

AQRP Project 14-005

**Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ
Measurements and Validation**

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Quality Assurance Project Plan

QAPP Category: III

Type of Project: Data Evaluation or Use for Secondary Purpose

QAPP Requirements: This QAPP requires descriptions of project and objectives; organization and responsibilities; scientific approach; quality metrics; data analysis, interpretation, and management; reporting; and references.

QAPP Requirements:

Audits of Data Quality: Cat III = 10% Required
Report of QA Findings: Required in final report

TITLE SHEET

This document is a Level IV Quality Assurance Project Plan for Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation. This project is managed by the staff at Texas A&M University.

Distribution List

Below is a list of individuals and their organizations that need copies of the approved Quality Assurance (QA) Project Plan and any subsequent revisions, including all persons responsible for implementation (e.g., project managers), the QA managers, and representatives of all groups involved. Paper copies need not be provided to individuals if equivalent electronic information systems can be used.

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APPROVALS

**This QAPP was approved electronically on February 2, 2015 by Vincent M. Torres,
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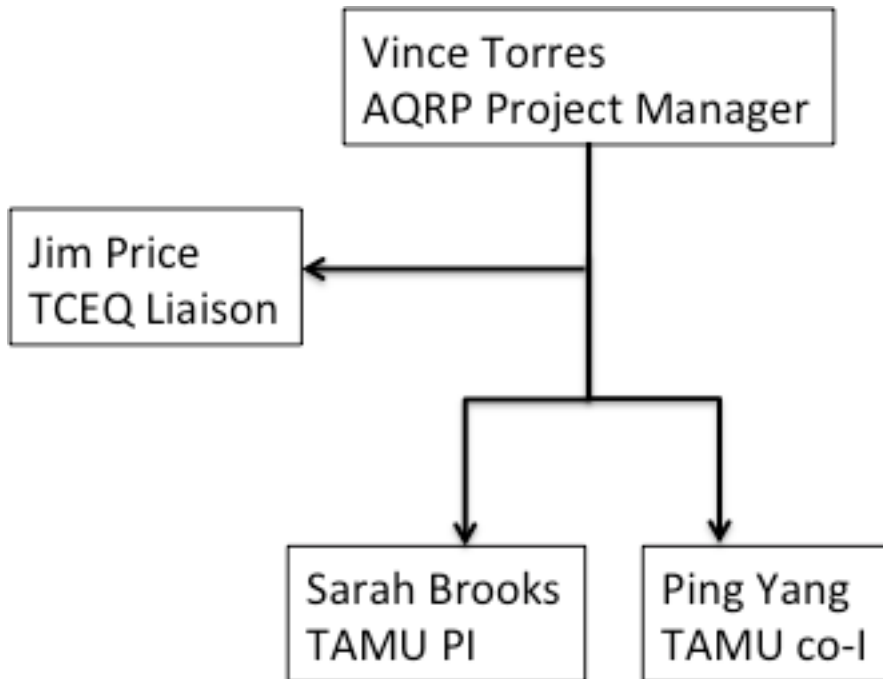
1. PROJECT DESCRIPTION AND OBJECTIVES

During the fall of 2013, the Houston area was the site of the 2nd field intensive of the National Aeronautics and Space Administration (NASA) Deriving Information on Surface conditions from Column and VERTically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign. During DISCOVER-AQ, we operated a new scattering instrument, the Cloud and Aerosol Spectrometer with Polarization (CASPOL) which measures the depolarization ratio of individual particles in the aerosol population. The polarization capabilities of CASPOL facilitate an effective approach to validate spaceborne aerosol retrieval, particularly Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) aerosol type classification. The CASPOL was operated on top of the 60 m tall Moody Tower (MT) on the University of Houston campus, a central urban location and site of many complementary measurements during DISCOVER-AQ. We now propose to analyze the CASPOL data set to determine the concentration, size distribution, and optical properties of aerosol from the wide variety of sources including urban pollution sources from downtown Houston and the industrial Ship Channel, and transported aerosol. Combined with additional measurements of organic carbon, black carbon and ozone, the CASPOL data set provides an opportunity to determine the primary aerosol sources and impacts of aging due to ozone modify aerosol optical properties. These in-situ data will be compared to Moderate-resolution Imaging Spectroradiometer (MODIS) and the CALIOP aerosol measurements to determine the sensitivity of remote sensing to changes in surface aerosol properties and air quality. The objective is to compare column observations provided by satellite instruments and near-surface atmospheric composition.

