Monthly Webex Tag-up, 24 September 2015

Agenda

Science Presentations

Pandora measurements during DISCOVER-AQ: near surface, tropospheric and total NO_2 columns

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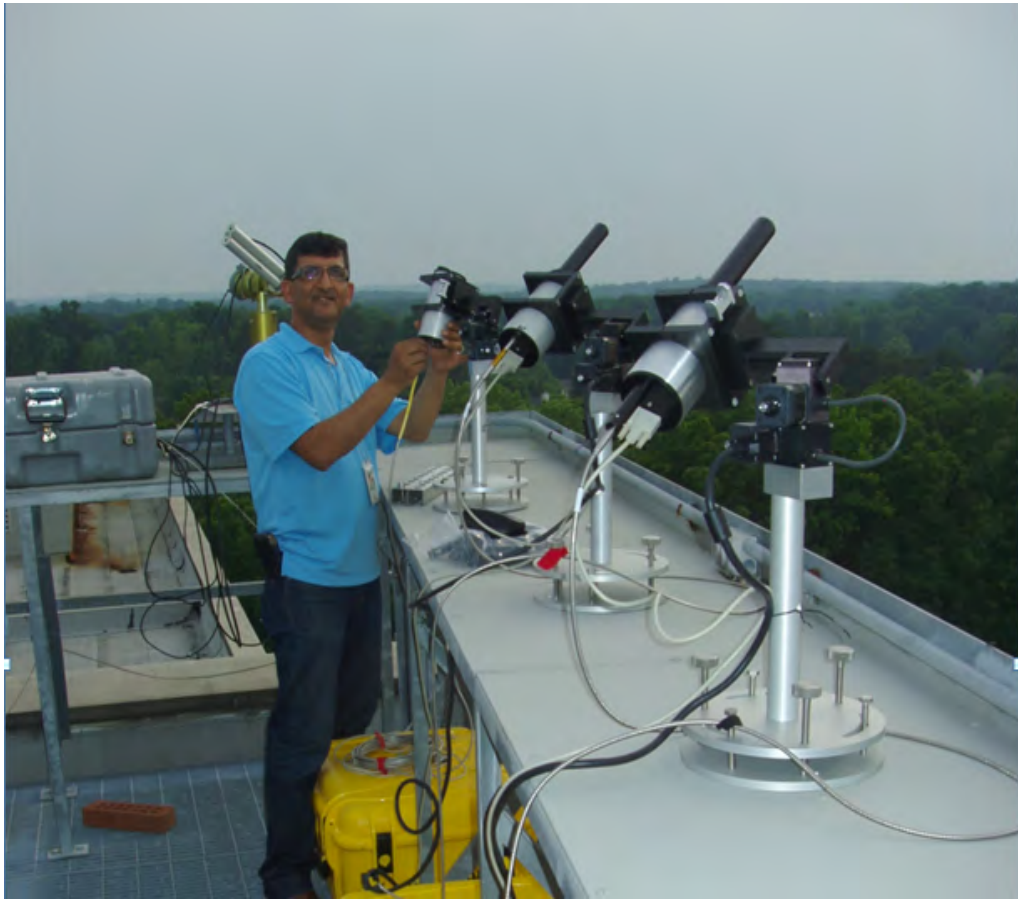
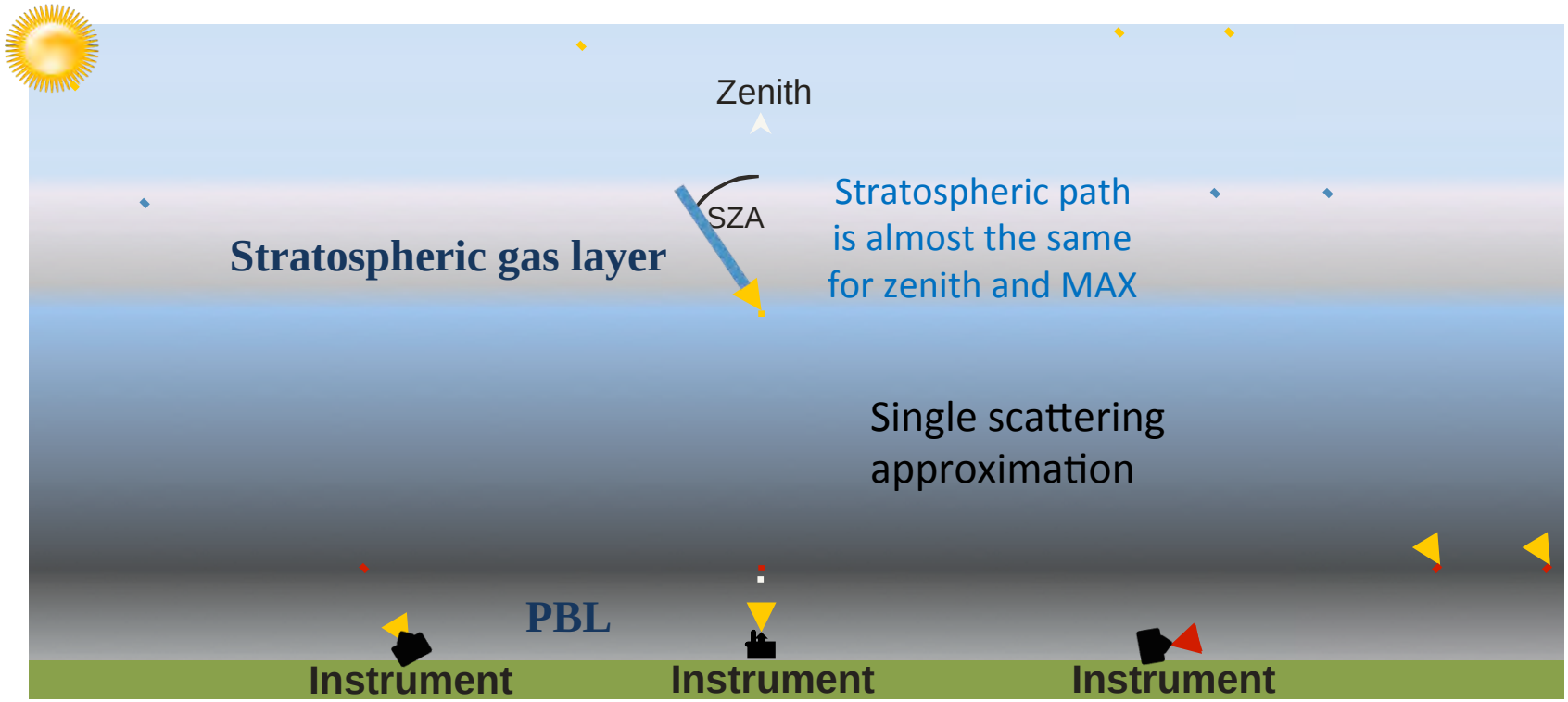


