Results and Findings from DISCOVER-AQ Denver 2014

Overview of ORD Ground-Based Measurements under EPA Collaboration with NASA

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EM – August 2016

1. **Evaluation and Comparison of Methods for Measuring Ozone and Nitrogen Dioxide Concentrations in Ambient Air during DISCOVER-AQ**
2. **Use of Air Quality Sensors during DISCOVER-AQ**
3. **The Use of Lidar Technology for Measuring Mixing Heights under the Photochemical Assessment Monitoring Stations (PAMS) Program**
4. **Multi-Perspective Observations of Nitrogen Dioxide over Denver during DISCOVER-AQ: Insights for Future Monitoring**

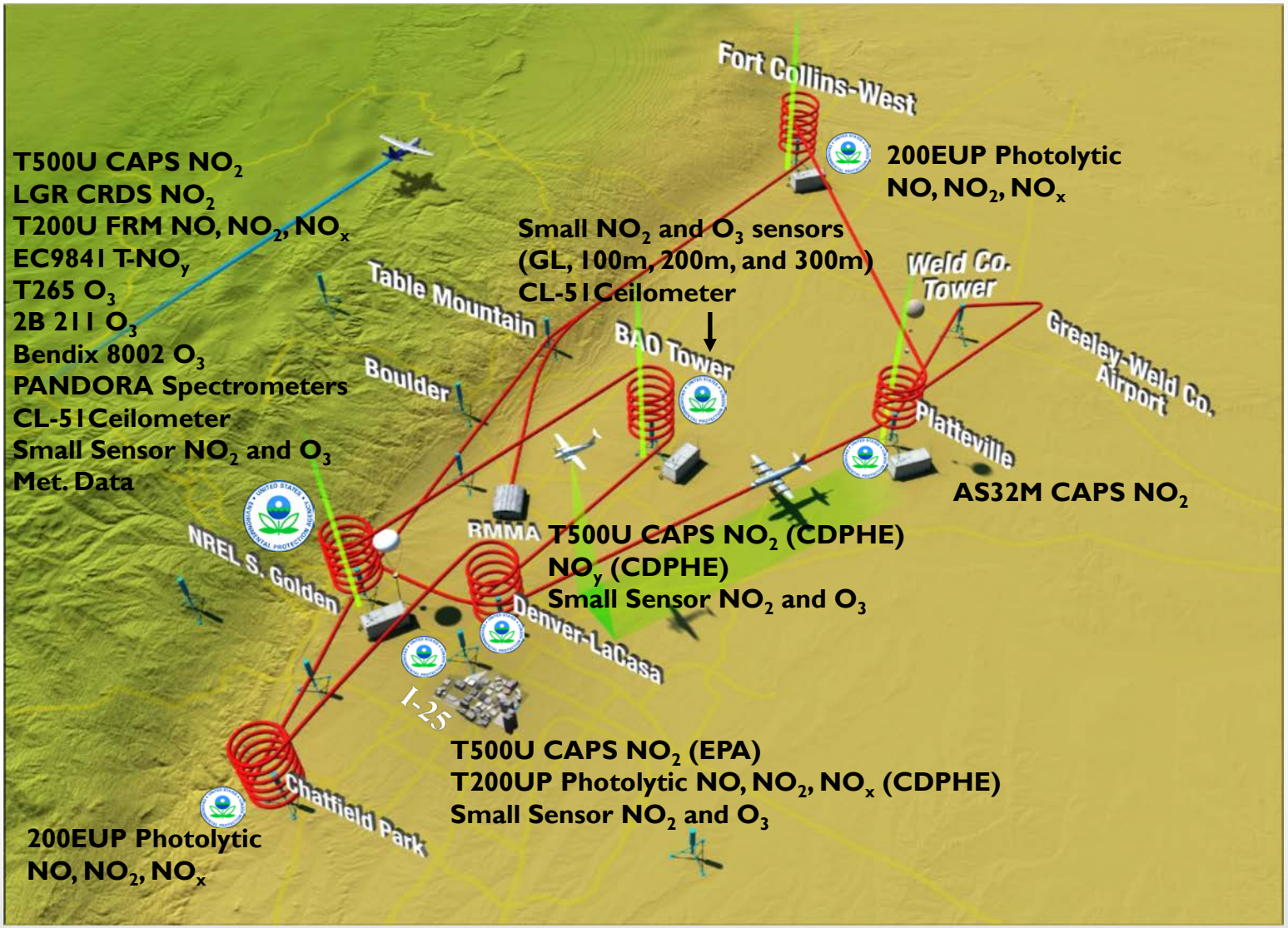
DISCOVER-AQ

- *DISCOVER-AQ:* Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality
- How can ambient air quality be reliably informed using non-traditional approaches, such as satellite remote sensing?
- Collaboration with NASA to explore temporal and spatial relationships between column and surface measurements at locations with differing air quality.
- Unprecedented 3-dimensional characterization of pollutants and precursors.
  - Result is an expansive database of satellite, aircraft, ground-based measurements for gaseous air pollutants (i.e., NO_2, NO_y, O_3, …) and particulate matter over urban areas with persistent air quality problems
    - Final Denver data set is publicly accessible in NASA archive.
- EPA research used to inform:
  - NAAQS compliance monitoring methods
    - Federal Reference (FRM) and Equivalent (FEM) methods
  - Value of new monitoring approaches (in-situ, small sensors, and remote sensing)
  - Evaluation and improvements for Community Multiscale Air Quality (CMAQ) fine-scale modeling

Benefits of EPA/NASA Collaboration on DISCOVER-AQ

- Reference method research will benefit state, local and tribal organizations by providing state of the science tools for use in regulatory monitoring:
  - New O_3 FRM (included in October 2015 Ozone NAAQS Rulemaking)
  - Direct optical NO_2 methods in near roadway settings
  - NO_y methods as a potential FRM for NO_x/SO_x secondary NAAQS
- Enhanced understanding and use of satellite and remote sensing methods for air quality applications
  - Exceptional event analysis
  - Improve understanding of surface pollutant distributions
  - Improve emission estimates
  - Assist in ground based monitoring site selection
- Evaluation of small sensor technology for supplemental air quality monitoring
  - Citizen science applications
  - Understanding vertical and spatial distribution of air pollutants
- DISCOVER-AQ intensive field campaigns are a driver for innovation with respect to fine-scale CMAQ evaluation
- Total DISCOVER-AQ air quality research investment in excess of $30 million
  - EPA-ORD approximately $2.7 million
  - NASA approximately $30 million

Denver, CO Observation Strategy July-August 2014

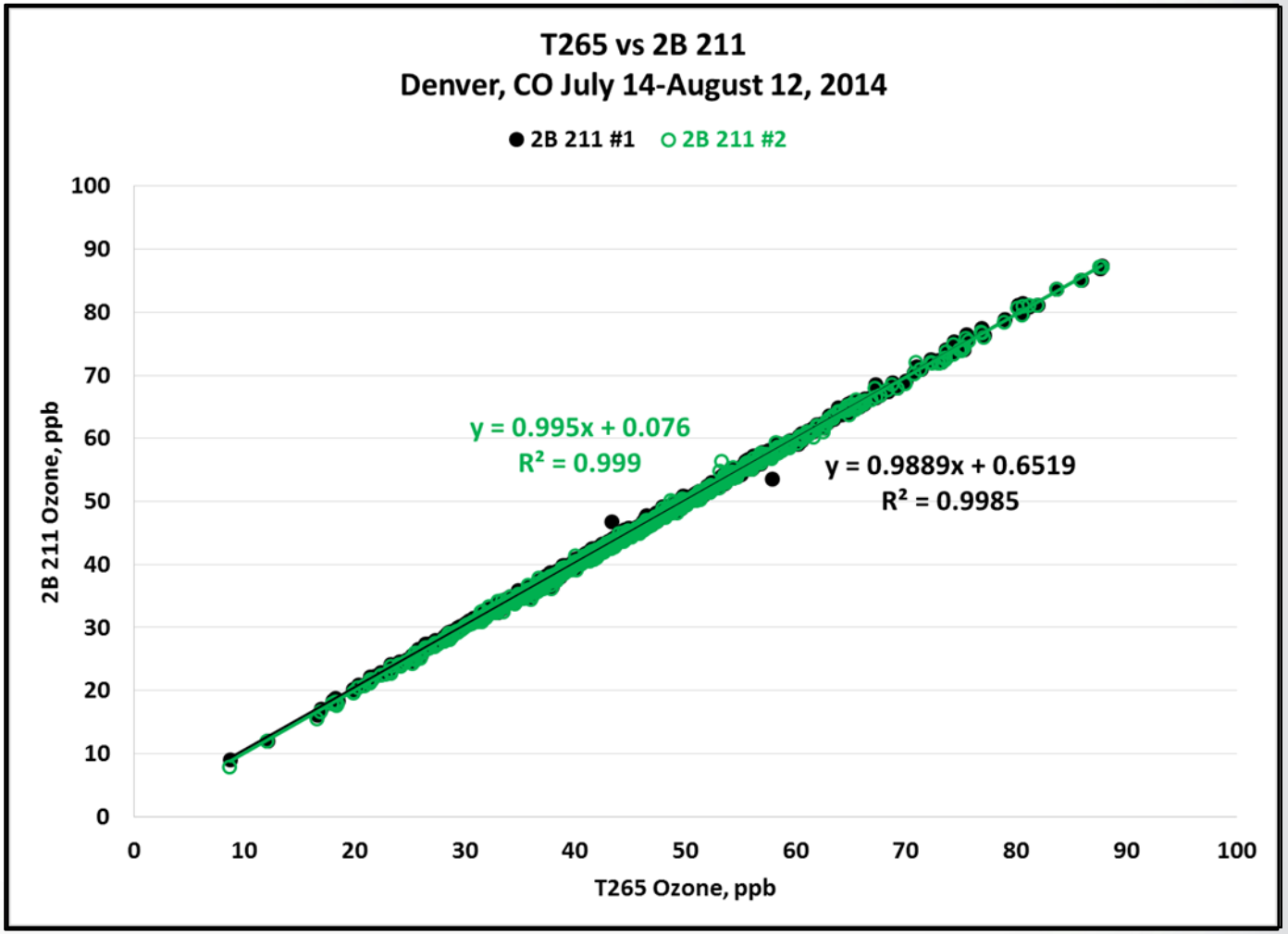


FRM/FEM Methods Research Under DISCOVER-AQ: O_3

- **ORD has leveraged DISCOVER-AQ deployments as ambient evaluations of new potential FRMs/FEMs.**
- **ORD has evaluated and proposed a new O_3 FRM based upon NO-chemiluminescence (NO-CL).**
- **The new FRM will mitigate many of the measurement issues associated with current methods (including measurement interferences by VOCs and water vapor).**
- **The new O_3 FRM was promulgated as part of the O_3 NAAQS rulemaking package and published in the FR on October 26, 2015.**

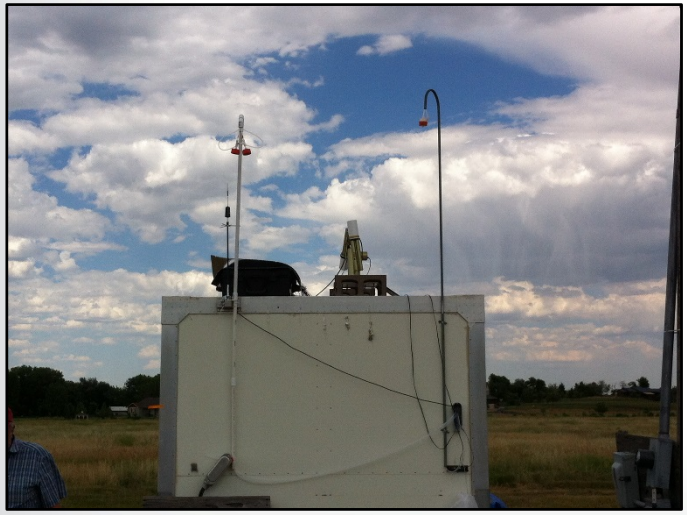
FRM/FEM Methods Research Under DISCOVER-AQ: O_3

