B200 are expected to provide data down to resolution of 1 km for aerosol backscatter and NO_2. DISCOVER-AQ observations and regional model calculations will be evaluated using variogram and autocovariance statistical analyses [*Crawford et al.*, 2009; *Chatfield et al.*, 2009; *Follette-Cook et al.,* 2009] to assess subgrid variability as well as the consistency in modeled and observed variability when observations are degraded to model resolution. These analyses will also be useful in the determination of optimal resolutions for future satellites. Multi-scale modeling will also be used to assess the impact of model resolution on nonlinear chemical processes. This will include calculations using the Langley photochemical box model to assess ozone production rates based on observations at 1 hz and averaged over longer periods to represent stages of reduced resolution. Regional model calculations will also be available at multiple resolutions (4 and 12 km) to assess these impacts.

2.2.2. Data Management:

The data management plan for DISCOVER-AQ will follow procedures evolved from more than 20 years of airborne field studies under NASA's Tropospheric Chemistry Program. The majority of DISCOVER-AQ scientists are familiar with these procedures through previous participation in NASA airborne campaigns. For DISCOVER-AQ there will be two phases of data sharing: field data submission and post-deployment data archival.

Field Data Submission: For field data submission, airborne investigators will provide preliminary data to the science team within 24 hours of completing a science flight. Exceptions may occur when flights are scheduled for consecutive days. For ground stations, data will be provided each day for the previous 24 hours. This data will be for science team use only and is intended for the purpose of monitoring progress in achieving mission objectives and to identify any problems with instrument performance that could impact operations. These data will not be retained in any form and will be expunged from the archive at the end of each deployment.

Post-deployment Data Archival: Post-deployment data archival will occur no later than 4 months after completion of a deployment. Data will be archived and publically accessible via the NASA Tropospheric Chemistry Integrated Data Center (http://www-air.larc.nasa.gov/). This data center resides at NASA Langley and has supported Tropospheric Chemistry campaigns since the late 1980s. DISCOVER-AQ data will conform to the ICARTT data format (http://www-air.larc.nasa.gov/missions/etc/IcarttDataFormat.htm) developed by NASA and NOAA airborne science communities in 2004 to support joint operations and on track to be endorsed as the standard airborne data format by NASA's Data Standards Process Group. This format has been adopted for numerous airborne data sets sponsored by NASA, NOAA, NSF, and international research teams. In addition to data archival, the Data Center provides important value added services such as data merging of observations on a common platform to a common timeline. These merged data sets often replace the raw data files as the resource most widely used by science teams for data analysis. Assessments of measurement consistency will also be provided when intercomparison opportunities arise. Upon completion of the full 5-year mission, Data Center personnel will arrange for the data to be hosted by the Langley ASDC which is responsible for long-term archival of tropospheric chemistry data sets.

DISCOVER-AQ data will have value to numerous collaborating partners (e.g., EPA, MDE, TCEQ, CARB). This archival plan ensures that immediate public access to the science data will be available to these partners as well as any other interested parties.

2.3. Science Team

Table 2.2 outlines the DISCOVER-AQ science team which includes 21 investigators comprising five subgroups: 1) Leadership, 2) P-3B in situ airborne measurements, 3) B200 remote sensing airborne measurements, 4) Ground-based measurements, and 5) Data analysis and modeling

Leadership: This group is responsible for the successful execution and oversight of the DISCOVER-AQ experiment. Their specific duties are outlined in detail under section 4.1 (Management Approach). In addition to their oversight roles, Drs. Crawford, Pickering, and Chen will also be engaged in analysis and modeling activities.

Measurement Co-Investigators (P-3B/B200/Ground): Each investigator on these teams are responsible for a portion of the DISCOVER-AQ observations with the following common responsibilities. Instrument delivery, integration, and operation; timely archival of data collected; collaboration with the modeling and analysis team in the analysis of observations.

Modeling and Analysis Co-Investigators: Each investigator on this team is responsible for a portion of the scientific analysis of DISCOVER-AQ observations. This includes aerosol and trace gas retrievals, multivariate statistical analysis, and regional modeling. These investigators are expected to collaborate extensively with the measurement teams to ensure that observations are properly interpreted.