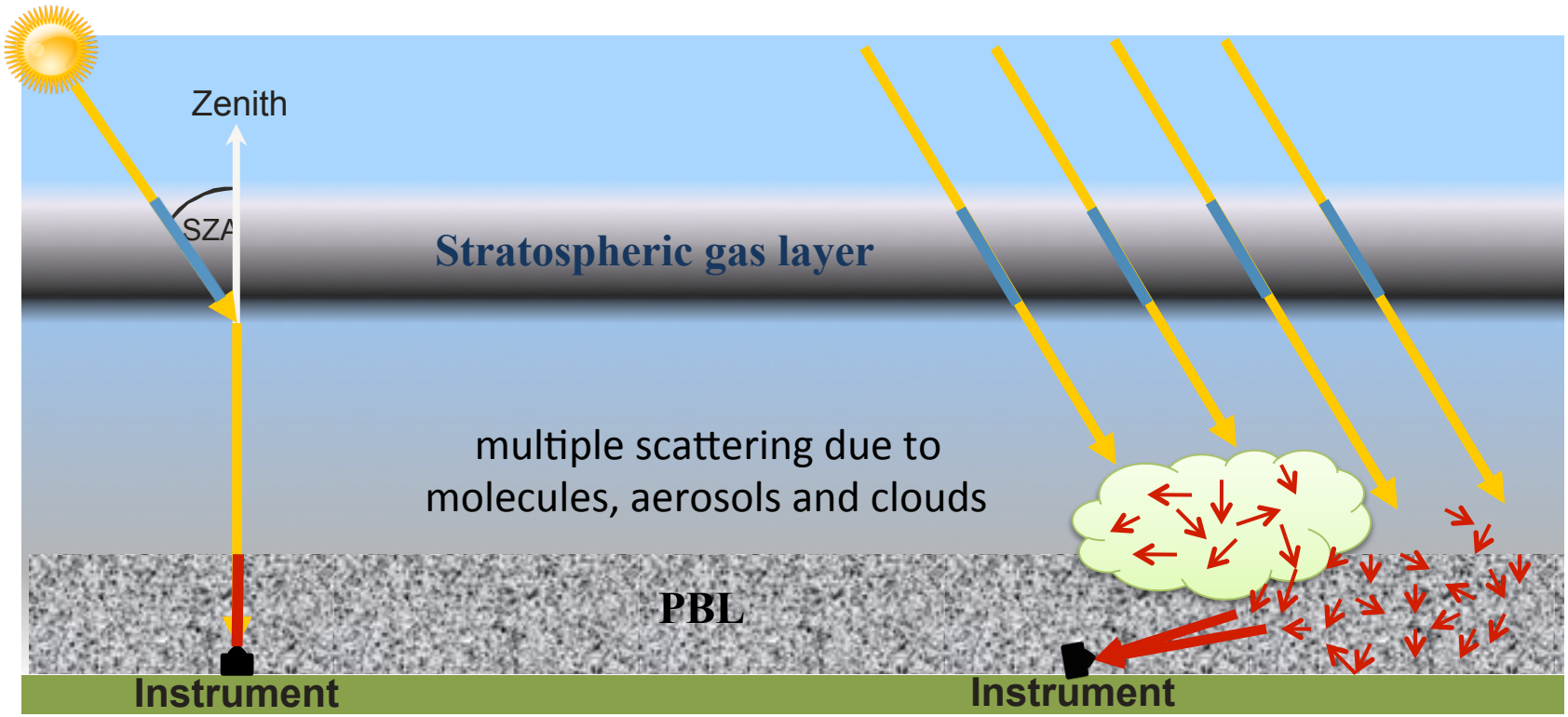
Pandora observation geometries (UV/VIS)

Direct Sun	Zenith Sky	Multi-Axis



almost equal path length through stratosphere and troposphere	longer path length through **stratosphere** than troposphere	longer path length through **troposphere** than stratosphere

Multi-axis observation geometry



- Wavelength
- Aerosol profile and aerosol properties
- Clouds
- Viewing zenith and relative azimuth angles
- Solar zenith angle
- Surface albedo
- Gas profiles

Box Air Mass Factors (bAMF)

- **Sensitivity of the measurements are typically expressed in terms of weighting functions (air mass factors)**
- **box AMFs are used to show profile independent AMF in each atmospheric layer**

$$bAMF(\lambda,\mu)_j = \frac{-WF^{LIDORT}(\lambda,\mu)_j}{I(\lambda)\cdot VOD(\lambda, gas\ profile)_j}$$

Air Mass Factors (AMF)

Non - linear Case

- AMF = **f** (species profile and total abundance)
- Absorption > 1%
- Aerosols, SO_2*, O_3 in UV