2. ORGANIZATION AND RESPONSIBILITIES

KEY PERSONNEL

The following flow chart identifies the key personnel at each organization who are responsible for the quality assurance (QA) and deliverables listed in this document.



PROJECT SCHEDULE

The schedule for this project and key milestones are listed in Table 1 below.

Tasks:

- Feb. 27, 2015 Task 1. Post- DISCOVER-AQ CASPOL calibrations and quality control
Task 2. Identification of Aerosol Types in the CASPOL data set
- May 29, 2015 Task 3. Comparison of in-situ aerosol properties to satellite-retrieved properties during DISCOVER-AQ
- Aug. 15, 2015 Task 4. Comparison of in-situ data and remote sensing products.
- Nov. 30, 2015 Task 5. Final publication and dissemination of results.

Deliverables:

Feb. 27, 2015 Deliverable 1: A set of files will be produced, 2 for each day. File format for the first file will include CASPOL time, total particle number, size distribution. The second file for each day will contain single particle backscattering, and depolarization data, which will be required to generate optical signature plots in Task 2.

Deliverable 2: Optical signature plots (backscattering vs. depolarization) for the specified categories, i.e. urban pollution, industrial pollution from the Ship Channel, or transported aerosol, according to the source regions identified by HYSPLIT.

May 29, 2015 Deliverable 3:

- 3A. Summary table of time periods in which MODIS and in-situ data are collocated.
- 3B. Summary table of time periods in which CALIOP and in-situ data are collocated.
- 3C. Summary table of in-situ time periods for representative aerosol types and conditions.

June, 2015 Highlight: A presentation of results accomplished during the first two quarters will be made at the June 2015 AQRW Workshop.

Aug. 15, 2015 Deliverable 4: A report summarizing which variations observed in-situ data can and which cannot be observed in remotely sensed data sets.

Nov. 30, 2015 Deliverable Task 5. A final publication of results will be prepared and submitted to the Journal of Geophysical Research or Aerosol Science and Technology.

Table 1. Project Deliverables and Tasks, with Due Dates.

3. SCIENTIFIC APPROACH

Task 1 Analyze CASPOL data collected during DISCOVER-AQ.

We operated the CASPOL instrument continuously from Aug 28 through October 4, 2013 from the top the 60 m tall Moody Tower (MT) on the University of Houston campus as part of DISCOVER-AQ. The CASPOL provides in-situ determination of aerosol concentration, size distribution, and depolarization ratio. Validation of remote sensing measurements of aerosols will be accomplished through in-situ measurements of aerosol size distributions, type, and particle-by-particle determination of depolarization ratio. We call special attention to the fact that in situ measurements by CASPOL provide valuable datasets for validating satellite-based aerosol property retrieval. From this perspective, the proposed research effort will have quite substantial broader impacts.

The coordinated Moody Tower measurements during DISCOVER-AQ provide time-resolved, 24-hour measurements of key trace gases and aerosols including ozone, carbon monoxide, nitrogen oxide and dioxides, and sulfur dioxide concentrations, aerosol optical depth, boundary layer height and basic meteorological parameters during the diverse conditions encountered in a coastal urban center in close proximity to multiple industrial sources of pollution. The height of MT is sufficient to reduce influence from nearby intermittent sources and yet is be more representative of surface air quality conditions in the Houston area than concurrent aircraft measurements.

In addition to ongoing measurements at MT, Dr. Rebecca Sheesley of Baylor University operated a seven-channel aethelometer and Particulate Matter with diameter of 2.5 μm and less ($\text{PM}_{2.5}$), and Total Suspended Particulates (TSP) filter samplers collocated with the CASPOL throughout the DISCOVER-AQ period. The mass loading of soot in particles and a first order estimate of degree of coating on soot particles will be determined by aethelometer data and the Organic Carbon to Element Carbon ratios (OC/EC) provided by Dr. Sheesley. In addition, the University of Houston operated a sun photometer during DISCOVER-AQ. This instrument, part of the Aerosol RObotic Network (AERONET) [Schuster *et al*, 2012], measures radiances at a set of visible and near-infrared wavelengths to determine column aerosol optical depth. Comparison to this sun photometer data and to the AERONET data in general will provide additional insight on horizontal and vertical variability in aerosol populations.