Table 2.2. 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_2O
Armin Wisthaler, Innsbruck	Non-methane hydrocarbons
Glenn Diskin, NASA LaRC	H_2O, 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_2O
Ground-based Measurements	
Jay Herman, UMBC	Pandora network for total trace gas columns of O_3, NO_2, and CH_2O
Anne Thompson, Penn State	NATIVE trailer in situ O_3, CO, NO, NO_y; aerosol lidar; ozonesondes.
Ray Hoff, UMBC	Lidar aerosol profiles, AERI, Raman H_2O, 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

3. Investigation Implementation

3.1. Measurement Platform System Capabilities

The airborne platforms selected for the DISCOVER-AQ mission are the P-3B and B-200. The P-3B is an ideal choice for a profiling aircraft for several reasons: 1) it is capable of hosting a comprehensive atmospheric chemistry and aerosol payload, 2) it is ideal for profiling the lower atmosphere, and 3) it has sufficient flight duration (8 hours) for sampling throughout the day.

The NASA B200 is ideal for the remote sensing payload since it has logged over 700 hours with HSRL onboard and can also accommodate ACAM with minor modifications. The B200 can also fly throughout the day, but must land for refueling given its 4.5 hour flight duration.

3.2. Instrumentation

The entire suite of instrumentation proposed for DISCOVER-AQ is TRL-9, and many instruments have heritage of a decade or longer. The following sections outline their specifications and capabilities as they apply to the requirements of DISCOVER-AQ science objectives in Table 2.1.

3.2.1. P-3B Instrumentation

Table 3.1. lists specifications for the P-3B in situ trace gas measurements. All of these investigators fielded their instruments onboard the NASA DC-8 during the recent ARCTAS field campaign in 2008 [*Jacob et al.*, 2009], and all have experience on other airborne platforms (e.g., NASA P-3B, NSF C-130, NSF HIAPER).

Table 3.2. lists specifications for the P-3B in situ aerosol measurements fielded by Dr. Bruce Anderson. With the exception of the last three instruments in the table, Dr. Anderson has fielded this measurement suite many times, most recently during ARCTAS. The final three instruments were fielded during ARCTAS by other investigators, thus their airborne implementation and integration is well demonstrated.

Table 3.1. P-3B in situ trace gas measurements[1]

Co-I	Technique or Instrument	Species	Precision	Uncertainty
Cohen	Thermal-Dissociation, Laser-Induced Fluorescence	NO_2	10 pptv	5%
		Total Peroxy Nitrates	40 pptv	10%
		Total Alkyl Nitrates	50 pptv	15%
		HNO_3	50 pptv	20%
Weinheimer	Chemiluminescence	O_3	0.1 ppbv	5%
		NO and NO_y	20 pptv	10%
		NO_2	20 pptv	10-20%
Fried	IR Absorption Spectrometer	CH_2O	60-80 pptv	12%
Vay	modified LI-COR 6252	CO_2	0.1 ppmv	0.25 ppm
Diskin	Diode Laser Spectrometer	CO	1 ppbv	1.5%
		CH_4	2 ppbv	0.2%
	Diode Laser Hygrometer	H_2O	0.1%	5%
Wisthaler	Proton Transfer Reaction-Mass Spectrometer	methanol	100 pptv	20%
		acetaldehyde	100 pptv	15%
		acetone	50 pptv	10%
		isoprene, MVK/MACR	20 pptv	10%
		acetonitrile	10 pptv	10%
		benzene, toluene, C8-aromatics, C9-aromatics	10 pptv	10%

1-response time for all instruments is 1 s with exception of Wisthaler which has 10 s response.