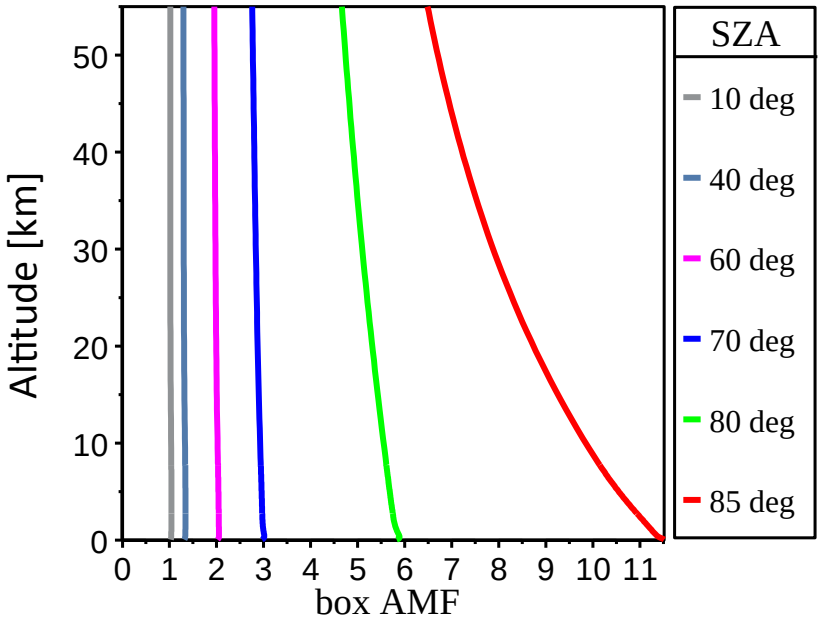
* High volcanic SO_2 loadings

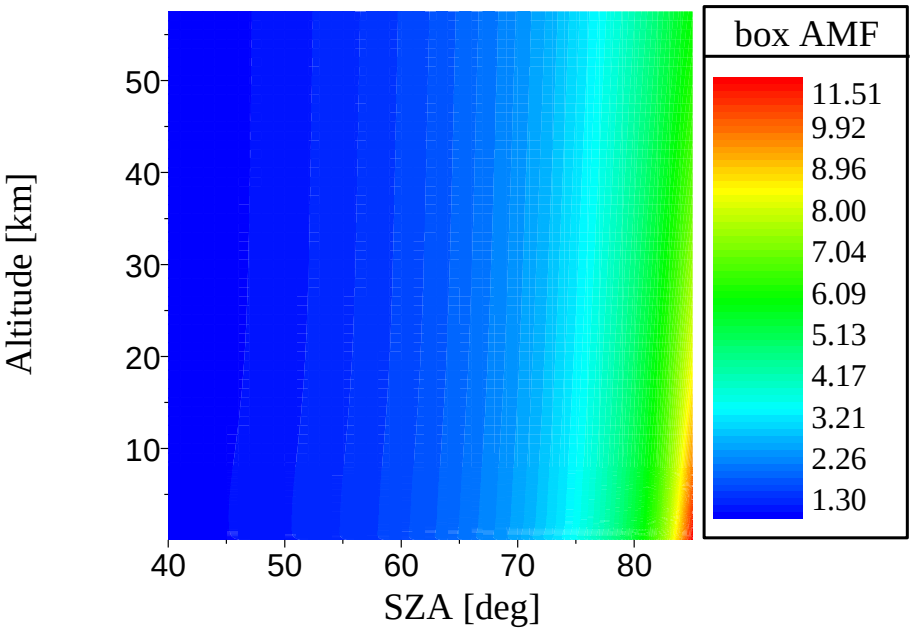
Linear Case

- bAMF ≠ **f** (species profile and total abundance)
- Absorption << 1%
- NO_2, HCHO, SO_2*, glyoxal, O_4
- One bAMF profile can be used for multiple gases and profiles under the **same atmospheric conditions**