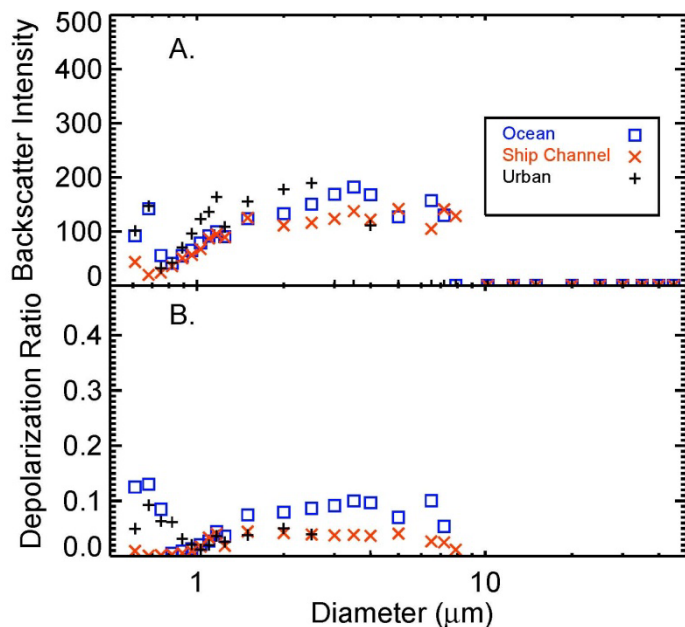
IB. CASPOL Instrument Details.

The CASPOL instrument determines the concentration, size distribution and optical properties for individual particles in a range of sizes, from $0.6 \mu\text{m} < \text{diameter} < 50 \mu\text{m}$, using a diode laser at a wavelength of 680 nm. The CASPOL measures light scattered by individual aerosol particles in the forward (4° to 12°) and backward (168° to 176°) directions utilizing three detectors. The forward scattering detector (f) provides the size measurement of the sampled particles, the two backward scattering detectors, β_{\parallel} , and β_{\perp} , measure the parallel and perpendicularly polarized scattered light respectively. In addition to providing measurements of aerosol number concentration and size distributions in real-time (one minute averages), the CASPOL measurements can be used qualitatively to indicate aerosol type and quantitatively to

derive lidar backscattering and depolarization signals at the wavelength of the CASPOL laser (680 nm). Using the two backscattering detectors, the aerosol depolarization ratio (ADR) at 680 nm is calculated for each particle size bin according to:

$$ADR = \frac{\beta_{\perp}}{\beta_{\parallel}}$$

To illustrate CASPOL response to aerosol populations of differing type, the backscatter and aerosol depolarization ratio as a function of particle size (determined by the forward scattering detector), preliminary CASPOL data collected under conditions of downtown Houston (Urban), transported aerosol arriving from the Gulf of Mexico (Ocean), and from an air mass from the ship channel (Ship Channel) are shown in Figure 1. (Source locations are identified by Hybrid Single Particle Lagrangian Integrated Trajectory Model (HYSPLIT) back trajectories as discussed below.)



As can be seen, the transported aerosol population (Ocean) contained particles with much higher depolarization ratios than either the Urban or Ship Channel

cases. The two local sources are also clearly different than one another. First, the aerosol population from the Ship Channel contains much larger particles, and secondly, submicron particles from the Urban case are highly depolarizing, whereas those from the ship channel have depolarization ratios near zero. In summary, variation in aerosol types present in the Houston environment can be observed and classified by the CASPOL. CASPOL measurements will be used along with other aerosol composition measurements at the Moody Tower to provide an indication of aerosol type present in Houston throughout the DISCOVER-AQ campaign.

Task 1 Deliverable: At the end of Task 1, all CASPOL data will be quality controlled and separated by class according to source. Data collected during and after precipitation events will be eliminated, as will any periods during which the CASPOL was operating offline for maintenance, drying, or flow testing. A set of files will be produced, 2 for each day. File

format for the first file will include CASPOL time, total particle number, size distribution. The second file for each day will contain single particle backscattering, and depolarization data, which will be required to generate optical signature plots in Task 2 below.