Table 3.2. P-3B in situ aerosol measurements (Co-I Bruce Anderson)

Technique/Instrument	Response	Parameter	Precision	Size Range
Condensation Particle Counters (TSI 3025, TSI 3010)	1 s	Ultrafine, Nonvolatile CN	10%	>0.003
TSI Scanning Mobility Particle Sizer	60 s	Aerosol Particle Size	20%	0.01 – 0.3
DMT Ultra-High Sensitivity Aerosol Spectrometer	1 s		20%	0.08 – 1.0
MetOne Optical Particle Counter	1 s		40%	0.3 – 10
Aerodynamic Particle Sizer (TSI 3321)	1 s		20%	0.5 – 20
DMT Cloud Condensation Nuclei counter	1 s	Cloud Condensation Nuclei Spectra	NA	<10
Nephelometer (TSI 3563)	1 s	Scattering at 450, 550, and 700 nm	5e-7 mM or 5%	<10
Particle Soot Absorption Photometer	5-60 s	Absorption at 467, 530, and 660 nm	5e-7 mM or 5%	<10
RR Nephelometers	20 s	Humidity Dependence of Scattering	NA	<10
DMT Single Particle Soot Photometer	1 s	Black Carbon	20%	0.1 – 1.0
Particle into Liquid Sampler/Ion Chromatograph	300 s	Soluble Ion Composition	NA	0.01 – 1.0
Particle into Liquid Sampler/Total Organic Carbon	30 s	Water Soluble Organic Carbon	NA	0.01 – 1.0

Table 3.3. lists specifications for the P-3B navigational and meteorological observations. While these observations are often considered to be turn-key, experience has shown that loss of data or lack of adequate QC for these data can be detrimental to mission success. Mr. John Barrick has more than a decade of experience in providing these observations on the P-3B and will be responsible for collecting and reporting these data during DISCOVER-AQ.

Table 3.3. P-3B navigational and meteorological measurements (John Barrick)

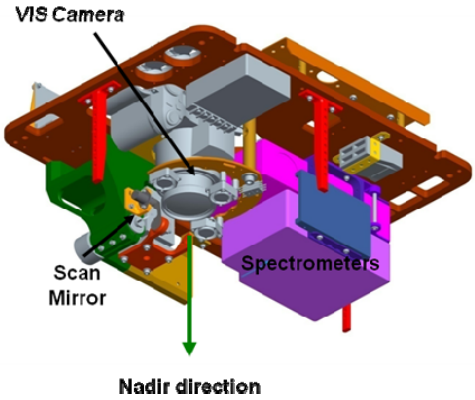
Parameter	Response	Technique/Instrument	Precision
GPS Location	1 s	GPS/Trimble TNL-3000	15 m
GPS Altitude	1 s		50 m
Pressure	1 s	MEMS/Rosemount MADT 2014	0.3 mb
Pressure Altitude	1 s	Calculated/Rosemount MADT 2014	5 m
Radar Altitude	1 s	Radar Altimeter/ Honeywell AA-300	3 m
Pitch, Roll, and Heading	1 s	INS/Honeywell Laseref	0.2 °
Wind Speed and Direction	1 s		3 m/s; ± 10 °
Ground Speed and Track	1 s		1 m/s; 0.5 °
True Air Speed	1s		2 m/s
Temperature	1 s	PRT/Rosemount E102 Non-Deiced	0.2 °C
Dew/Frost point	2 - 30 s	Edgetech Vigilant 137 3-Stage Chilled Mirror Hygrometer	0.5 - 1.0 °C
NO_2 Photolysis Frequency	1 s	Metcon jNO_2 Filter Radiometers	8%

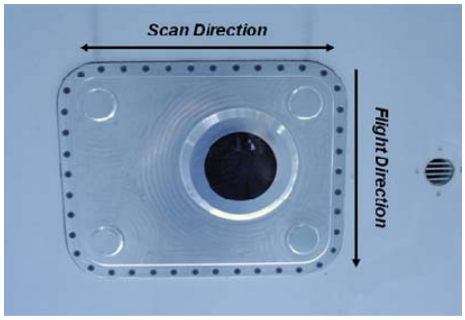
3.2.2. B200 Instrumentation

Table 3.4. lists specifications for the B200 remote sensing measurements, both of which are TRL-9. Since 2006, HSRL has logged more than 700 hours of science flight in ten field campaigns in support of NASA, DOE, NOAA, and EPA [*Hair et al.*, 2008; http://science.larc.nasa.gov/hsrl/]. ACAM [*Kowalewski and Janz*, 2009] is the newest and least documented portion of the DISCOVER-AQ measurement suite, although it has logged over 50 flight hours onboard NASA's WB-57. For that reason, additional technical details for ACAM are provided below.