* Background SO_2 and low volcanic loadings

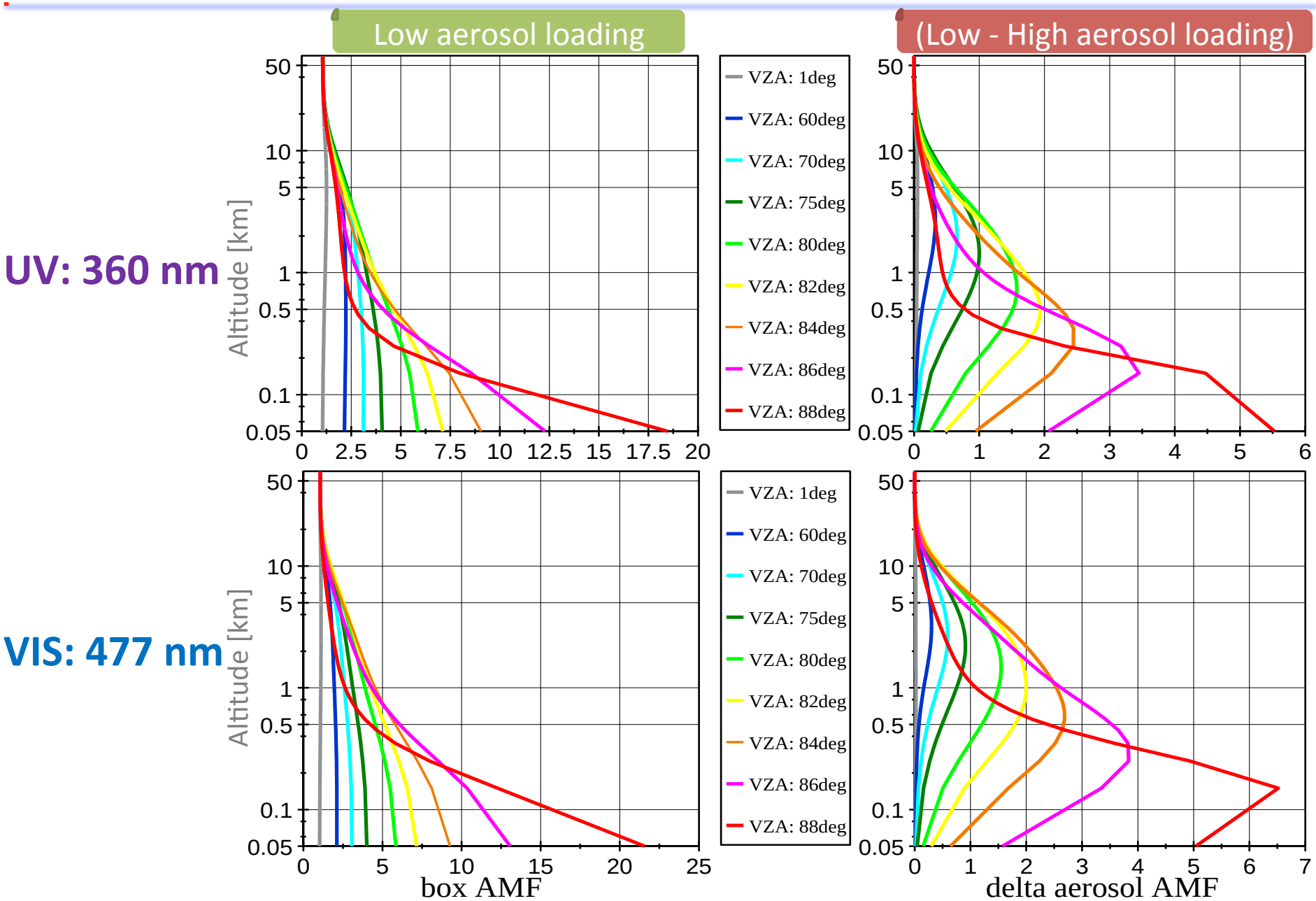
Direct sun box AMF



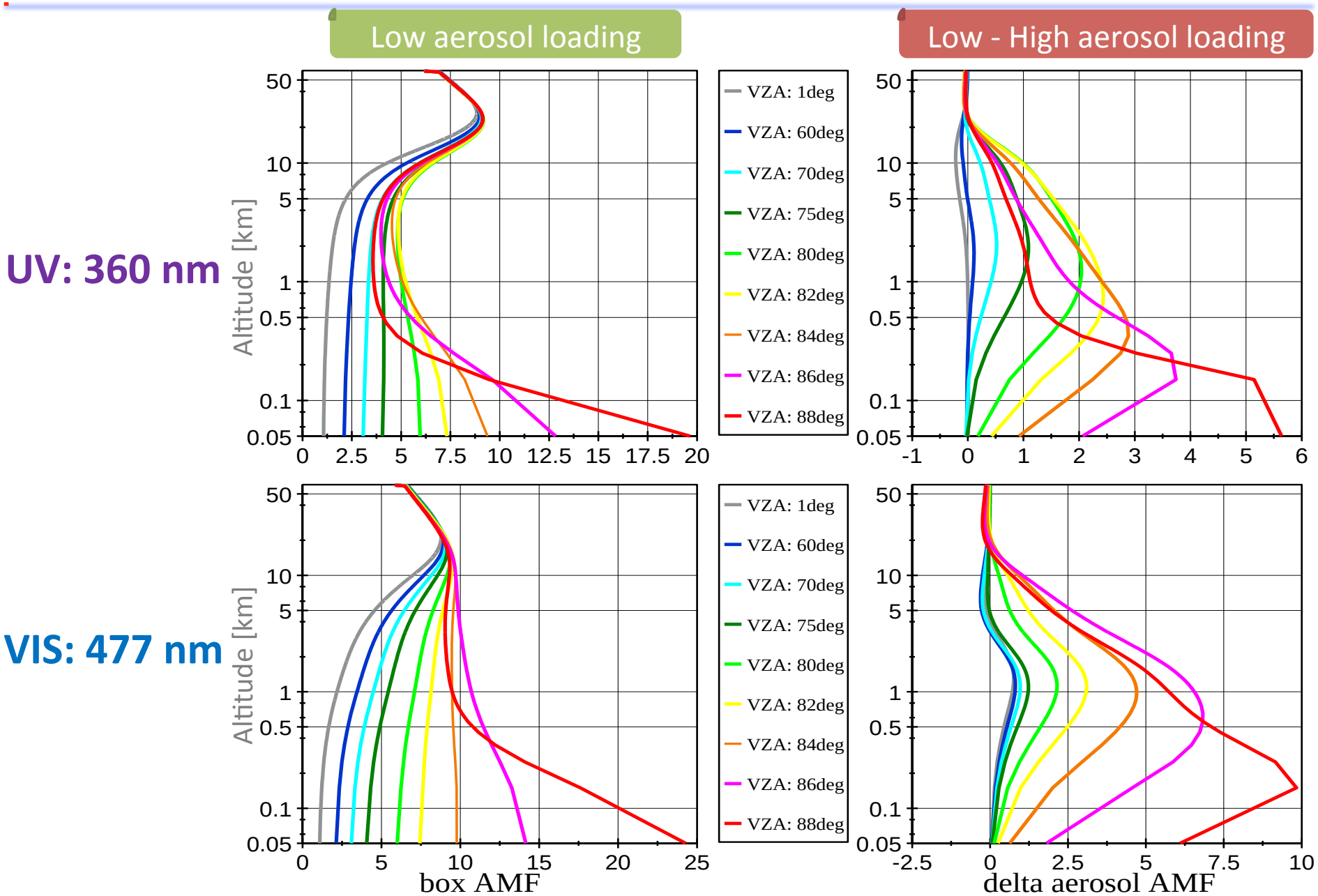


- **almost equal path length** through stratosphere and troposphere at SZA < 70°
- al large SZA more sensitivity to **lower troposphere** than stratosphere
- week wavelength dependence

Multi-axis box AMF: **SZA: 20°** RAA: 90°



Multi-axis box AMF: **SZA: 85°** RAA: 90°



Pandora measurements provide NO_2:

-> **Total column**

-> **Tropospheric Column**

-> **Near surface concentration**

-> **Some profile information**

-> **along a narrow field of view (1.5°) in a specific azimuthal direction**

Air volume "probed" by MAX-DOAS is not easy to identify due to multiple scattering

Pandora profiling algorithms

1. Real time DOAS fitting

ΔSCD: NO_2, HCHO, O_3, SO_2, H_2O and O_2O_2

Combination of different elevation angle measurements

➔

Near surface concentrations, tropospheric total columns, some profile information

Wavelength calibration,

Stray light correction,
Trace gas profiles

2. Direct Intensity fitting

Optimal estimation using on-line radiative transfer calculations (VLIDORT)

➔

Aerosol Ext. Coef. Profile, SSA, ASY factor, Surface Albedo
Gas profiles (CURRENTLY ONLY O_3)

Real-time analysis: DOAS fitting

Direct sun and sky spectra

Read Pandora data

Calibration file (cross sections, Ring spectrum)

Surface T, P, RH, temperature at 27 km

Read auxiliary data

stratospheric NO_2 (Odin/ OSIRIS) climatology, NDACC AMF lookup tables

DOAS fitting (gas specific: 5 fitting windows)

no inversion

Near surface volume mixing ratio from selected angles: gas and O_2O_2

Tropospheric column calculation from DS and MAX-DOAS (gas specific)

Profile parameterization (gas specific)

Write **near-surface vmr, Trop. Column, profile parameters**

Real-time analysis

- **Combination of direct sun and MAX-DOAS data**
- **Traditional DOAS fitting at multiple wavelength windows**
- **Total tropospheric column from direct sun and MAX-DOAS**
- **Near surface concentration from low elevation angles of trace gas and O_2O_2 (gas specific)**
- **Profiles are derived from near surface concentration, total tropospheric column, normalized scan patterns**
- **No radiative transfer calculation and inversion necessary**