- **Similar to all other ambient air studies, good agreement was observed between the Bendix 8002 (ET-CL), the T265 (NO-CL) and the 2B 211 (SL-UV) methods for 1 Hr average and Maximum Daily Eight Hour Average (MDA8) ozone concentrations during the July-August 2014 Denver, CO evaluation.**



FRM/FEM Methods Research Under DISCOVER-AQ: NO_2, NO_x, and NO_y

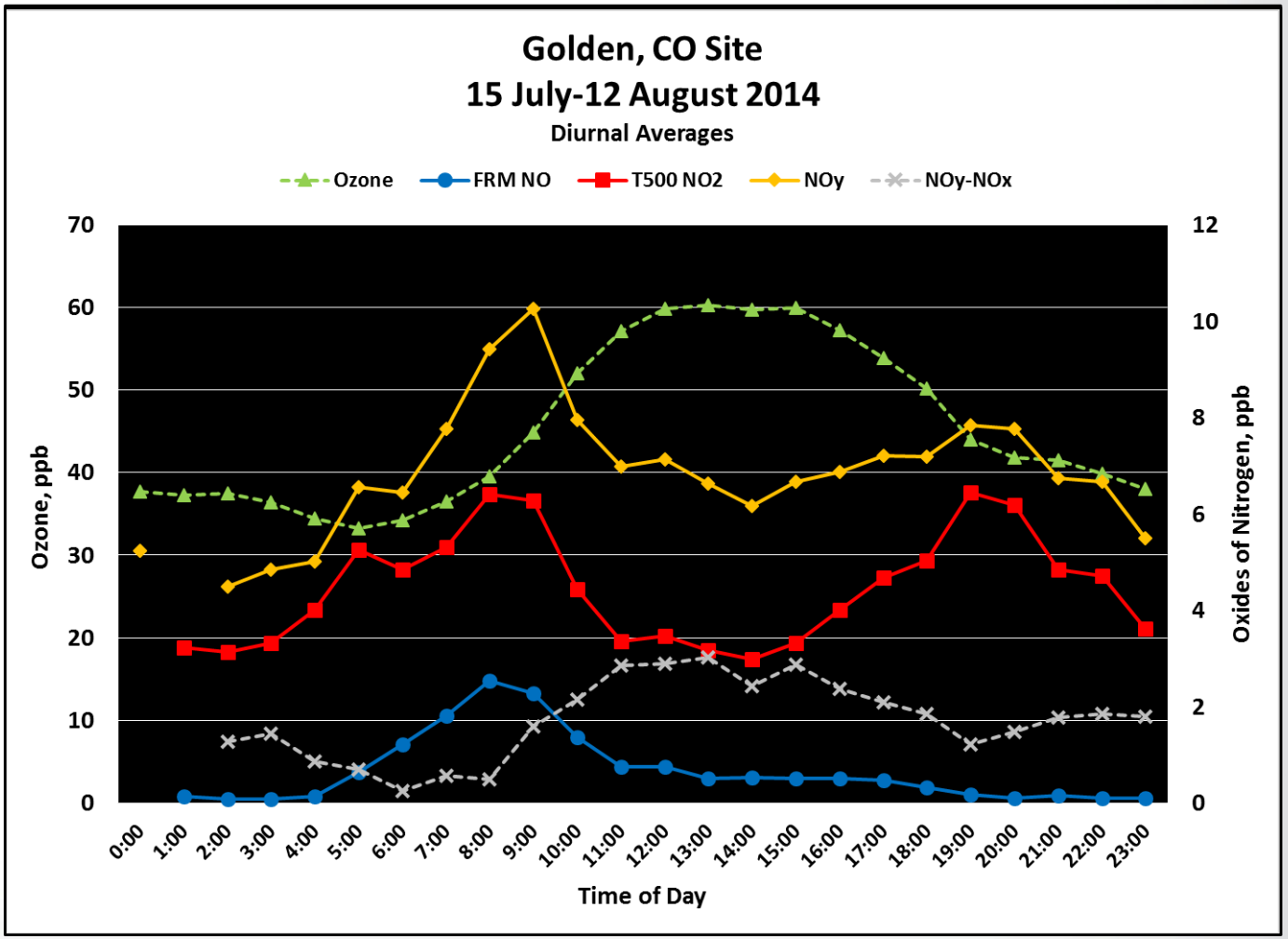
- **DISCOVER-AQ provided the opportunity to evaluate the current FRM against more selective NO_2 methods.**
- **Ambient deployments also allowed for the investigation and evaluation of methods for oxides of nitrogen (NO_x) and total reactive oxides of nitrogen (NO_y).**



- **NO_2 method evaluations were performed during all DISCOVER-AQ deployments.**
- **NO_2 data were collected by ORD at 7 sites during the Denver DISCOVER-AQ study.**
- **ORD collected ~8 weeks of ambient data in a near roadway setting (I-25) during and after the Denver DISCOVER-AQ study.**

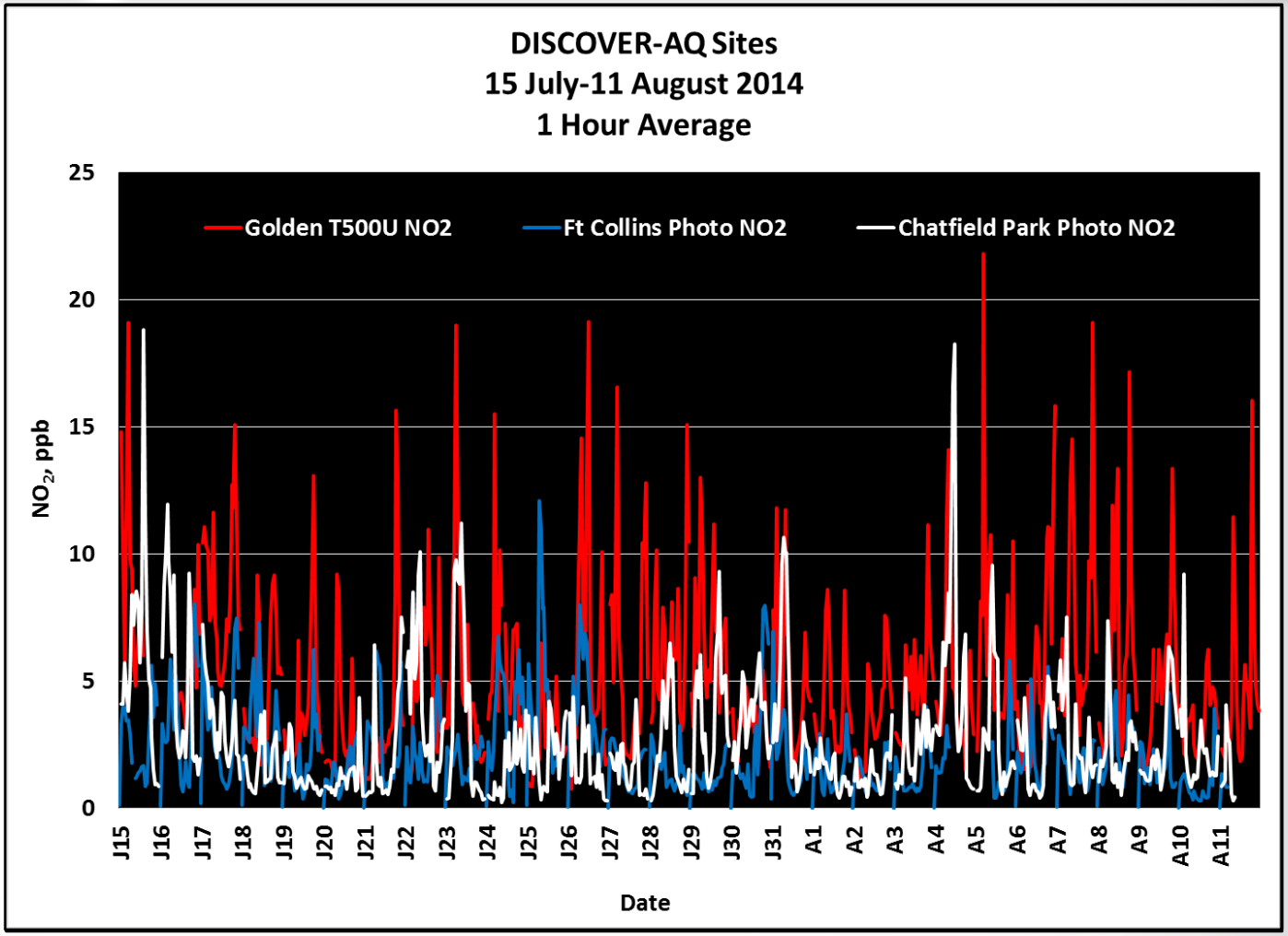
Oxides of Nitrogen Measurements Golden, CO Site

- Peaks in 1 Hr NO, NO_2, and NO_y concentrations are observed during periods generally associated with local traffic patterns.
- Differences between NO_y and NO_x (NO_y-NO_x=NO_z) are correlated (similar diurnal patterns) with ozone. Both ozone and NO_z are photochemically formed.
- Hourly average results (for each hour of the day) averaged over the month long study period further show the traffic impacts on peak NO, NO_2 and NO_y concentrations and the similar diurnal patterns of NO_y-NO_x and ozone.



Oxides of Nitrogen Measurements DISCOVER-AQ Sites

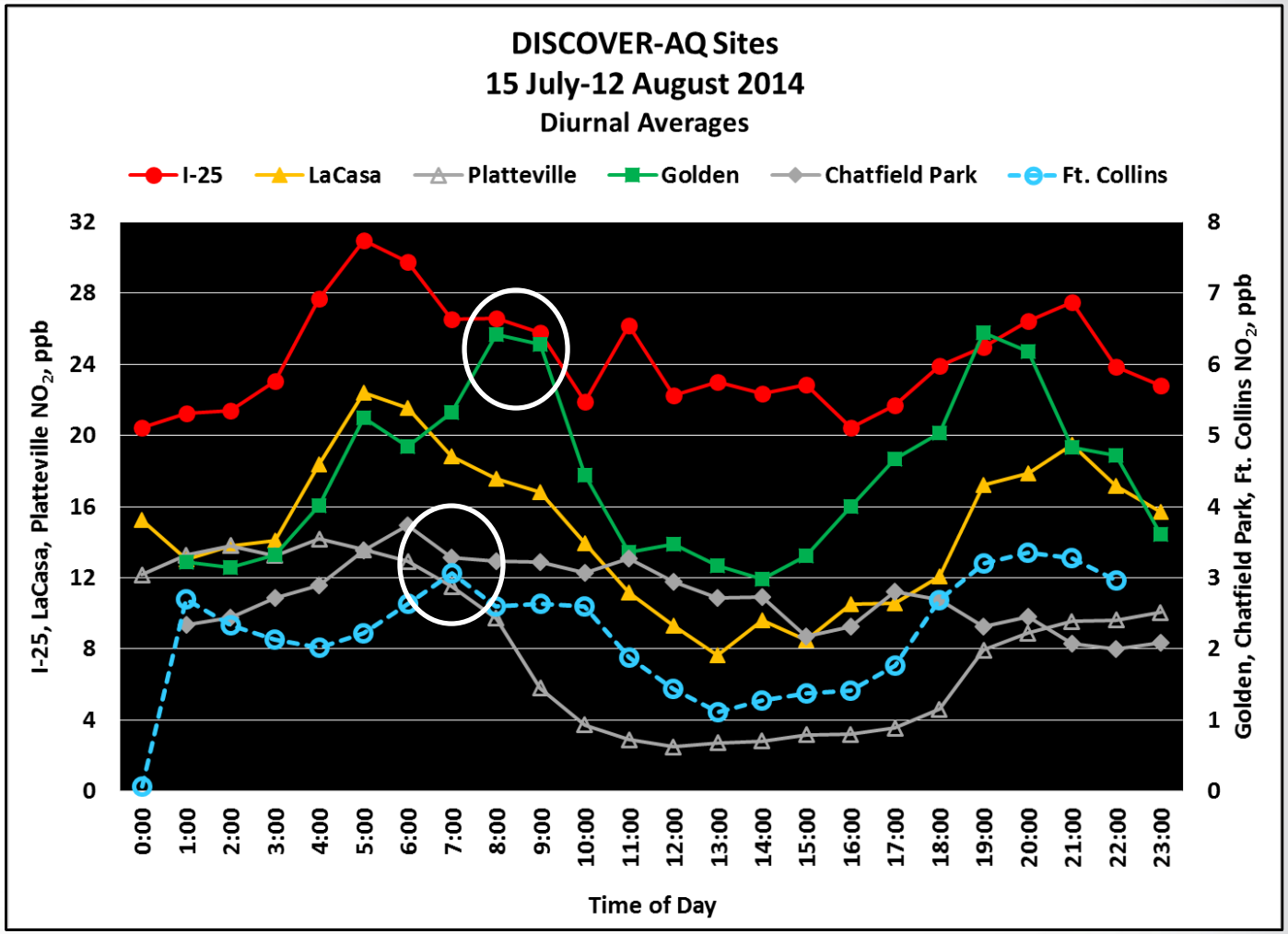
- NO_2 concentrations observed at LaCasa and I-25 (near roadway) and Platteville are significantly higher than those at the other DISCOVER-AQ sites.
- Data averaged to 1 hour to get a better picture of diurnal patterns in peak concentration.
- NO_2 concentrations at I-25 and LaCasa sites appear to be impacted by traffic and local sources.
- Peaks in NO_2 concentration at Platteville occur during overnight hours.
- Peaks in NO_2 concentration at other sites show traffic and loacal source impacts