Table 3.4. B200 Instrumentation

Co-I (Instrument)	Parameter	Resolution	Approx. Precision
Hostetler (HSRL)	Aerosol Backscatter (532 and 1064 nm)	10 sec (~1 km) hor. 60 m vert.	0.0002 $(km\text{-}sr)^{-1}$
	Aerosol Extinction (532 nm)	1 min (~6 km) hor. 300 m vert.	0.01 km^{-1}
	Depolarization (532 and 1064 nm)	10 sec (~1 km) hor. 60 m vert.	0.005 (532 nm) 0.01 (1064 nm)
	Aerosol Optical Depth (532 nm)	1 min (~6 km)	0.01
Janz (ACAM)	Slant Column O_3	1 km x 1 km	0.1 DU
	Slant Column NO_2	1 km x 1 km	$1x10^{15}$molec/cm^2
	Slant Column NO_2	1 km x 7 km	$5x10^{14}$ molec/cm^2
	Slant Column CH_2O	1 km x 7 km	$2x10^{15}$ molec/cm^2



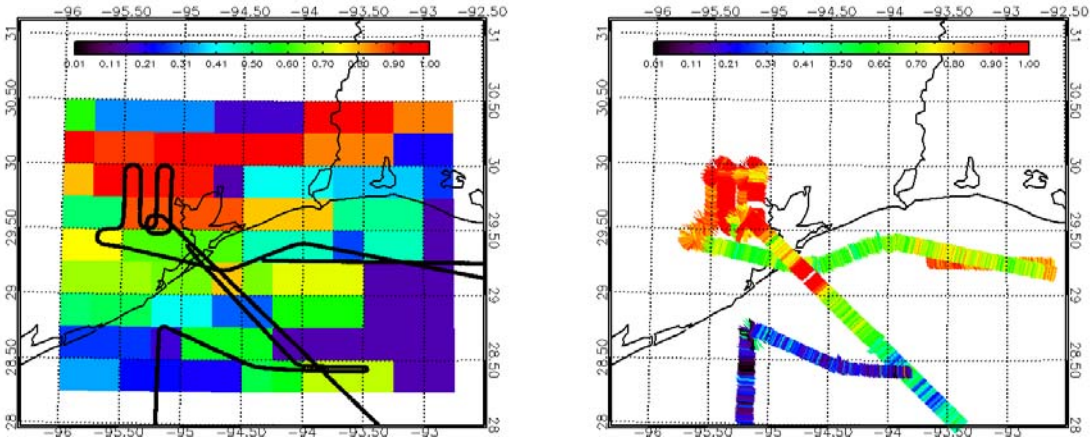


ACAM: The Airborne Compact Atmospheric Mapper was designed and built at the NASA Goddard Space Flight Center. ACAM has participated in three campaigns to date aboard NASA's WB-57 aircraft. The primary science objectives of ACAM are to provide remote sensing observations of tropospheric and boundary layer pollutants, such as NO_2, CH_2O, O_3, SO_2, and aerosols as well as provide visible imagery for cloud and surface information.

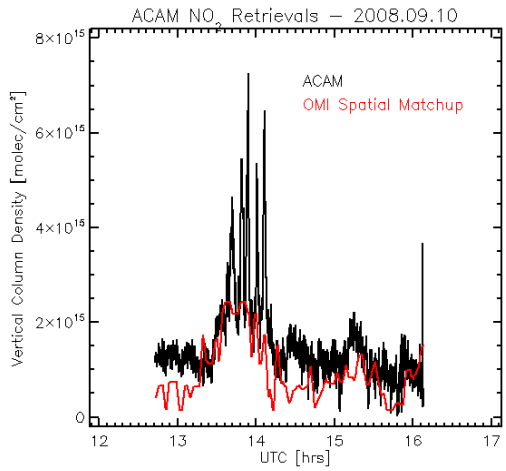
Through its participation in flight campaigns, ACAM has provided visible images for cloud and surface information in support of NASA's Aura satellite instruments and other platform payloads. Lessons-learned from these initial missions, and various improvements in the environmental control and operation of the sensors, have led to improvements in ACAM's ability to detect slant-column concentrations of key trace gases for a given spatial resolution element. Additionally, improved in-field absolute calibration of the ultraviolet (UV) and visible (VIS) spectrographs have enabled exploring absolute radiance transfers with satellite instruments (e.g., OMI) at the sub-5% accuracy level. Shown above is a 3D model of the internal instrument layout that has been flown previously and a photo of the environmentally controlled housing with a UV compatible viewport. Future flights will replace