Real-time analysis: tropospheric NO_2

Trop. NO_2 column = Total column from DS data – stratospheric column

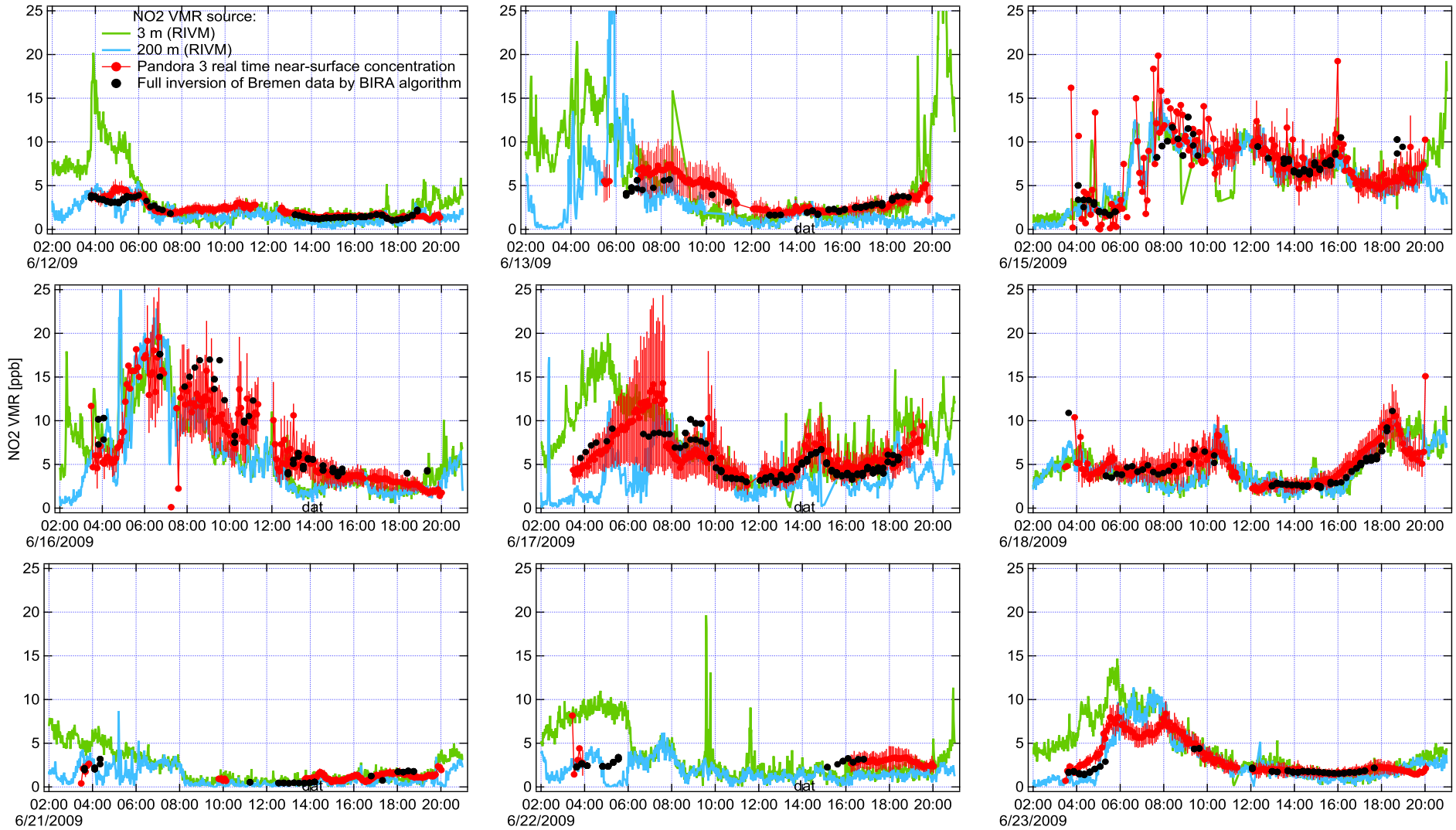
A) Stratospheric column from DS data

- Separation of stratospheric and tropospheric columns based on T-sensitivity (low residuals and high pollution level, 75º SZA)
- Linear interpolation between morning and evening stratospheric columns at 75º SZA to estimate stratospheric column at SZA < 75º

B) Stratospheric column from zenith sky data

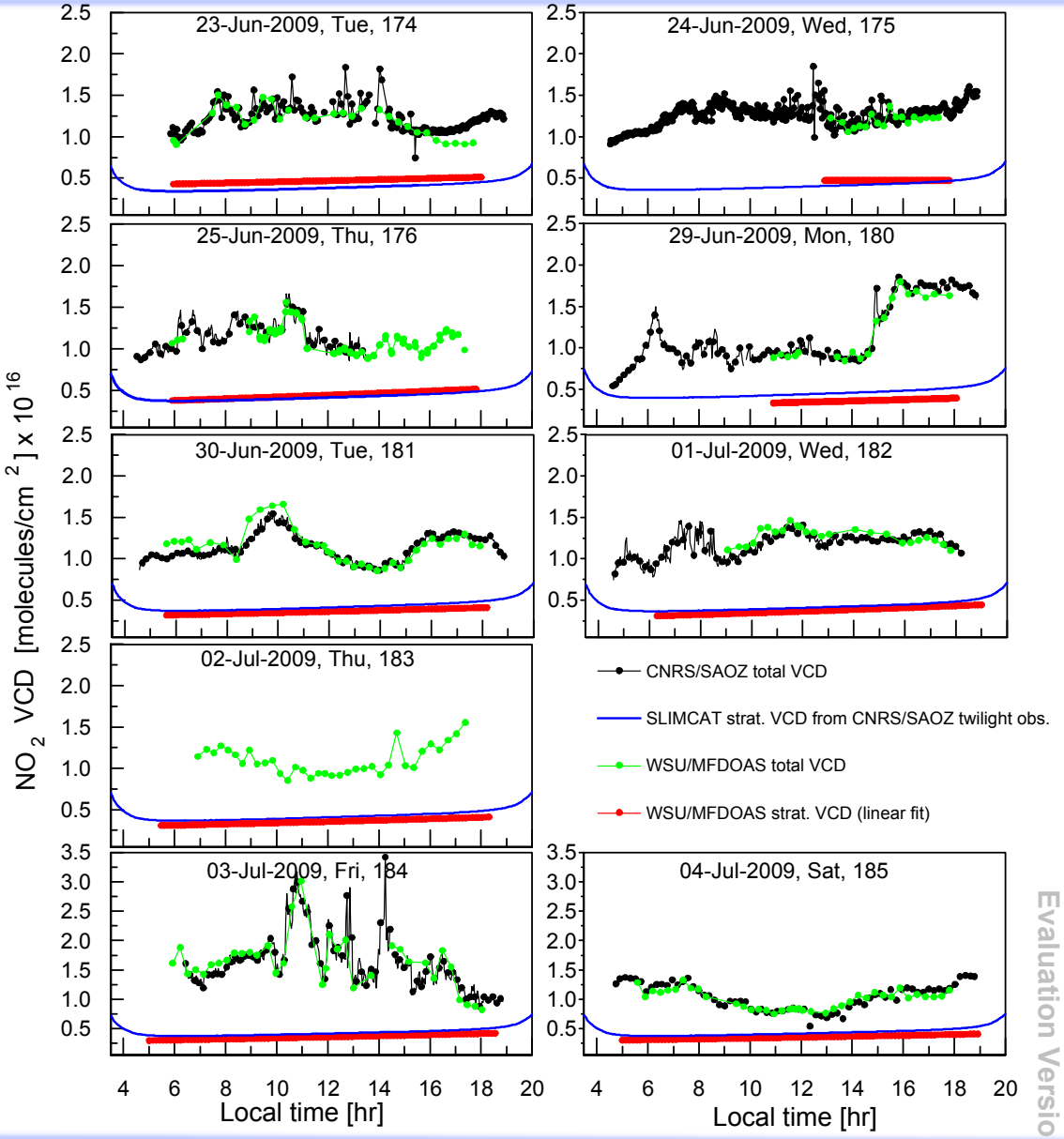
- NDACC settings for SZA 86-90deg
- Interpolation to SZA < 75deg using scaled Odin/OSIRIS stratospheric NO_2 climatology

Near-surface NO_2: OE vs real time



Proof of concept: CINDI-2009 (Cabauw, the Netherlands)