Task 2 Identification of Aerosol Types in the CASPOL DISCOVER-AQ data set

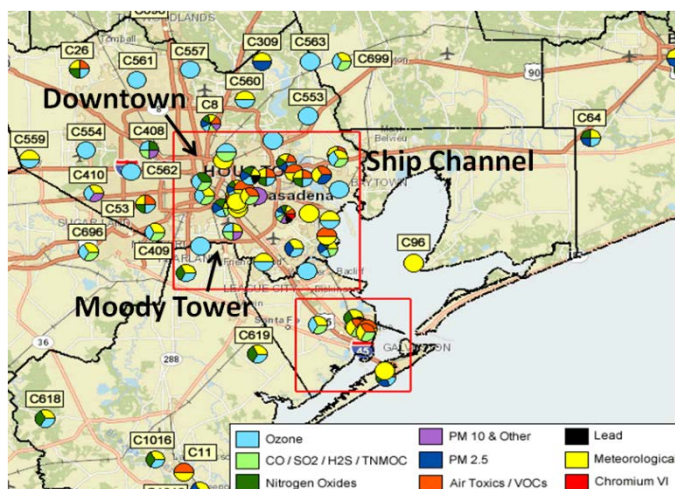
A. Classification of aerosols

First, we will classify sampling periods according to source locations using 5-day HYSPLIT back trajectories [Draxler and Rolph, 2003]. Because the CASPOL measures forward and backscattering and depolarization ratio of individual particles, the relationship between aerosol properties (concentration and type) and backscattering intensity and depolarization ratio can be accurately constrained for a variety of aerosol types including those shown in Figure 1 above as well as transported continental background and biogenic aerosols and mineral dust. After initial classification, we will evaluate whether the CASPOL data are unique for each aerosol source type. If unique optical signatures are observed, aerosol classification in future work may rely on the CASPOL signatures.

B. Refinement of Classification within urban type

The impacts of pollution on aerosol are complex [Ma et al, 2013]. We anticipate that coincident gas phase pollutants will modulate the aerosol properties. One impact of pollution on aerosols is that gas phase ozone interacts with soot aerosol, increasing its hygroscopicity. Hence aged (oxidized) particles will take up water and may be present as solution droplets at ambient relative humidities. (The aerosols may, in turn, reduce ambient ozone concentrations by absorbing light). Ozone data collected at the Moody Tower by researchers from the University of Houston, will be used to classify the CASPOL ozone exposure level. Ozone has been observed to age soot particles when exposed to ozone in concentrations of 30 ppbv or more [Pöschl et al, 2001]. Hourly averages of ozone concentration will be identified as low (0 to 33 ppbv), medium (33 to 66 ppbv) or high (66 to 100 ppbv). In addition, OC/EC ratios will be classified as high (>10) or low (<10) CASPOL data collected under each of those classifications. A typical urban value for OC/EC is 6 [Seinfeld and Pandis, 2006]. If the ozone and OC/EC levels are both low, the aerosols will be assumed to be fresh. If the ozone concentration is high and the OC/EC ratio is

above 10, the aerosols will be classified as aged. For any other ozone concentrations and OC/EC ratios, the aerosol will be assumed to be partially aged.



As can be seen in Figure 2, ozone and PM_{2.5} are monitored at a large number of Continuous Air Monitoring Stations (CAMS) within the Greater Houston Area.

Figure 2. Daily averaged air quality data for October 30, 2013. TCEQ data is available <http://www.tceq.texas.gov>.

PM₁₀ is also monitored at a few stations in the region. Hourly averages of TCEQ mass measurements of PM_{2.5} and PM₁₀ (blue and purple slices of the pie charts in Figure 2, respectively) will be compared to the CASPOL data throughout the project to evaluate how representative the aerosol sampled by CASPOL at Moody is of the ambient aerosol in the Greater Houston Area.

Task 2 Deliverable: HYSPLIT backtrajectories will be run for all quality controlled CASPOL DATA.