Oxides of Nitrogen Measurements DISCOVER-AQ Sites

- **Hourly average results (for each hour of the day) averaged over the month long study period show the differences in average NO_2 concentrations and diurnal patterns at the various sites during the study period.**

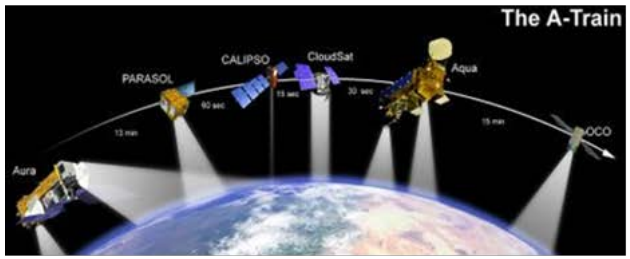
- **Sites on the western slopes (Golden, Ft. Collins) show slight delays in peak concentrations illustrating transport of pollutants up slope throughout the day.**



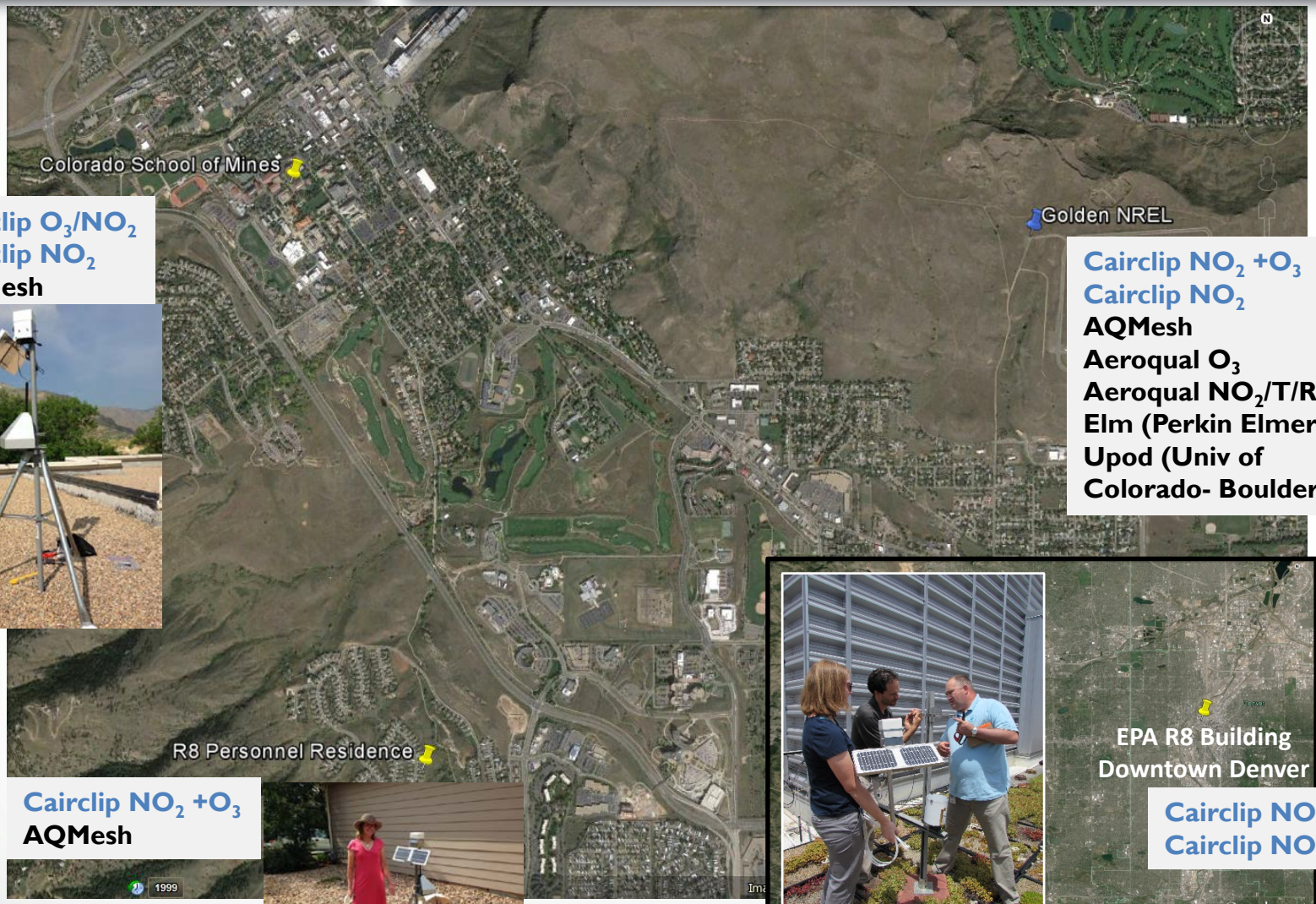
FRM/FEM Methods Research Under DISCOVER-AQ

Changing the Paradigm

- **This research also provides tools for evaluation and assessment of new technologies (sensors, remote sensing spectrometers, satellites, aircraft measurements) for monitoring ambient air pollution.**



Citizen Science Network
Denver, CO



Cairclip O_3/NO_2
Cairclip NO_2
AQMesh

Cairclip NO_2 +O_3
Cairclip NO_2
AQMesh
Aeroqual O_3
Aeroqual NO_2/T/RH
Elm (Perkin Elmer)
Upod (Univ of Colorado- Boulder)

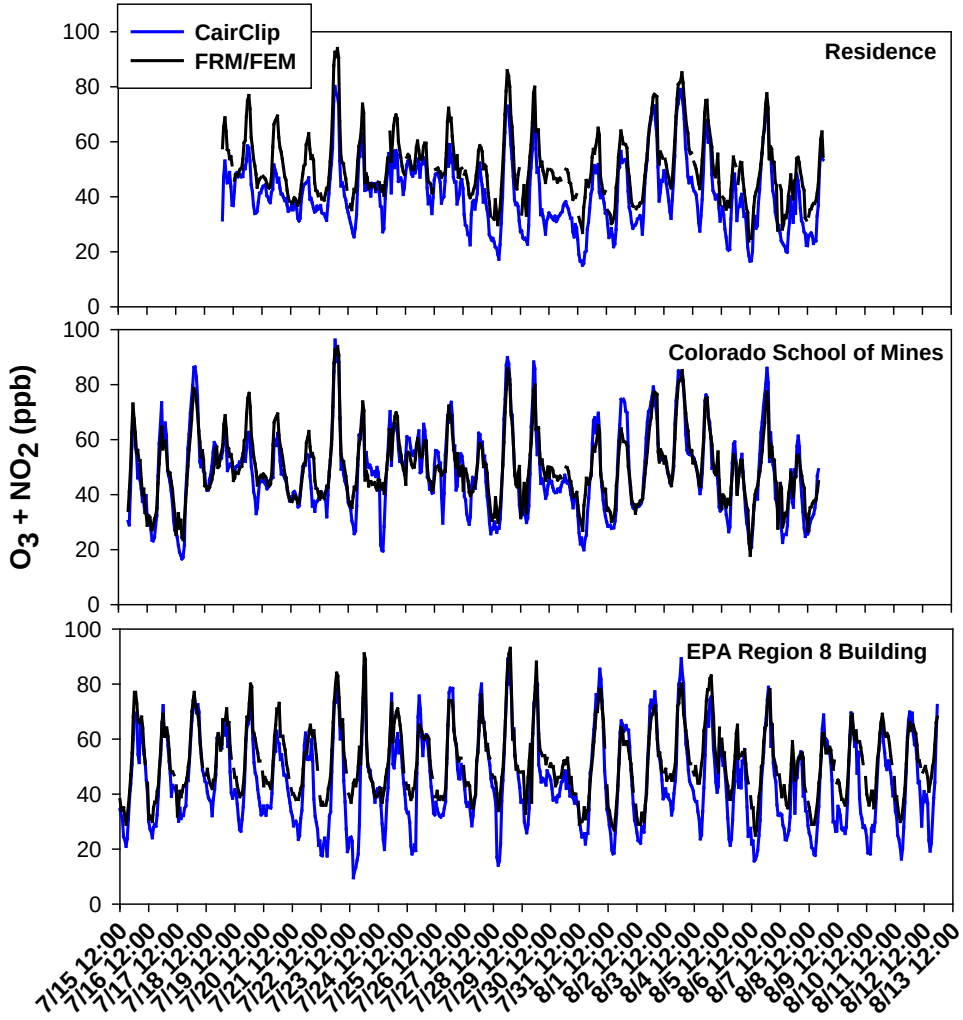
Cairclip NO_2 +O_3
AQMesh

Cairclip NO_2 +O_3
Cairclip NO_2

Sensor Evaluation and Citizen Science
Denver, CO

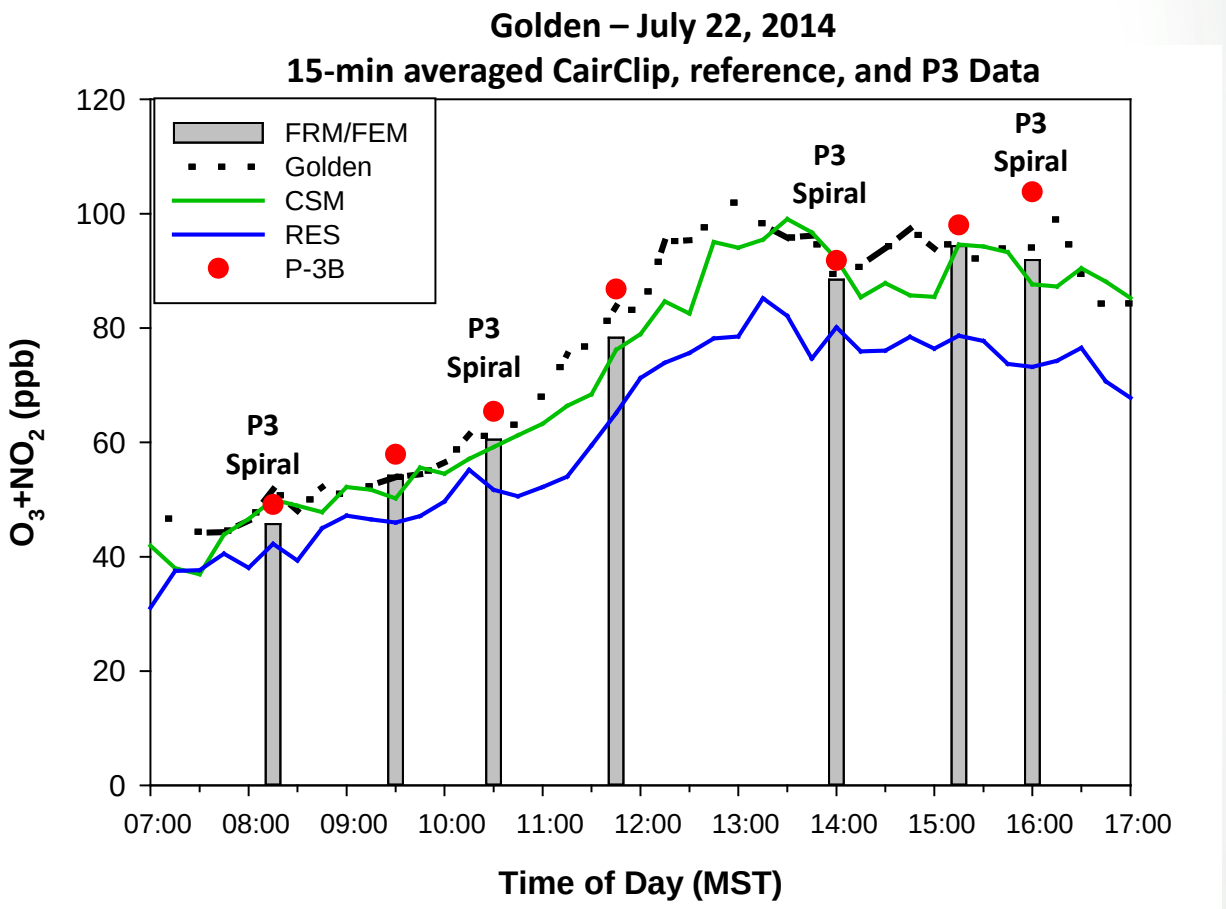
- Hourly averaged CairClip (O_3/NO_2 version) and reference data
- Sensor measurements are comparable to reference measurements