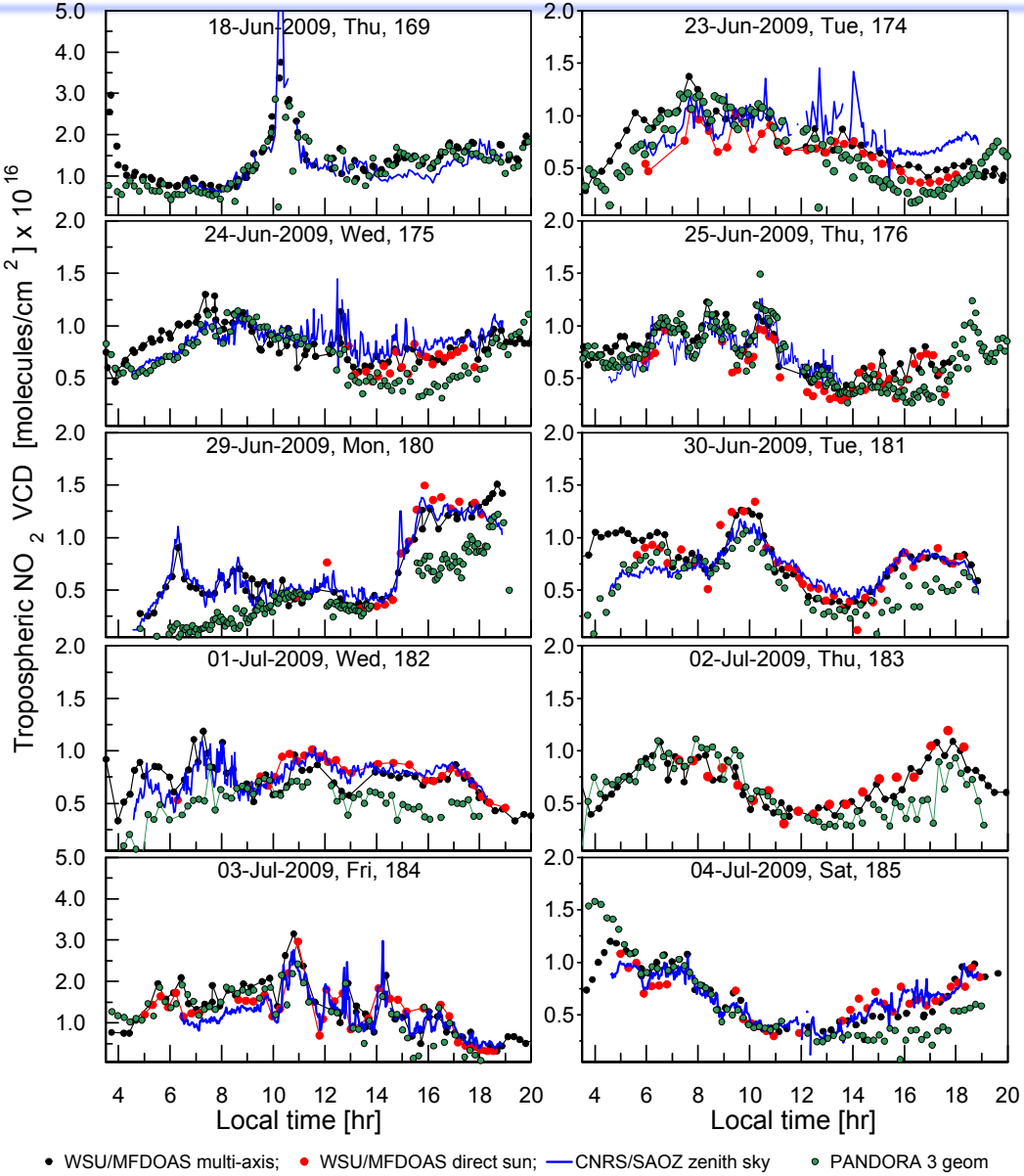
Total NO_2: OE vs near-real time



Evaluation Version

Proof of concept: CINDI-2009 (Cabauw, the Netherlands)

Tropospheric NO_2: OE vs near-real time

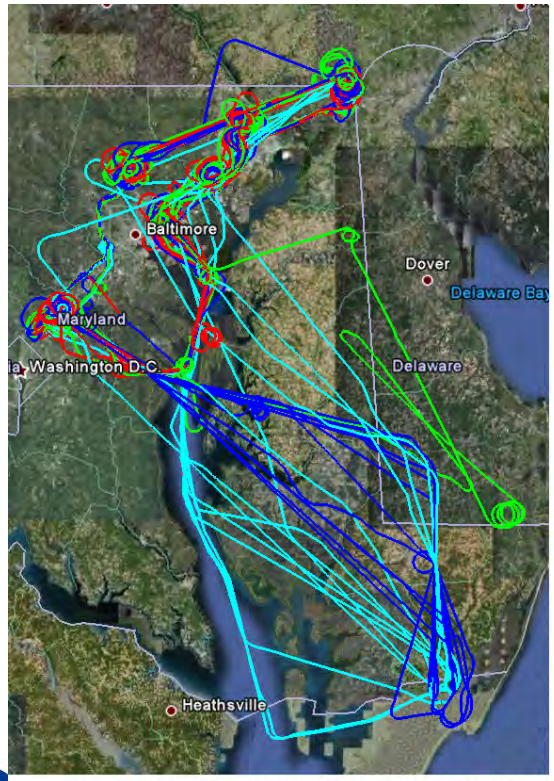


Proof of concept: CINDI-2009 (Cabauw, the Netherlands)

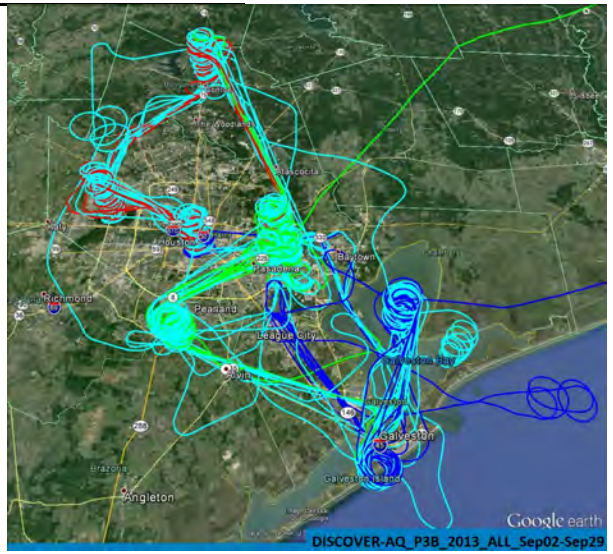
DISCOVER-AQ campaigns

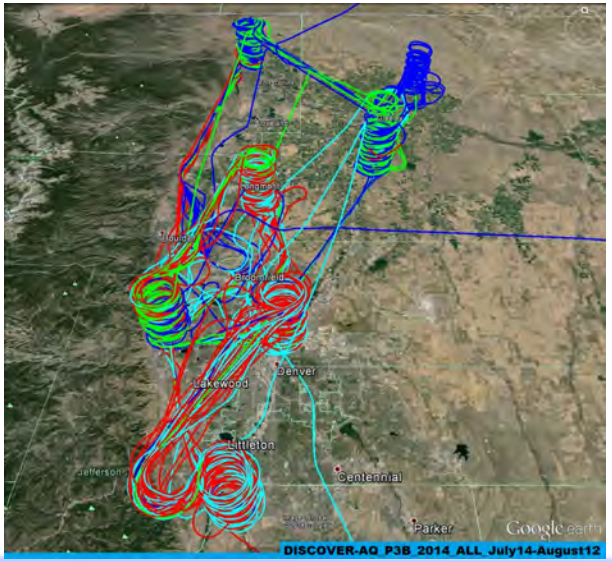
Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality – NASA sponsored mission

- **Baltimore-Washington, D.C. 2011**
- **California 2013:** direct sun and 2 profiling sites
- **Texas 2013:** direct sun and 2 profiling sites
- **Colorado 2014:** direct sun and 2 profiling sites