All CASPOL data will be sorted into categories, i.e. urban pollution, industrial pollution from the Ship Channel, or transported aerosol, according to the source regions identified by HYSPLIT. Further categorization will be conducted based on data from additional in-situ measurements. A summary table designating in which category data from all time periods belongs will be produced. Data from each time period will be collected in a single file for each category. From these files, CASPOL data from will be used to generate optical signature plots (backscattering vs. depolarization) for the specified category. Plots will be inspected for characteristic differences which may allow source region identification directly from CASPOL in future studies.

Task 3. Comparison of in-situ aerosol properties to satellite-retrieved properties during DISCOVER-AQ

The main objective of the NASA DISCOVER-AQ mission is to improve pollution monitoring from satellites for better air quality forecasting and warning systems and aerosol source identification. While aerosol retrievals were performed for a number of different satellite instruments during DISCOVER-AQ, we will build on the strengths and experiences of the proposal team and focus on the MODIS instrument operated onboard the Terra and Aqua satellites and CALIOP on the CALIPSO satellite, which flies in formation with Aqua.

The MODIS instrument is a radiometer that measures reflected solar and emitted terrestrial radiation in 36 bands between 0.4 and 14.4 μm. MODIS is a scanning instrument with a 2030 km swath which means that each MODIS instrument gets a daytime view of Houston with a favorable viewing angle at least every 3 out of 4 days. Because MODIS retrievals are based on reflected solar radiation, they are only made during the daytime. MODIS retrieves aerosol properties by comparing measured reflectances to modeled reflectances from a wide range of aerosol simulations. The modeled reflectances depend on a number of assumptions about aerosol composition, size distribution, and absorption and scattering properties, as well as environmental conditions including surface properties, atmospheric profile, and viewing geometry. The impacts of these assumptions and their global applicability are not certain. For example, our proposal team has shown that neglecting non-sphericity of dust and certain pollutant particles can lead to underestimations of Aerosol Optical Depth (AOD) [Feng *et al.*, 2009].

Aerosol retrievals from passive sensors such as MODIS are very sensitive to cloud

contamination. Essentially, AOD cannot be retrieved by satellites in the presence of cloud cover. This means that although the DISCOVER-AQ campaign took place over many days, there are a limited number of cases with widespread aerosol retrieval coverage over Houston from MODIS on Aqua, and several more days with limited coverage over the Greater Houston area. Because the Houston area is heavily urbanized, the surface is relatively reflective. The “Dark Target” MODIS aerosol retrievals have been shown to have decreased accuracy over large urban areas, but there is uncertainty as to whether this is due to surface reflectivity or the aerosol models used in the retrievals [Levy *et al.*, 2010]. Of particular interest for this project will be the upcoming release of the newest version of MODIS aerosol product, Collection 6 [Levy, *et al.*, 2013, 2013], which will include the “Dark Target” retrievals as well as the “Deep Blue” retrievals [Sayer, 2013] that were designed to work over bright surfaces. The Collection 6 Dark Target retrievals will be available at standard 10-km resolution, as well as an improved 3-km resolution product, while the Deep Blue retrievals will be at 10-km resolution. The Collection 6 properties retrieved over land will include total aerosol optical depth at 0.47, 0.55, and 0.65 μm and qualitative information about aerosol type and size parameters.

CALIOP, the lidar instrument on the CALIPSO satellite, provides a vertical profile of attenuated backscattered radiation at two wavelengths, 532 and 1064 nm. In addition, the depolarization ratio (ratio of the perpendicular component to parallel) is profiled at 532 nm. CALIOP backscatter profiles and depolarization signatures make it possible to discriminate between spherical and nonspherical particles, such as dust and liquid aerosol droplets, and water droplets and ice crystals [Winker, 2010] and are used in the creation of the CALIPSO cloud and aerosol layer products [Vaughan, 2009;]Cho et al, 2008]. Figure 3 shows the CALIOP depolarization ratio to backscatter relationships for each of CALIOP’s six retrieved aerosol types: clean marine, dust, polluted continental (urban), clean continental (remote background aerosol), polluted dust (dust which has travelled away from the source region) and smoke (from biomass burning). Aerosol optical depth retrievals by CALIOP depend on the assumed aerosol type model and comparisons with the ground-based **AEROSOL ROBOTIC NETWORK** (AERONET) measured optical depths depended on scene type [Schuster, 2012]. AERONET and CALIOP had the greatest AOD differences for the dust scenes.