Note: R8 Building sensor data compared to Denver CAMP state monitoring site



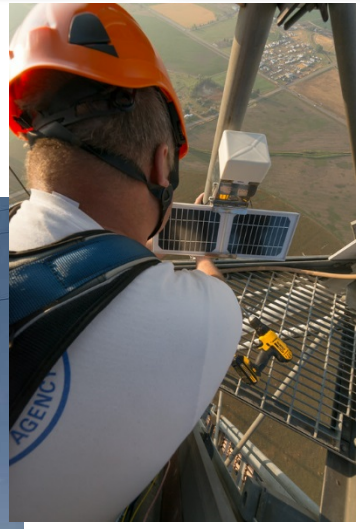
Sensor Evaluation and Citizen Science
Denver, CO

- **P3 Aircraft O_3 and NO_2 measurements limited to below 1000 m (AGL) altitude**
- **Good agreement obtained between aircraft and ground based (including sensors) results**

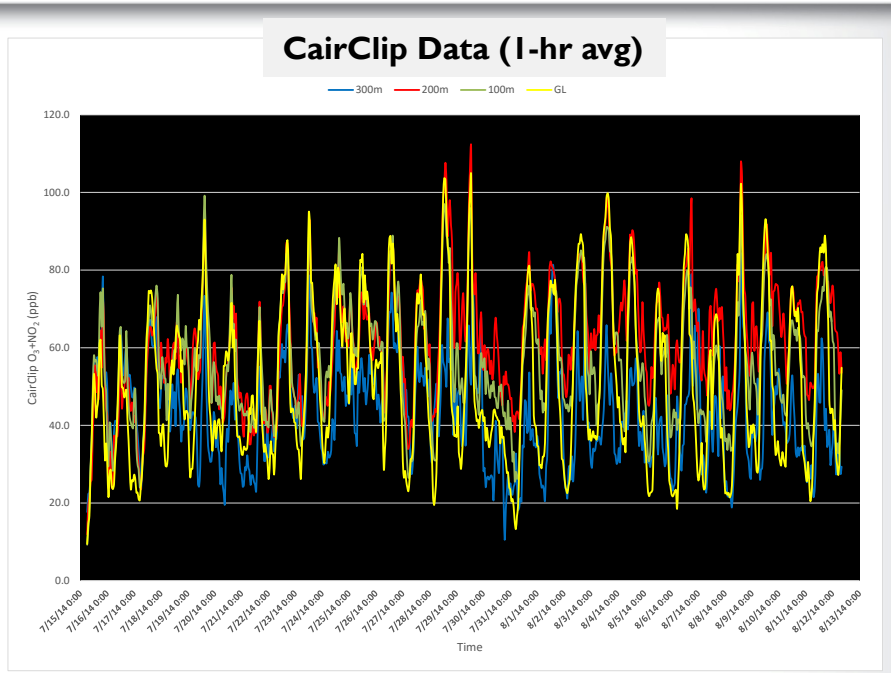


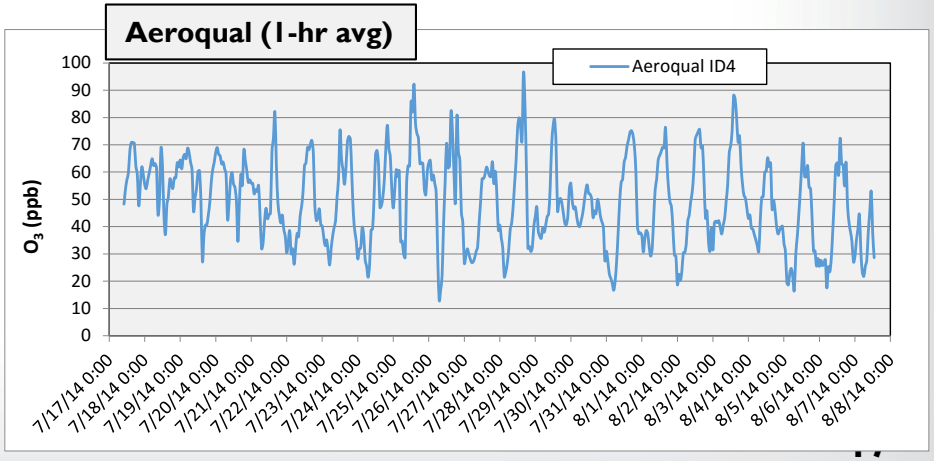
Sensor Evaluation – BAO Tower Denver, CO

Evaluating vertical distribution of pollutants at NOAA's BAO Tower

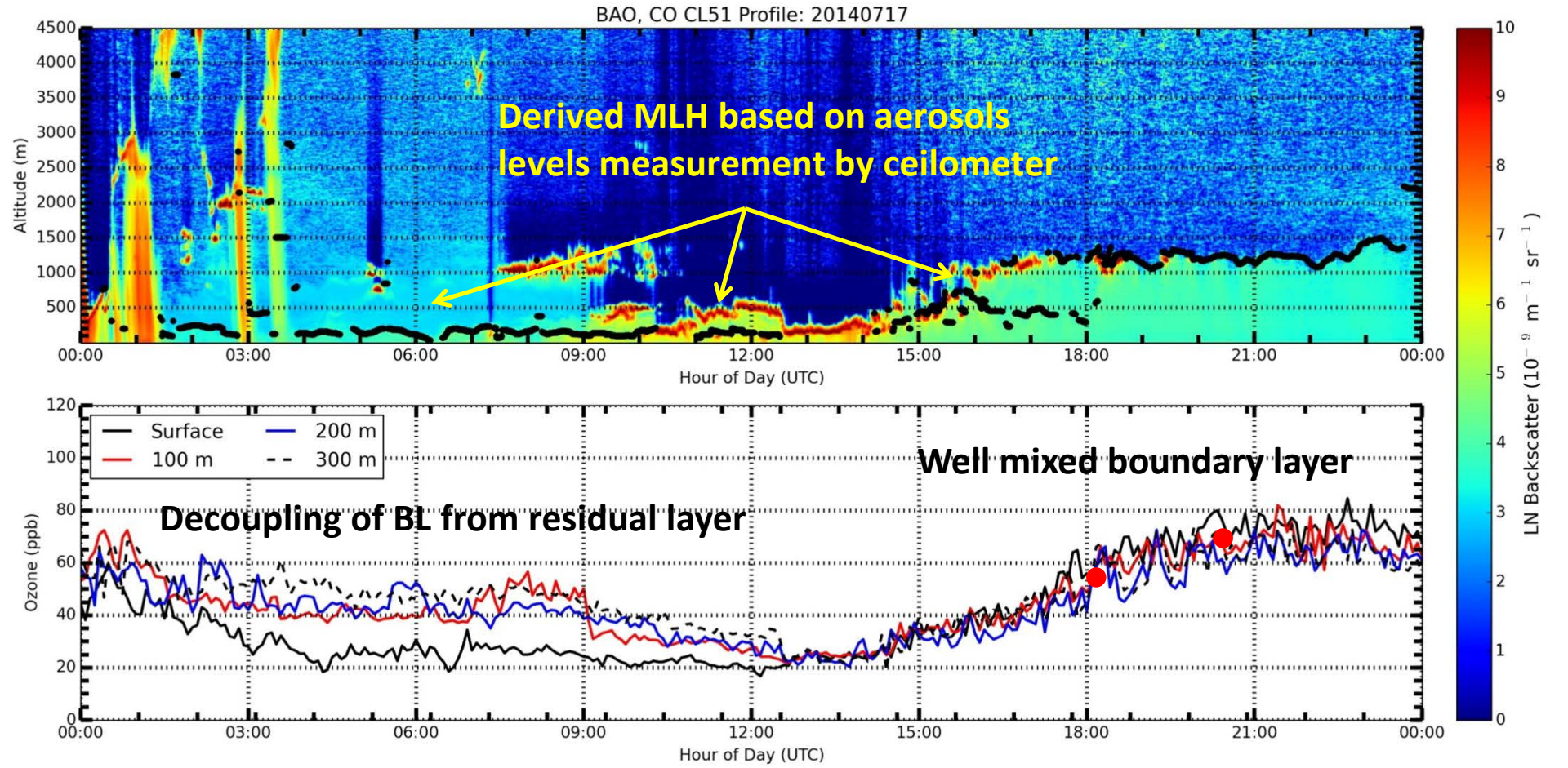


Ground Level
CairClip
Aeroqual O3
AQMesh





Preliminary Data – DISCOVER-AQ Boulder Atmospheric Observatory - Erie, CO July 17, 2014



- **ORD added a CL-51 ceilometer at BAO Tower to characterize MLH.**
- **Top Image: aerosol backscatter overplotted with derived mixed layer heights.**
- **Bottom image: Sum of Ozone and Nitrogen Dioxide measurements with CAIRCLIP sensors on BAO Tower. Sensors located at 3m, 100m, 200m, and 300m AGL. Red dots are P3 measurments during BAO Tower spiral.**
- **Combined measurements appear to capture decoupling of boundary layer from residual layer between surface and 100m due to night time radiational cooling and growth of boundary layer on the next day.**

Remote Sensing Discussion Topics

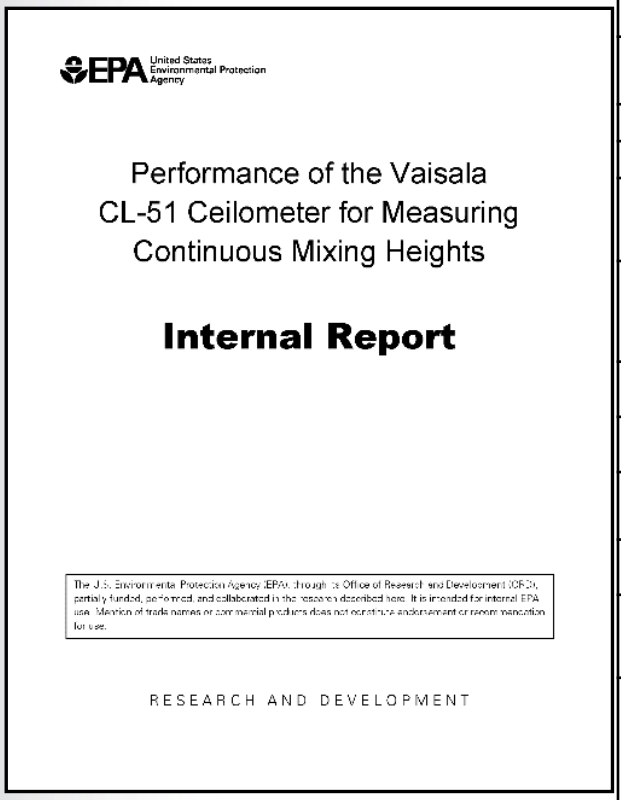
Vaisala CL-51 Ceilometer

- Field Evaluation of Mixing Height
- BL-View vs. STRAT
- Data Considerations – full backscatter profile vs. hourly mixing height