DISCOVER-AQ_2011_ALL_P3B_July1-July29

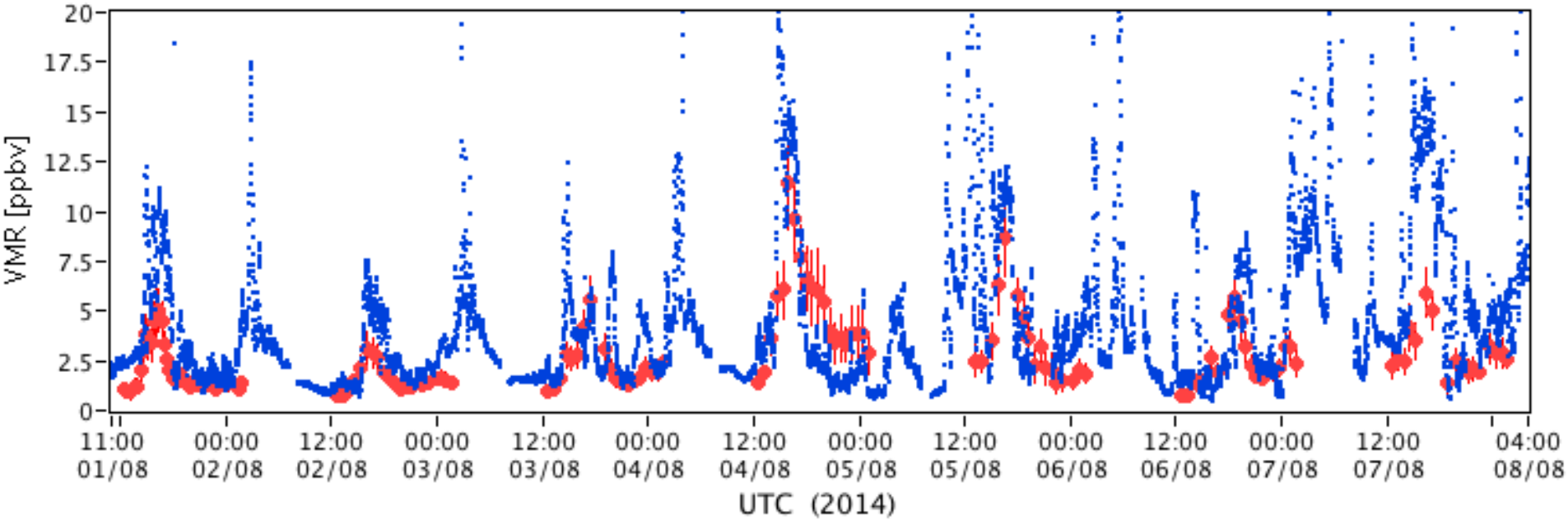




DISCOVER-AQ campaigns

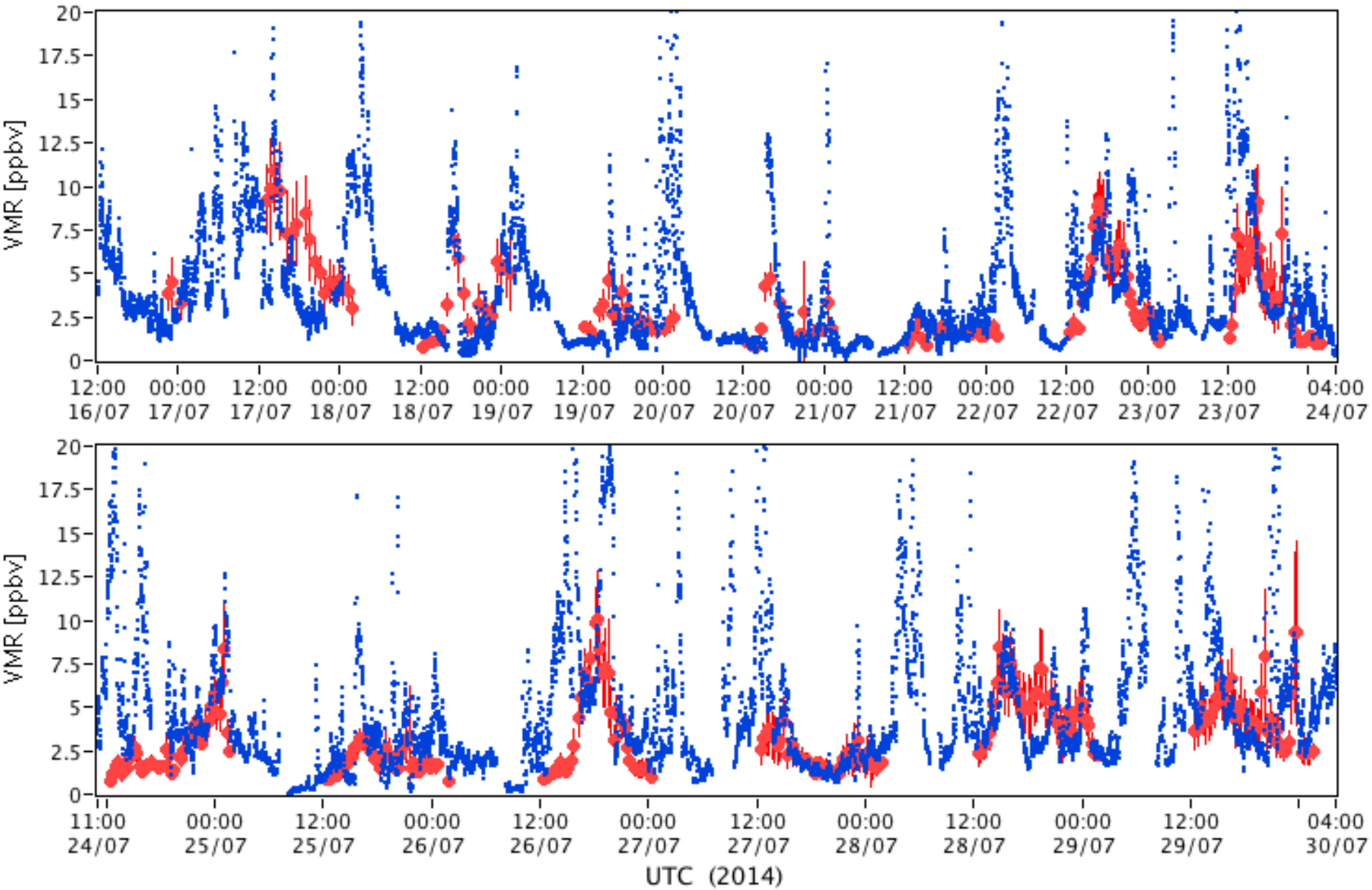
- All Pandora data have been analyzed and will be posted on DISCOVER-AQ website by 15 October 2015
- Recommendations for inter-comparisons:
  - Account for azimuthal orientation (provided in the data files)
  - Account for vertical sensitivity (AMF provided in the files)
  - Account for a narrow field of view (1.5°)
  - Direct sun and multi-axis tropospheric columns can be different due to spatial heterogeneity
  - Avoid data collected at SZA > 80°

NO_2 surface vmr: Golden, CO (2014)