Because CALIOP has the ability to vertically profile backscatter and depolarization ratio, comparisons between it and the CASPOL are highly desired. However, CALIOP is not a scanning instrument which means that it has limited coverage. During the CASPOL measurement period, CALIOP passed within 35 km of Moody Tower on three daytime occasions (around 17:45 UTC on 8/31, 9/16, and 10/02) and within 83 km on three nighttime occasions (around 8:25 UTC on 9/4, 9/11, 9/20, and 9/27). The nearest overpass to the Moody Tower measurement site was 29.5 km away on 8/31.

Task 3 Deliverable:

- A. Identification of time periods in which MODIS and in-situ data are collocated.***
- B. Identification of time periods in which CALIOP and in-situ data are collocated.***
- C. Identification of in-situ time periods for representative aerosol types and conditions.***

Task 4 By inspection of the coordinated data sets, we propose to answer the following questions about MODIS and CALIOP retrievals

1. *How sensitive are MODIS retrievals over the Houston Area to aerosol type?*

First, we address the question of whether uncertainty in the MODIS aerosols retrievals over urban areas is due to aerosol assumptions or surface reflectivity. We will use aerosol data available across the full region to give each MODIS retrieval (day and pixel) a predominant aerosol type based on assumptions from each of the MODIS algorithms from Collection 5 and Collection 6 and meteorological condition classification. Then, we will compare the MODIS aerosol optical depth and aerosol type assumptions to AERONET optical depths and CASPOL aerosol typing. Next, we will look specifically at MODIS pixels that include Moody Tower to determine if variability detected by the CASPOL is reflected in the MODIS retrievals. If so, this will enable future use of the CASPOL data to improve MODIS aerosol models.

2. *How do the CASPOL depolarization ratios and aerosol typing compare with CALIOP?*

CALIOP Data can be processed to produce remotely sensed optical signature plots, which are nearly identical to the CASPOL data. While CASPOL and CALIOP both provide information about aerosol backscatter and depolarization ratio, there are distinct differences between the measurements. For example, CASPOL provides information about individual particles, while CALIOP retrieves averaged information over 5 km horizontally and approximately 30 m vertically. Additionally, the CALIOP retrievals are based on a number of assumptions about aerosol lidar ratio and depolarization ratio for aerosol types. The CASPOL measurements provide us an exciting and novel opportunity to evaluate the CALIOP aerosol assumptions and propose improved aerosol type models.

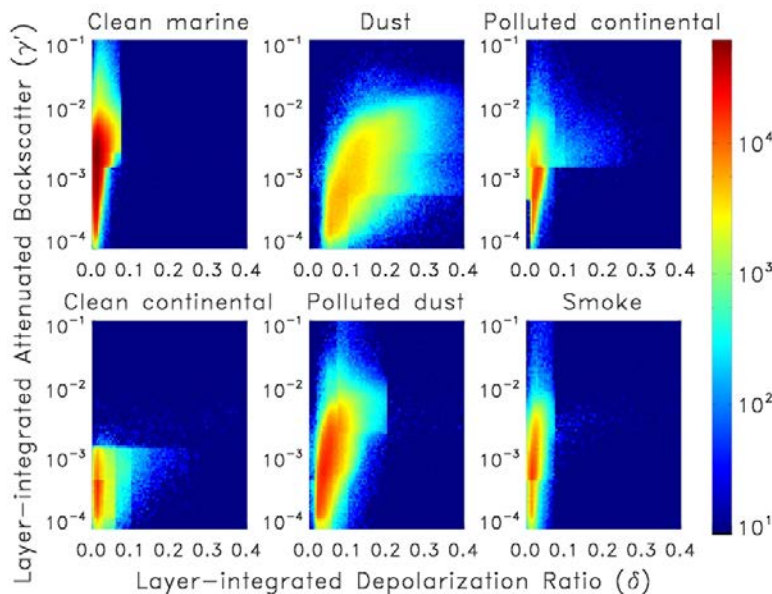


Figure 3. The CALIOP lidar depolarization-backscatter relationships (at 532 nm) for six aerosol types, from the CALIPSO Cloud and Aerosol layer product. [H-M Cho, 2011: *Studying clouds and aerosols with lidar depolarization ratio and backscatter relationships. Ph.D. thesis, Texas A&M University*]. Global observations during the entire year of 2008 are included. The color of each pixel presents the frequency of occurrence for a depolarization-backscatter box with 0.01 by 0.002 sr^{-1} interval.