PANDORA Ground Based Spectrometer, TropOMI and TEMPO Missions

- Nexus with new PAMS requirements

Field Evaluation of CL-51


EPA United States Environmental Protection Agency

Performance of the Vaisala CL-51 Ceilometer for Measuring Continuous Mixing Heights

Internal Report

The U.S. Environmental Protection Agency (EPA), through its Office of Research and Development (ORD), partially funded, performed, and collaborated in the research described here. It is intended for internal EPA use. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

RESEARCH AND DEVELOPMENT

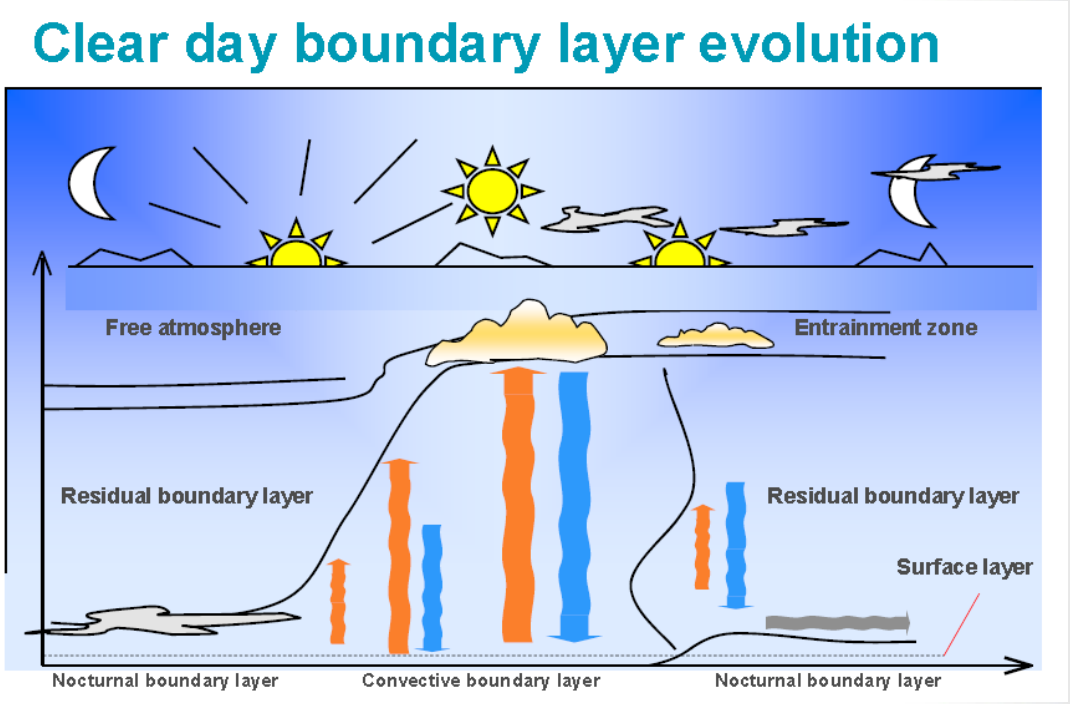
Instrument Names	CL-51	Sonde	CL-31	NASA P-3B Profiles	MPL
Variable Measured	aerosol backscatter	T, RH, O3	aerosol backscatter	T, RH, O_3, & extinction	aerosol backscatter
LIDAR Wavelength (nm)	910	NA	910	NA	532
MLH or PBL	MLH	PBL	MLH	PBL & MLH	MLH
Platform	Surface	Balloon	Surface	Aircraft	Surface
Location	Hampton, VA, Golden and Erie, CO	Hampton, VA, Golden and Erie, CO	Erie, CO	Golden and Erie, CO	Golden, CO
Study Timeframe	December 2013-2015; July-August 2014	December 2013-2015; July-August 2014	July-August 2014	July-August 2014	July-August 2014
Temporal Coverage	Continual	Day/week	Continual	Flight Day	Continual
Spatial Coverage	Point	<10 km	Point	<10 km site spiral	Point
Temporal Resolution	36 s	1 s	2 s	< 20 minutes	60 s
Vertical Resolution	10 m	5 m	10 m	~100 m	30 m
PBL/MLH Method	Gradient	Hefter (T inversion) & Gradient	Gradient	T inversion & Gradient	Gradient
Approximate Instrument Cost	$39,000	Receiving station, ozonizer test unit, and start-up kit - $25,000, plus $200/sonde (iMET)	$32,000	NA	$100,000

Boundary Layer Height/Mixing Layer

- -The Convective (daytime) Boundary Layer (CBL) is characterized by roughly uniform vertical profiles of Moisture (RH) and Potential Temperature. Potential Temperature is often the most common measurement used to characterize Planetary Boundary Layer Heights (PBLH).

- -Atlas and Korb (1981) presented the use of aerosol profile measurements via LIDAR as a method to indicate BL Heights.

- -When sufficient aerosols are present, the aerosol gradient (Mixing Layer Height) at the top of the Convective Boundary Layer is well correlated with the PBLH characterized by the thermodynamic gradient.



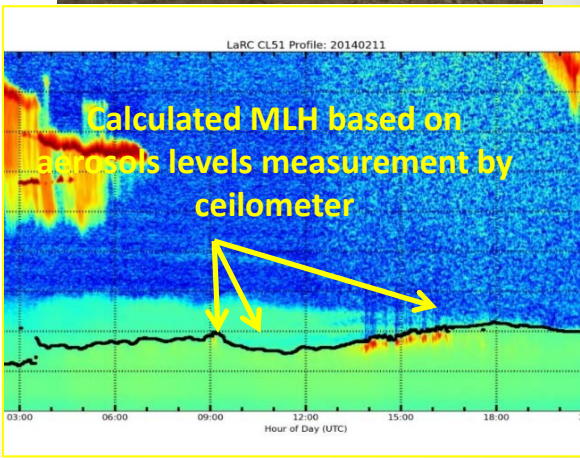
Mixing Layer Height and Air Quality

- The Mixing Layer Height (MLH):
  - Controls the volume of air available for the mixing of pollutants in the lowest layer of the atmosphere.
  - Varies through out the day impacting the level of pollutant concentrations at the surface.
  - A critical parameter in chemical transport modeling.
  - A key variable in satellite trace gas retrievals, and also understanding the column density measurements relative to surface concentrations.

- The PAMS program now requires hourly MLH (2019 Implementation).

- As part of on-going in-field remote sensing research, NERL evaluated the use of CL-51 ceilometer to measure mixing heights at the following locations:
  - CAPABLE research site (NASA LaRC, Hampton, VA)
  - DISCOVER-AQ Denver (Golden, CO and Boulder Atmospheric Observatory Erie, CO).
  - KORUS-AQ Olympic Park, Seoul and Tahwea Forest, South Korea

EPA CL-51 ceilometer adjacent to Space Science and Engineering Center, University of Wisconsin Mobile Lab during DISCOVER-AQ



Vaisala CL-51Ceilometer

Vaisala CL-51 Ceilometer Stated Characteristics:

- **Cloud reporting range: 0…43,000 ft (0…13km)**
- **Backscatter profiling range: 0…49,200 ft (0…15km)**
- **Can operate in all weather**
- **Fast measurement - 6 second measurement cycle**
- **Reliable automatic operation**
- **Good data availability**
- **Eye safe diode laser (LIDAR)**

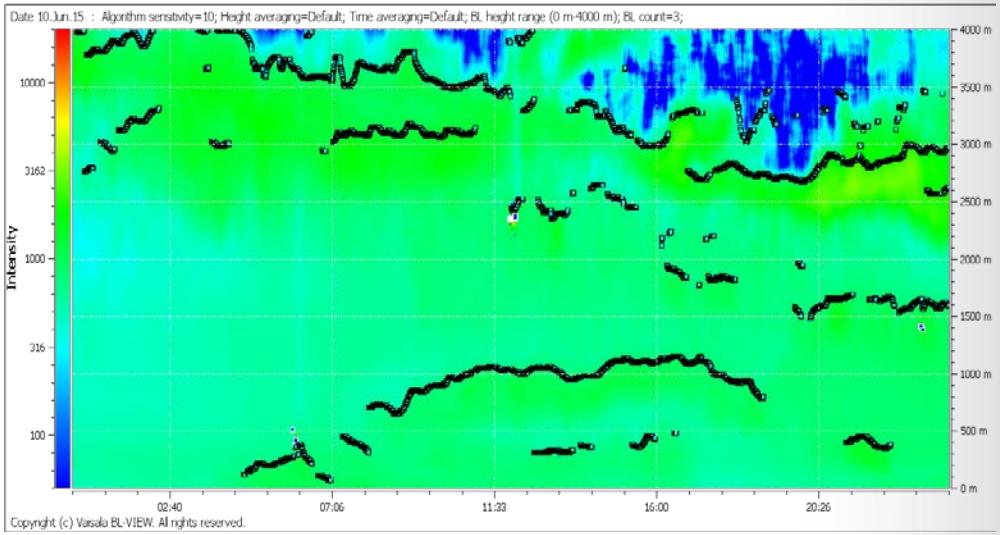
CL-51 positioned next to Space Science and Engineering Center, University of Wisconsin Mobile Lab

Within in the U.S. peer-reviewed literature contains limited evaluation of the CL-51 derived mixing layer height compared to radio-sonde boundary layer height.

CL-51 Comparison was conducted using the Vaisala BL-View Software for the CL-51 MLHs

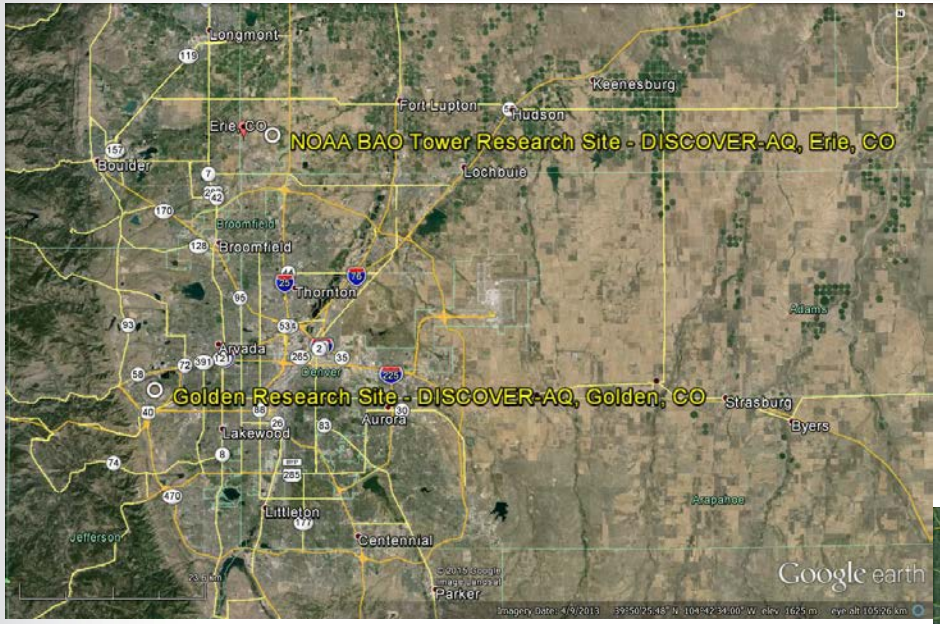
- **BL-View Software:**
  - Uses a proprietary gradient method algorithm
  - Identifies up to 3 aerosol layers for consideration of MLH
  - Layers assigned quality index (QI) 1 to 3; 3 highest confidence
  - Use of variable time and altitude averaging
- **Advantages:**
  - Standardization of the retrieval parameters
  - Flexible User Interface which allows user-specified sensitivities
- **Disadvantages:**
  - Database system that makes access to raw data difficult
  - Unable to log the entire backscatter profile via BL-View
  - Inability to batch process archived data

Characteristic backscatter curtain plot generated in BL-View for 10-June, 2015 at CAPABLE Research Site - Hampton, VA



Smoke from the Canadian forest fire was observed by increased backscatter in the 2500 – 4000 m range.