the still image camera with an HD video camera and will also incorporate an upward looking telescope for reference calibrations.

The scan mirror that illuminates the fiber-coupled spectrometers sweeps out a +/- 23 degree Field-of-regard across-track in the nadir direction. The single pixel field of view varies with altitude and integration time and will be approximately 300 m for the DISCOVER-AQ flight tracks. ACAM utilizes the Differential Optical Absorption Spectroscopy (DOAS) method to obtain slant column densities of measurable trace gas absorption in the spectral range of interest. The two panel figure below shows some results from the most recent WB-57 deployment (September 2008). Shown in the figure are normalized NO_2 column densities for both the OMI 0.25 degree gridded tropospheric product and the ACAM derived values for the same day.



OMI 0.25 degree gridded product [left]. ACAM retrievals [right]. Values are normalized to the peak response. Houston [Sept. 10, 2009]



The figure to the right shows the effect of the different spatial resolution of the two instruments. The higher frequency peaks seen are at the 1.5 km spatial resolution of ACAM on the WB-57. This type of data can be used to explore the effects of various spatial resolutions on regional scale air quality model performance. The Houston data also shows sensitivity to CH_2O and ozone although further work is required to optimize the retrievals of these trace gases. An upward looking reference calibration scheme is being added in order to improve the retrieval capabilities of tropospheric ozone and the UV spectrometer has already been upgraded in preparation for DISCOVER-AQ objectives for better sensitivity to CH_2O in the 345-355 nm wavelength region. In addition to the UV/VIS spectrograph, ACAM also contains a VIS/NIR spectrograph (450-900 nm, 2 nm resolution) which will be used to provide information for planning of the GEO-CAPE ocean science instrumentation.

3.2.3. Ground Instrumentation

Table 3.5 lists specifications for the Pandora instruments [*Herman et al.*, 2009]. While this instrument is at TRL-9, the DISCOVER-AQ strategy requires these instruments to be integrated into the AQS network, thus fabrication of twelve new Pandora instruments is planned during the first year of the proposed work. Pandora consists of an optical head (shown on right) connected to a cooled temperature controlled Avantes spectrometer (280 to 525 nm res. 0.5 nm) by a fiber optic cable. An existing new spectrometer instrument, based on the shadowband principle, Cleo, is being deployed with a few of the Pandoras to provide independent aerosol measurements over a wide wavelength range (320 to 825 nm). The control and analysis software are mature.

Table 3.5. Pandora capabilities

Instrument	Response	Parameter	Precision	Uncertainty	Range	Resolution
Pandora	4 s	Total Column O3, NO2, CH2O, SO2, H2O, BrO	0.01 DU	0.1 DU		
Pandora +Cleo	15 min / 5 s	Aerosol Properties	τ<0.1, SSA 0.1	0.05		
Cleo	5 s				320 - 825 nm	1 nm
Pandora	10 min	Ozone profile	1 DU	height dep.	0-50 km	3-5 km
	10 min	NO2 profile	0.01 DU	height dep.	0-50 km	1 km

Table 3.6 lists instrumentation and specifications for the NATIVE trailer. This asset has deployed numerous times in support of NASA field campaigns (e.g., INTEX, TC4, and ARCTAS).