Task 4 Deliverable A summary of MODIS aerosol optical depth and aerosol type for each for the cases by the CASPOL. CALIOP remotely sensed optical signature plots for each case identified in the CASPOL data. A report summarizing which variations observed in-situ data can and which cannot be observed in remotely sensed data sets.

4. QUALITY METRICS

Quality control (QC) checks on data collected during the field campaign are critical to successful generation of the data. The QC checks used during generation of the original in-situ CASPOL data as well laboratory calibrations of the CASPOL data after the field deployment to check for any changes in instrument performance. Data acceptability is determined by considering detection limit, sample inlet conditions, ambient conditions, with removal of data collected during precipitation and during the time between precipitation and the next maintenance of the inlet line, and data set completeness. Laboratory calibrations serve to determine precision and accuracy in particle sizing of the CASPOL instrument.

Audits of data quality were performed by visual inspection of the data in conjunction with the instrument housekeeping variables, inlet line temperature and relative humidity, and recorded ambient conditions. Since this is the first deployment of the CASPOL instrument, the data cannot be compared to previous deployments. Data that passes these examinations will be deemed acceptable. Data that fails will be further evaluated for possible explanations of any apparent discrepancies. In instances where no clear explanations are found, the data will be removed from the CASPOL data set. Data from additional in-situ instruments will have been QC checked by the respective PIs of complimentary AQRP projects. Ten percent of the in-situ data will be audited by Brooks. At least 10% of the secondary data used in the analysis (i.e., CASPOL, in-situ organic carbon, black carbon, and ozone measurements will be independently reviewed by a member of the research team who did not conduct the analysis for quality assurance purposes.

Remotely sensed data that will be used in the analyses for this project already have undergone extensive QA/QC procedures prior to being included in official NASA MODIS and CALIOP data products and disseminated amongst NASA data user groups. As above, at least 10% of the secondary data used in the MODIS and CALIOP datasets will be independently reviewed by a member of the research team who did not conduct the analysis for quality assurance purposes.

5. DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

Data analysis techniques are described in Section 3. Interpretation of these data may contribute to a better understanding of particulate matter sources and concentrations, and quantification emissions in Texas. Analysis of coincident in-situ and satellite data collected during DISCOVER-AQ will provide insight of the feasibility of using remotely sensed data to observe ground level air quality. Analysis of these data will provide a means to assess the formation and sources of particulate matter pollution impacting Texas air quality. Data generated during the course of this project will be backed up in multiple places including server operated by the Department of Atmospheric Sciences at Texas A&M University and on external hard drives maintained by the PIs. The data will be maintained for a minimum of 3 years after the completion of the project.

6. REPORTING

Reporting for this project will include:

- A. Monthly and quarterly reports including accomplishments, problems encountered and corrective actions, goals for the next reporting period.
- B. Separate monthly financial reports.
- C. Draft final and final reports describing all activities and summarizing all findings.

The final report will include time series of all collected data, identification of the air mass type associated with each time segment of data, and optical signature plots for each specified category. The results of the Quality Assurance Findings will be included in the final report. In addition, the final data report will include MODIS and CALIOP data for each time period collocated with the CASPOL data. The final report will also include a written assessment of the sensitivity of MODIS and CALIOP data products to variations in aerosol concentrations and properties observed near the surface. Finally, the report will include recommendations for future work.

All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at <http://aqrp.ceer.utexas.edu/> will be followed.

A draft of a journal manuscript based on the work performed as part of this project will be presented to the TCEQ upon submission to the journal. The manuscript is likely to include a summary of aerosol properties observed during DISCOVER-AQ and evaluation of the CALIOP aerosol assumptions and proposed improved aerosol type models based on comparison to the in-situ data collected during DISCOVER-AQ.

7. REFERENCES

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