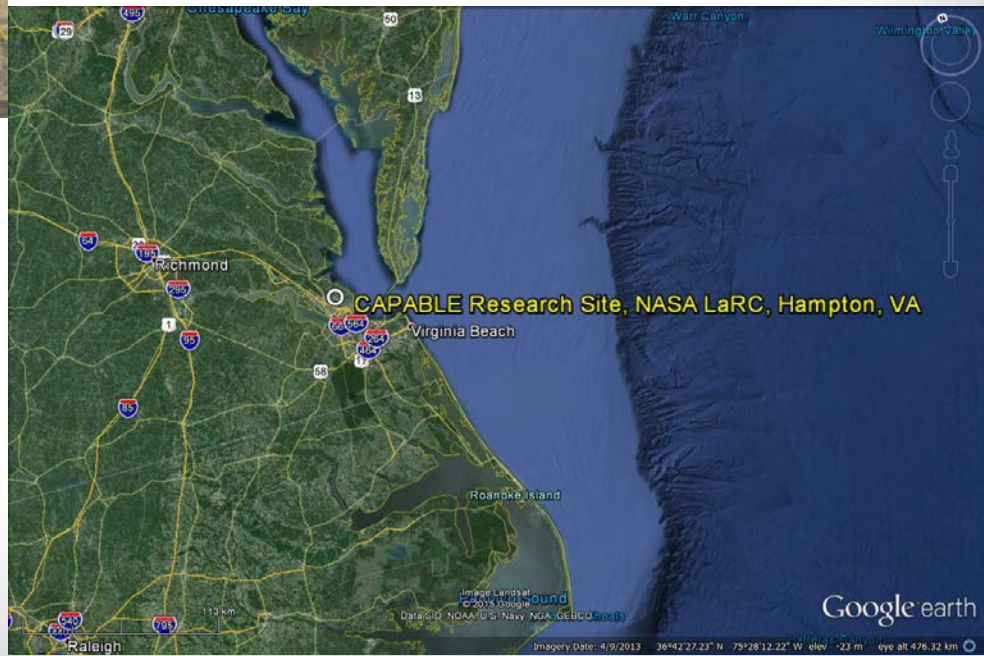
Field Evaluation locations for CL-51



NOAA BOA Tower Site (Erie, CO)
– start of High Plains

Golden NREL Site
-On a mesa -intermountain site

Both sites low aerosol loading

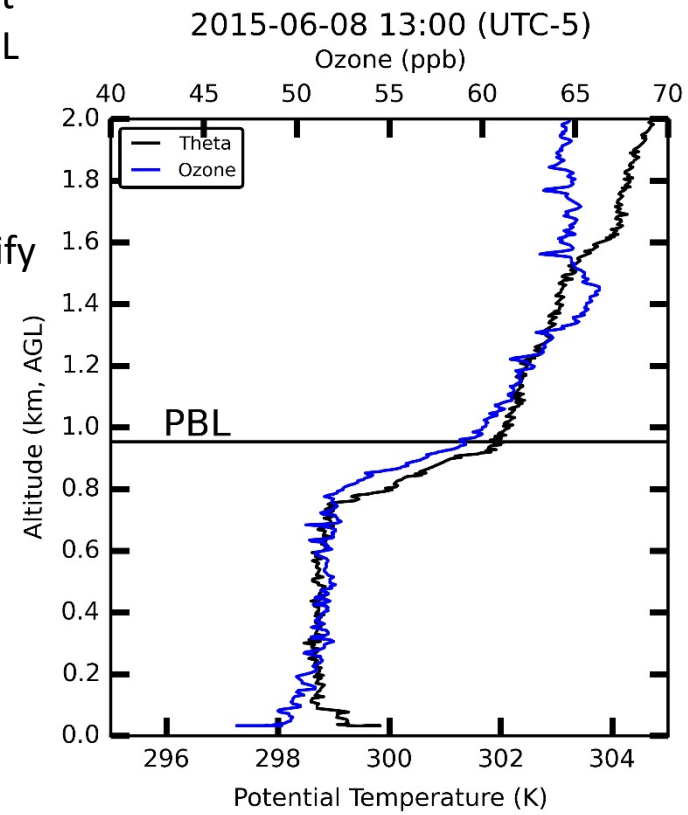


NASA Langley (Hampton, VA)
- Near sea level – coastal site

Low-moderate aerosol loading – with marine influence

Boundary Layer Height/Mixing Layer

- Radiosondes are typically viewed at the “gold standard” to measure PBL height via potential temperature. Water vapor and pollutant concentrations, such as ozone or aerosols, can also be used to identify PBL/ML heights.

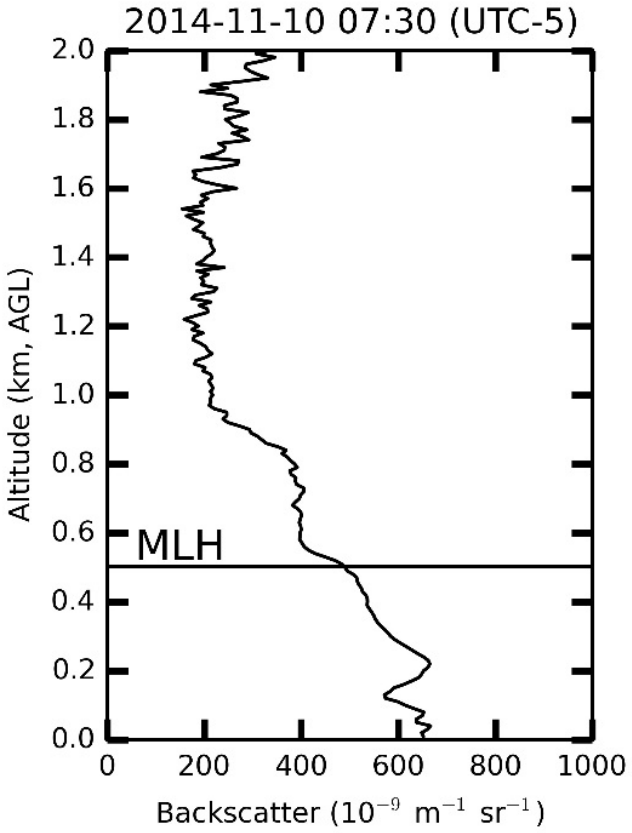


Atmospheric profile of potential temperature and ozone concentration collected with ozondesonde

Boundary Layer Height/Mixing Layer

- Radiosondes are typically viewed at the “gold standard” to measure PBL height via potential temperature. Water vapor and pollutant concentrations, such as ozone or aerosols, can also be used to identify PBL/ML heights.

- The aerosol concentration typically builds up within the PBL as most of the aerosol sources are near the surface and the entrainment zone or capping inversion acts as a lid. In contrast, the aerosol concentration is much low in the free troposphere, allowing this gradient to be identified as the mixing layer.



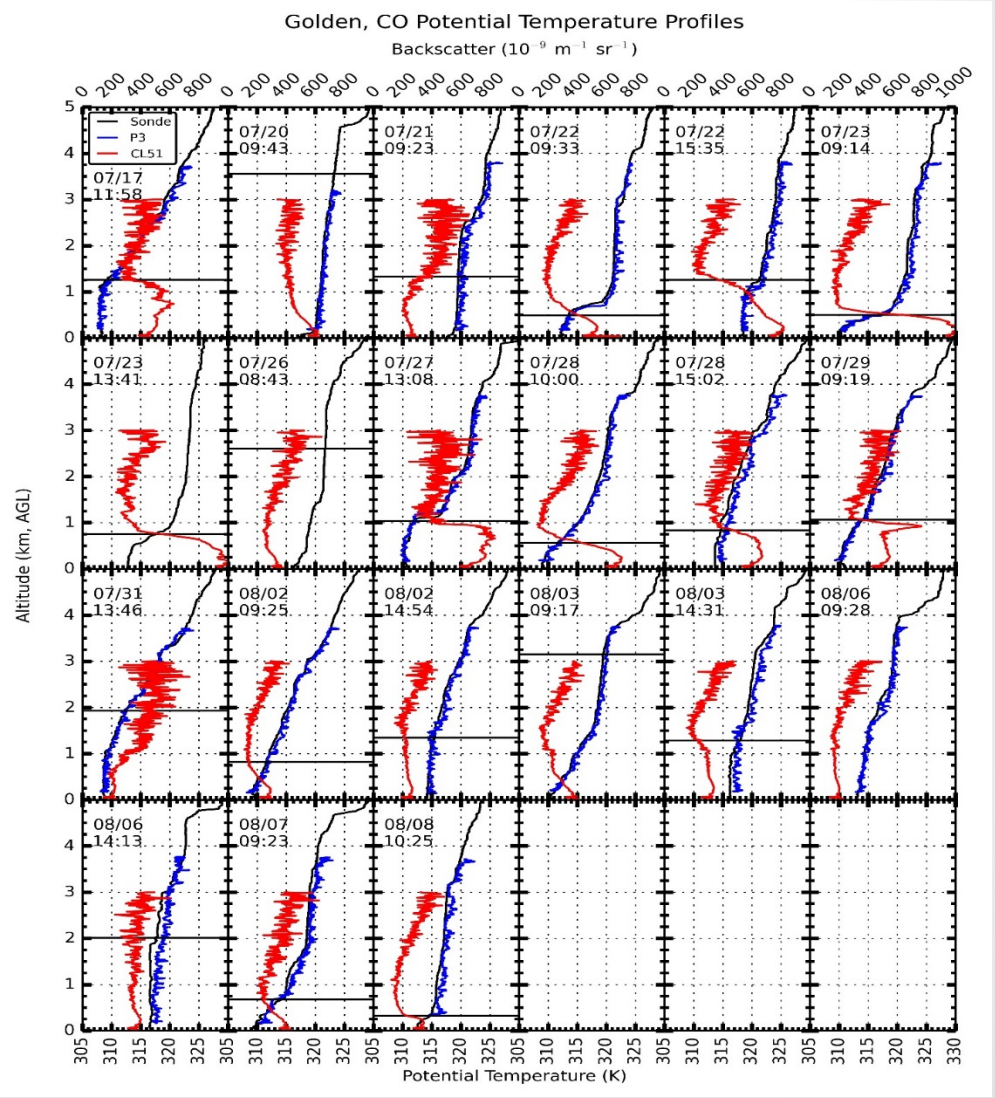
Atmospheric profile of normal range-resolved aerosol backscatter collected with ceilometer (Vaisala CL-51)

CL-51 positioned next to Space Science and Engineering Center, University of Wisconsin Mobile Lab

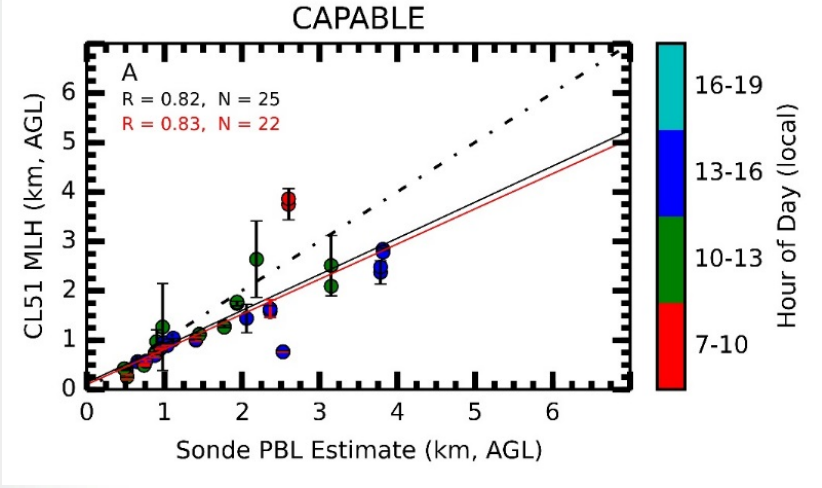
NASA P-3B Spirals used to Evaluate Spatial Representation of Sonde PBLH