Table 3.6. NATIVE instrumentation

Instrument	Response	Parameter	Precision	Uncertainty
Thermo Scientific 42C-Y	60 s	NO and NO_y	50 pptv	3%
Thermo Scientific 49C	20 s	O_3	1 ppbv	4%
Thermo Scientific 48C	60 s	CO	40 ppbv	5%
Thermo Scientific 43C	80 s	SO_2	0.2 ppbv	5%
R.M. Young 41382	10 s	Temperature	NA	0.3 deg C
R.M. Young 41382	10 s	Relative Humidity	NA	2%
R.M. Young 61202	10 s	Pressure	NA	0.3 hPa
R.M. Young 05103	1 s	Wind Speed and Direction	NA	0.3 m/s; 3°
Metcon 2-pi jNO_2 Filter Radiometer	1s	NO_2 Photolysis Frequency	NA	5%
UV Shadowband Radiometer (YES Inc. UVMFR-7)	30 s	Diffuse and Direct Irradiance, Total Column O_3		
Aerosol Lidar	Variable	Aerosol Backscatter		
Ozonesonde/Radiosonde Ground Station	Variable	O_3, Temperature, Pressure, Water Vapor		

Table 3.7 lists instrumentation located at the UMBC UMAP site. The first two lidars in the table will also be relocated in support of each deployment.

Table 3.7. UMBC instrumentation

Instrument	Response	Parameter	Precision	Uncertainty	Range	Resolution
MPL lidar (SigmaSpace)	60s	532 nm backscatter	$1x10^{-8}$ $(m\text{-}sr)^{-1}$	Range Dep.	0.5-20 km	15 m
Leosphere scanning lidar	60 s	355 nm backscatter	$1x10^{-8}$ $(m\text{-}sr)^{-1}$	Range Dep.	0.1-15 km	7.5 m
Elastic Lidar Facility (ELF)[1]	60 s	532 and 1064 nm backscatter	$1x10^{-8}$ $(m\text{-}sr)^{-1}$	Range Dep.	0-4-15 km	7.5 m
ALEX Raman Lidar[1]	300 s	H2O at 407 nm	<2 g/kg	Range Dep.	0.8-4 km	75 m
Sun-Photometer (Cimel CE318N-EBS9)[2]	15 min	λ AOD/ SSA Size Dist Θ	0.01/1.00 ~0.05 nm variable	0.01/0.02 ~0.05 nm variable	NA/0.00 to 1.00 0.05 to 20 um 3 to 160°	
TSI 3563 Nephelometer[1]	180 s	Aerosol scat., backscat. coeff.	$5x10^{-7}$ mM or 5%	<10%		
RSI 1400 TEOM[1]	600 s	PM2.5 (surface)	1 ug/m^3	3%		

1-UMBC UMAP instrumentation that will only be available to support the Baltimore-Washington deployment
2-Specifications also apply to the five dedicated AERONET sun-photometers procured for this project.

3.3. Assembly, Integration, Test

Since all instruments are at TRL 9 and have been previously fielded, there are no major uncertainties regarding their integration and testing. Standard practice for airborne field deployments is to conduct a short engineering check flight after payload integration is complete. This is followed by one or two test flights of short duration, typically four hours. In past deployments, this has been sufficient for all of the instruments in the proposed payloads to be determined as mission capable.

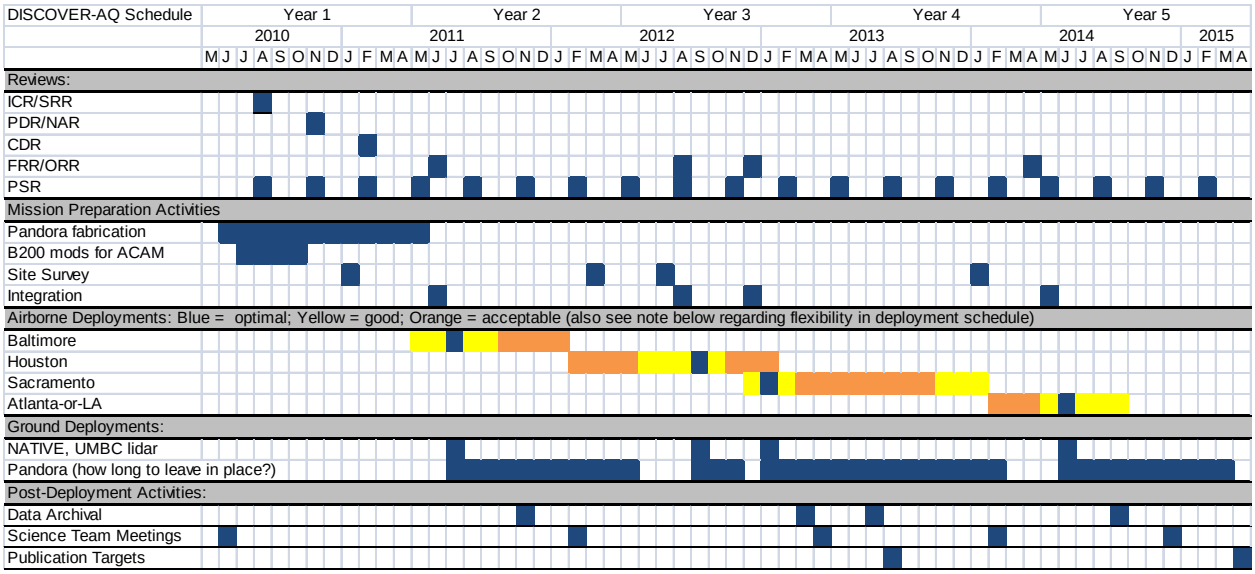
P-3B Integration: A preliminary integration floor plan for the P-3B has been provided by Mike Cropper of Wallops Flight Facility (not shown due to space constraints), and the payload has been determined to fall within P-3B weight and space limits. Instruments will be housed in standard, double-bay racks provided to instrument investigators by Wallops. Inlets for the instruments are already in existence and in most cases are also configured to work for both the NASA P-3B and DC-8. Instrument investigators will be responsible for their individual rack configurations to be inspected and approved by Wallops Flight Facility as is standard practice.

B200 Integration: Of the two instruments on the B200, HSRL is a resident instrument that has logged over 700 hours of science flight. Integration of ACAM will require minor modifications to the aircraft that have been assessed and cost estimated in consultation between ACAM investigators and the LaRC Research Services Directorate which is responsible for B200 operations.

Ground sites: Site selection for Pandora instruments, the NATIVE trailer, and UMBC lidars will be conducted in consultation with local authorities responsible for sites within the AQS network (see Letters of Support from local partners).

4.3. Schedule

The nominal schedule for DISCOVER-AQ is provided here. A brief discussion of the various schedule elements is provided below.



Reviews: Because this project does not require the development of any new hardware designs, the review schedule will be tailored to enable the commencement of science flights within one year of the beginning of the project. The ICR/SRR will focus on validating the measurement requirements and deployment strategy for meeting science objectives. The PDR/NAR will focus on the feasibility of deployment plans vis-à-vis air traffic coordination and selection of ground sites. The CDR will focus on the status of instrument preparation and aircraft integration plans. The FRR/ORR will be held just prior to each deployment to determine that all arrangements are in place and assets are ready for deployment. Quarterly PSR's will be held by the Project to evaluate progress in executing the mission, ascertain any new risks and review existing risks, and review schedule and budget against planned baselines. Although not explicit in the schedule, the Project will also support all necessary NASA KDP Reviews and will be involved in all applicable NASA ASRB Reviews.

Mission Preparation Activities: Major preparation activities include the fabrication of 12 Pandora instruments and modifications to the B-200 to accommodate the ACAM instrument. Individual instrument investigators will be responsible for any minor upgrades they plan for their instruments prior to deployment. Site surveys will take place at least six months prior to each deployment.

Deployments: The deployment schedule reflects the optimal deployment strategy while also communicating flexibility. If necessary, the order of deployment sites may also be rearranged. The option of leaving Pandoras in place to continue observations between deployments is being considered.

Post Deployment Activities: Science team meetings will be conducted annually and data submission to a public archive will occur no more than 4 months after completing each deployment. Publication targets allow for submission of findings from the initial flights early in year 4 and synthesis of results from all flight years at the conclusion of the project.