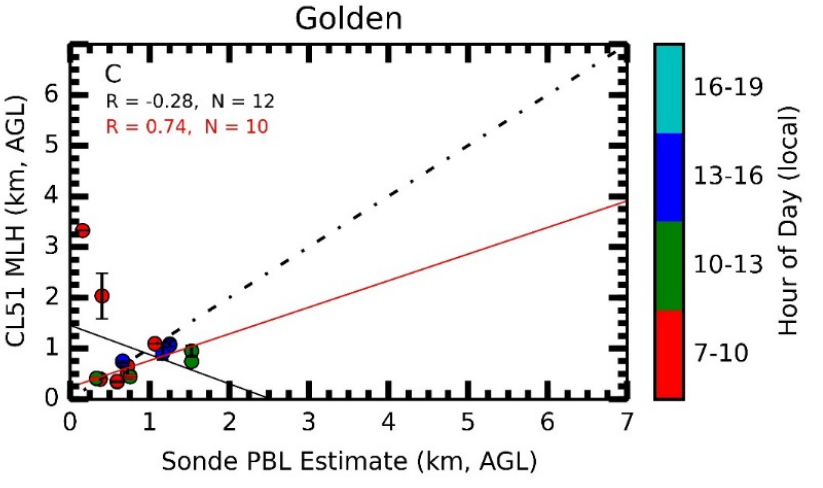
- Potential temperature (**NASA P-3B** and **Millersville University radiosondes**) and **CL-51 backscatter** profiles collected at the Golden NREL site. Horizontal lines indicate MLH as determined via BLView.

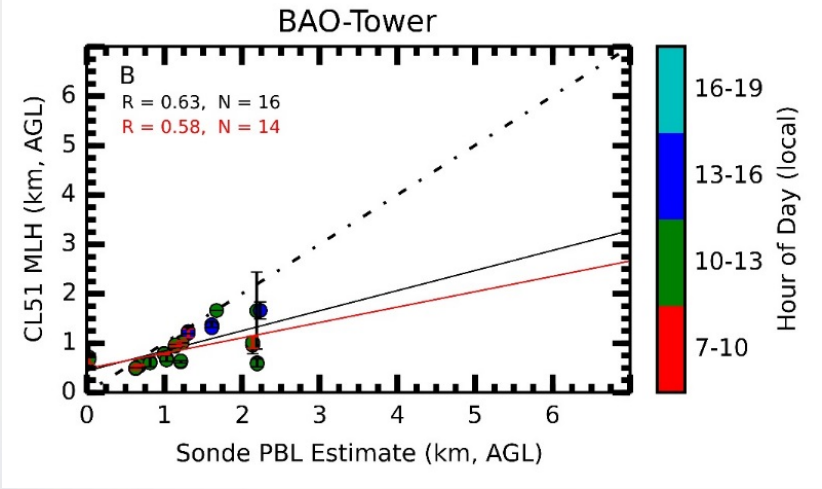
- PBL Height from NASA P-3B spiral (~5 km) shows good agreement with sondes.



CL-51Mixing Layer Height (aerosol gradient) vs. Planetary Boundary Layer Height (thermal gradient)



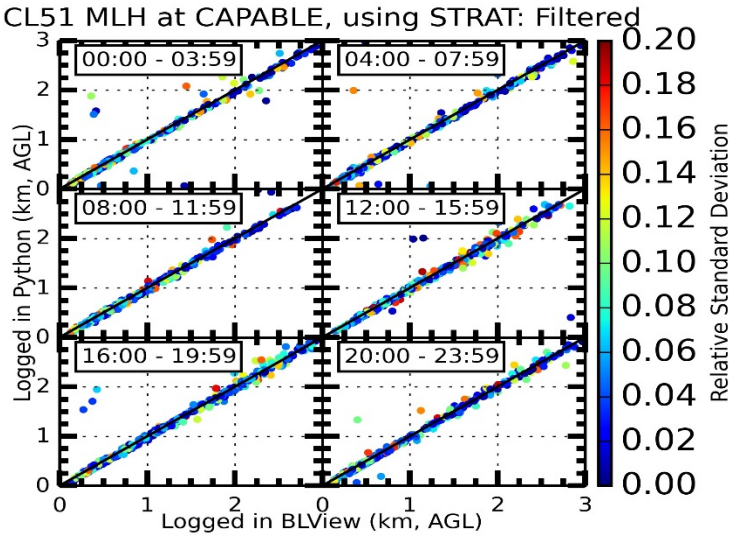


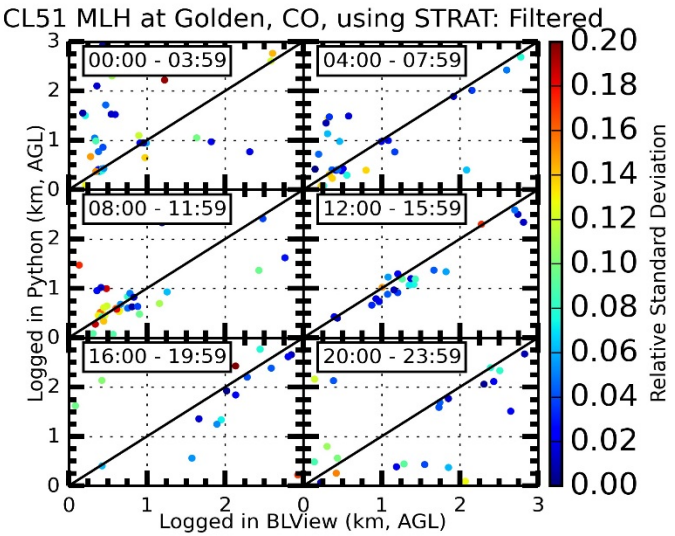


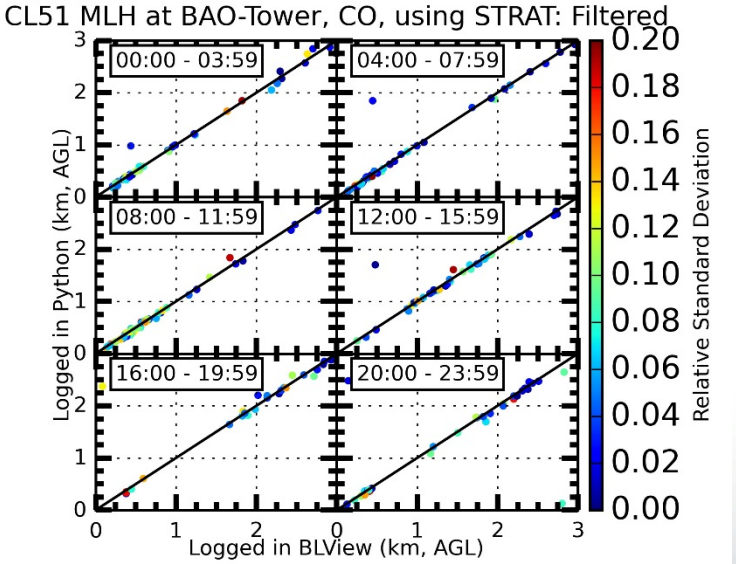
- **Total of 53 radio sondes used for evaluation**
- **CL-51 data averaged over 5-minutes to account for spatial differences with sondes**
- **R = unfiltered**
- **R = filtered; 5-minute σ > 0.20 km or RSD > 20%**

Knepp, T.N., J. S. Szykman, R. Long, R. Duvall, J. Krug, M. Beaver, K. Cavender, K. Kronmiller, M. Wheeler, R. Delgado, R. Hoff, E. J. Welton, E. Olson, R. Clark, D. Wolfe, D. Van Gilst, and D. Neil, *Assessment of Mixed-Layer Height Estimation from Single-wavelength Ceilometer Profiles,* submitted Atmos. Chem. Phys

STRucture of the ATmosphere (STRAT v1.04) algorithm







- **STRAT is a covariance wavelet technique (CWT) currently in use by the European Aerosol Research Lidar Network (EARLINET - http://www.earlinet.org/)**
- **Developed under a GNU General Public License**
- **Potential open-source alternative to BL-View**
- **Evaluated the impact of data logging via BL-View versus raw CL-51 output**
- **When MLH is averaged to time-scale of 1-hour, data logging method shows no significant differences for CAPABLE & BOA site**
- **Need to do a direct comparison MLHs via BL-View and STRAT**

Data Considerations

- Hourly Mixing Height is the required variable under PAMS
- CL-51 is capable of providing attenuated backscatter profiles up to 15km+
- Data logging the entire backscatter profile allows for:
  - Alterative algorithms to derive MLH, especially if other lidars (MPL, HSRL, CL-31s) are part of any network
  - Visual check on the derived MLH
  - Use of data to better evaluate exceptional events
- Consideration should be given to explore 1.) use of data systems capable to exploit the full value of any aerosol profile network, 2.) synergies with the NASA Micro-Pulse Lidar Network

Potential Consideration for Data Collection and Reporting of Ceilometer Data

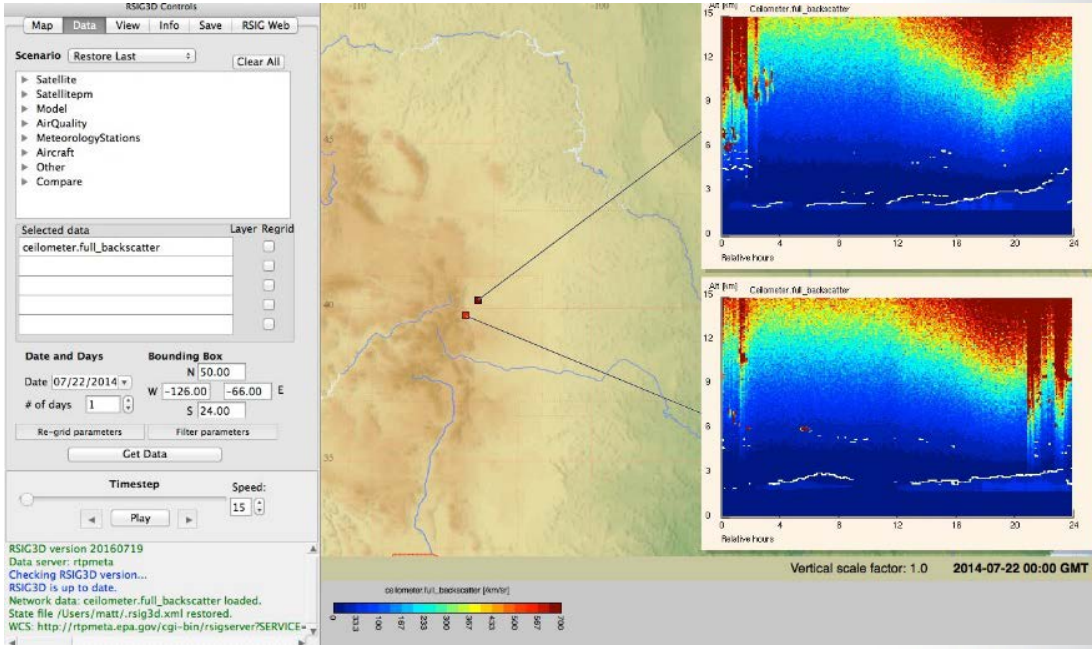
Applied Research Issue:

- PAMS only required an hourly average mixing layer with archive in Air Quality System Data (AQS) Base.

- That means 100% of the measured data not required to be retained.

Data not retained includes:

- raw measurement and normalized aerosol backscatter (0-15.5km, 10 m vertical resolution, every 36 secs).
- Aerosol layer heights, Cloud base heights, higher resolution (sub-minute) mixing height
- -EPA Office of Research and Development advocating for full archive (range resolved normalized backscatter and all aerosol layer heights).



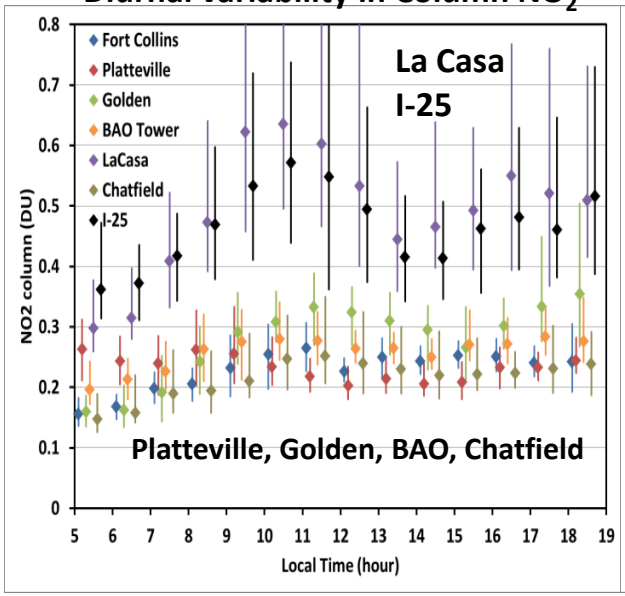
Example of CL-51 backscatter full profile and MLH from DISCOVER-AQ in EPA Remote Sensing Information Gateway 3D-Application

Pandora Ground-Based Spectrometer

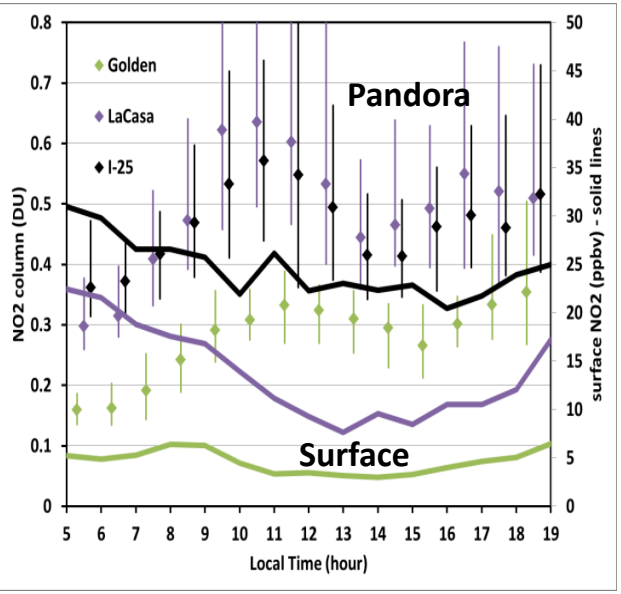
- Developed at NASA Goddard
- Total Column O_3, SO_2, HCHO, BrO, NO_2 and H_2O every 80 seconds
- NASA is exploring options to develop a PANDORA Network
- New PAMS requirements ("true" NO_2 and MLH) provide synergistic measurements to PANDORA
- PAMS + PANDORA (NASA) could potentially serve as a U.S. ground-based satelltie validation network

Pandora Column Density vs. Surface NO_2

Pandora
Diurnal variability in Column NO_2

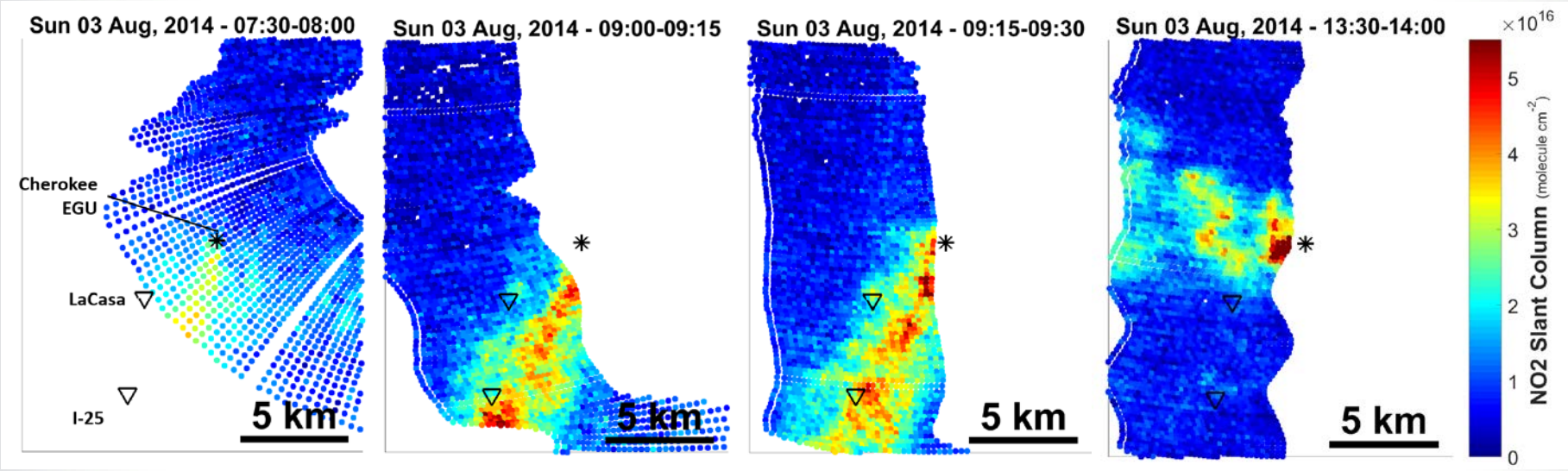


Column and Surface NO_2
Diurnal variability

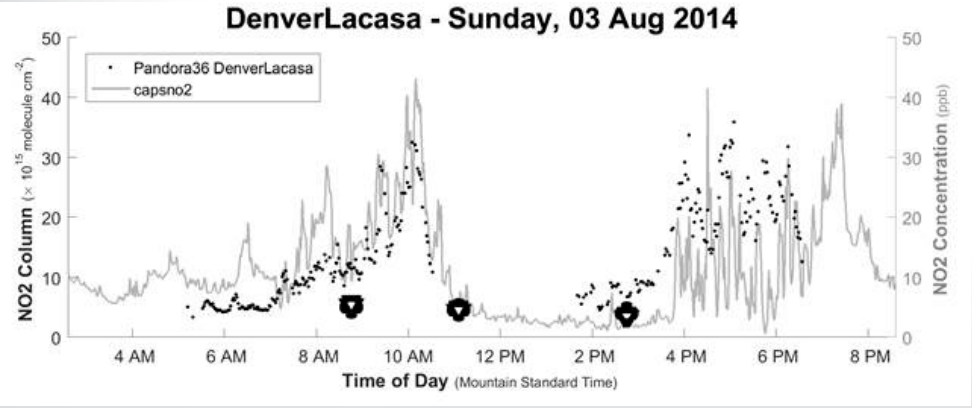


DISCOVER-AQ observations over Colorado in August-September 2014
(L) Diurnal variability in total column NO_2 observed by Pandora spectrometers.
(R) Comparison of diurnal variability in total column and surface NO_2 for the three sites with the highest NO_2 abundances.

GeoTASO NASA Airborne Spectrometer



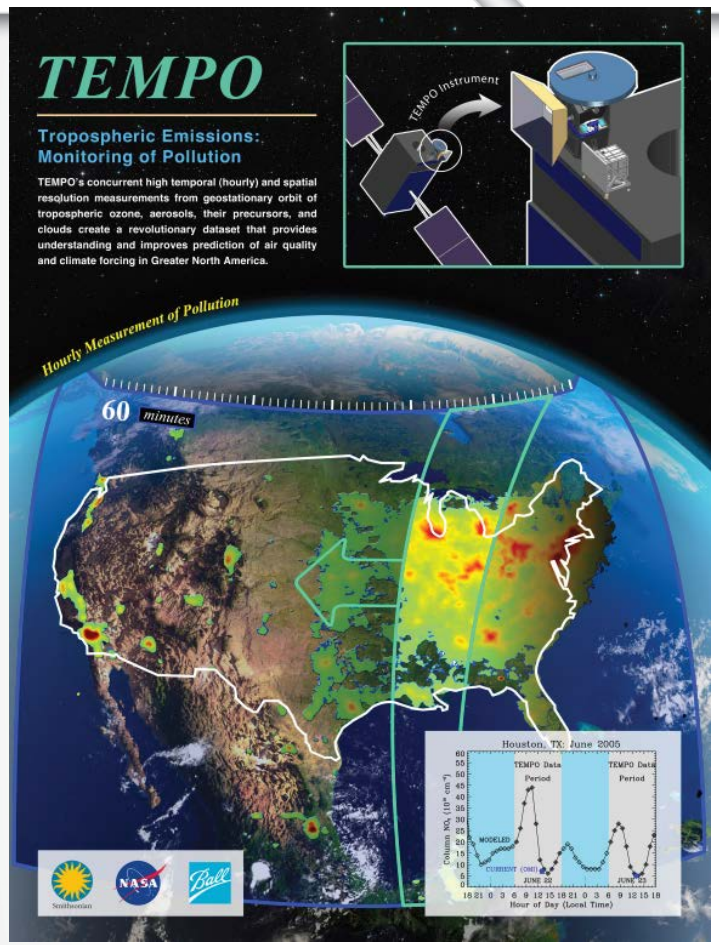
Data courtesy of **Caroline Nowlan**
Harvard-Smithsonian, CfA



In the morning, the Cherokee EGU NO2 plume was primarily to the east of the La Casa site. By early afternoon (right), the plume was to the north and west of the La Casa site, with almost no enhancement observed by GeoTASO directly overhead. In between those two time periods (bottom left), the NO2 plume likely passed overhead the La Casa site, based on PANDORA column and surface NO2 measurements.

A 1 ppb surface to 1 x 10^{15} molecule cm^{-2} column relationship observed in the morning indicates that a large fraction of the total column is near the surface, which makes it difficult for the P3B to fully sample the column

TEMPO: Hourly atmospheric pollution from geostationary Earth orbit



Selected Nov. 2012 as NASA's first Earth Venture Instrument

- Instrument delivery September 2017, with expected ~2019+ launch

Provides hourly daylight observations to capture rapidly varying emissions & chemistry important for air quality

- UV/visible grating spectrometer to measure key elements in tropospheric ozone and aerosol pollution
- Exploits extensive measurement heritage from LEO missions
- North American component of a constellation for air quality observations

TEMPO data and potential air quality application areas Emissions Inventories (improve or develop new methods, including mobile sources and area sources such as soil NOx)

- Inform air quality model development and evaluation
- Evaluation of impact of short term climate forcers (ozone, chemically produced aerosols) and climate-chemistry connections
- Data on smaller spatial scales better supports AQ assessment and planning activities: Source attribution, Exceptional Event Evaluations (Wildfires and Strat. Intrusions) and Trends
- Intercontinental transport of air pollution

TEMPO PI - Kelly Chance, SAO

Summary and Next Steps

- DISCOVER-AQ collaboration provides EPA with an opportunity to conduct mandated NERL research on Federal Reference and Equivalent Methods (FRM/FEM) integrated with new research areas (remote/satellite and sensor based measurements of air pollution)
  - New ozone FRM was promulgated as part of the Ozone NAAQS rulemaking published in the Federal Register October 26, 2015.
  - Near-roadway research results will impact existing and upcoming near-roadway NAAQS monitoring sites (2014-2016).
  - An increased understanding of data quality from small sensors will inform potential uses of sensor technology in air pollution monitoring.
  - CL-51 a viable options for PAMS MLH measurements; software and data considerations.
  - Initial results of PANODORA Spectrometers appear to add another valuable measurement dimension for air quality; consider should be given for development of a systematic air quality-satellite validation network.
- DISCOVER-AQ research has set the stage for a continued science collaboration between EPA and NASA (KORUS-AQ [Korean-US Air Quality Study, 2016], TEMPO [Tropospheric Emissions: Monitoring of Pollution, a future NASA space mission dedicated to monitoring air pollution from space, 2018+]

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Disclaimer

Although this work was reviewed by EPA and approved for presentation, it may not necessarily reflect official Agency policy.