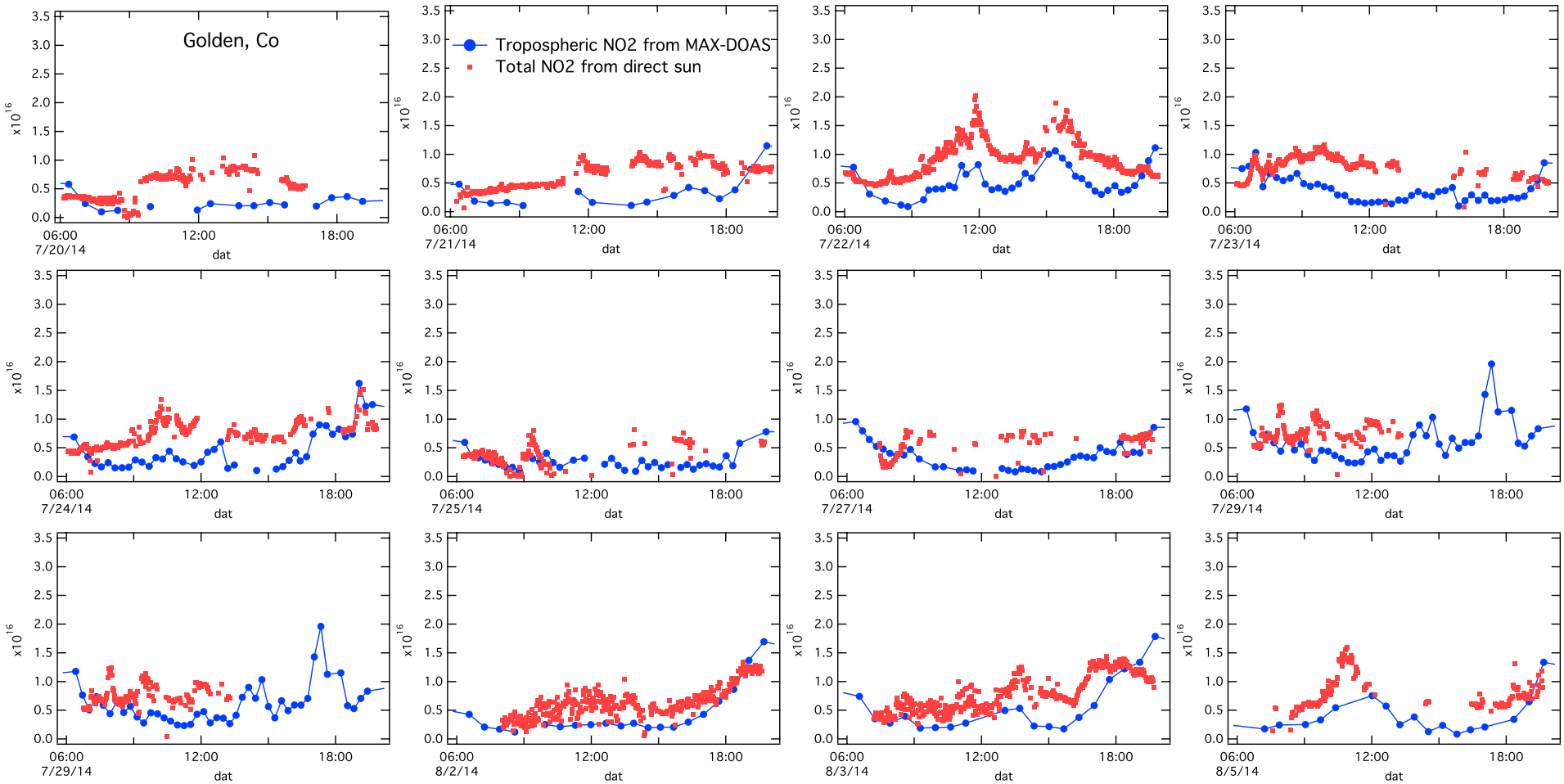


- in-situ ground-based CAPS NO_2 (Russell Long)
- Pandora 38 near-surface real time

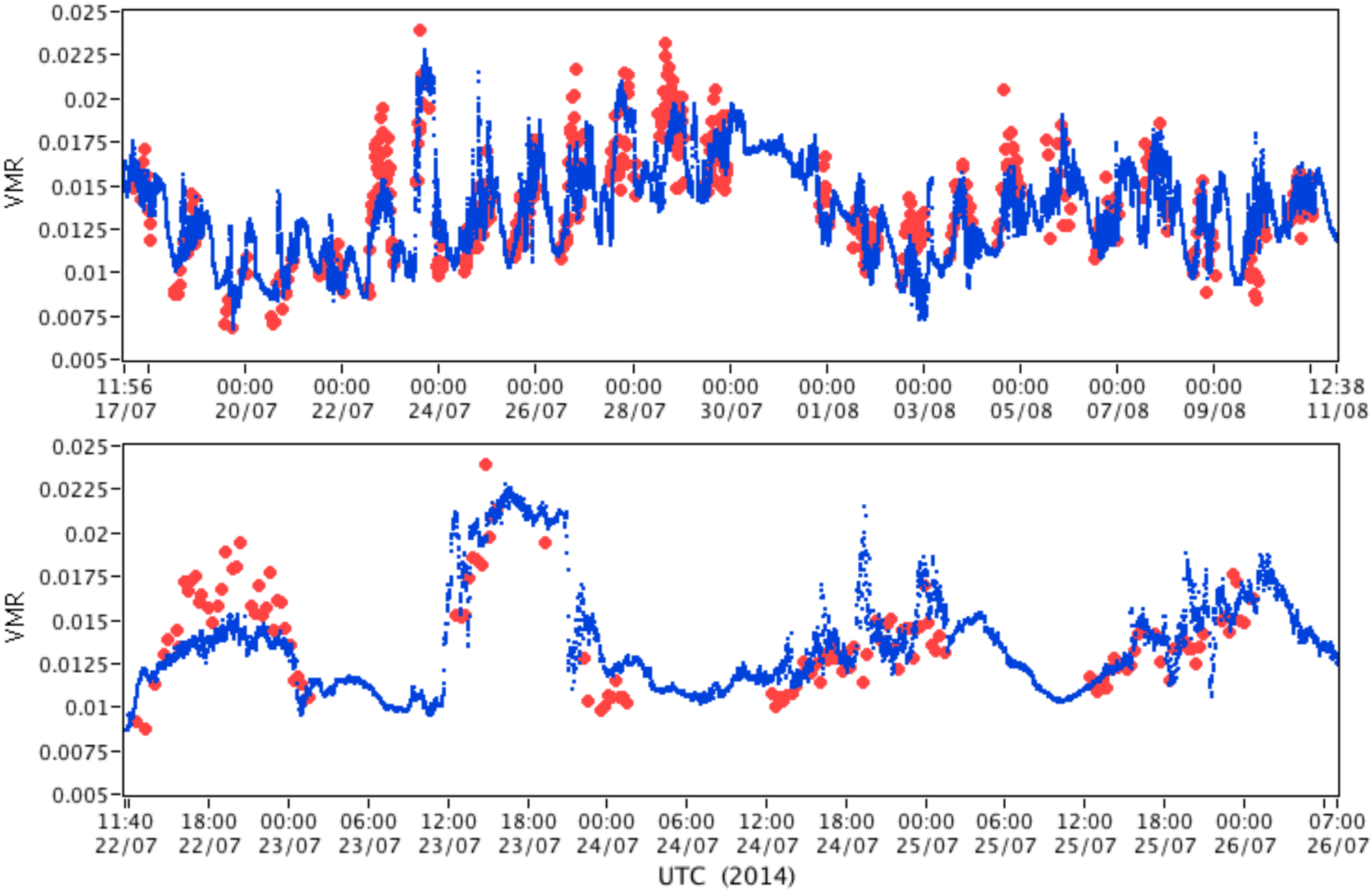
NO_2 surface vmr: Golden, CO (2014)



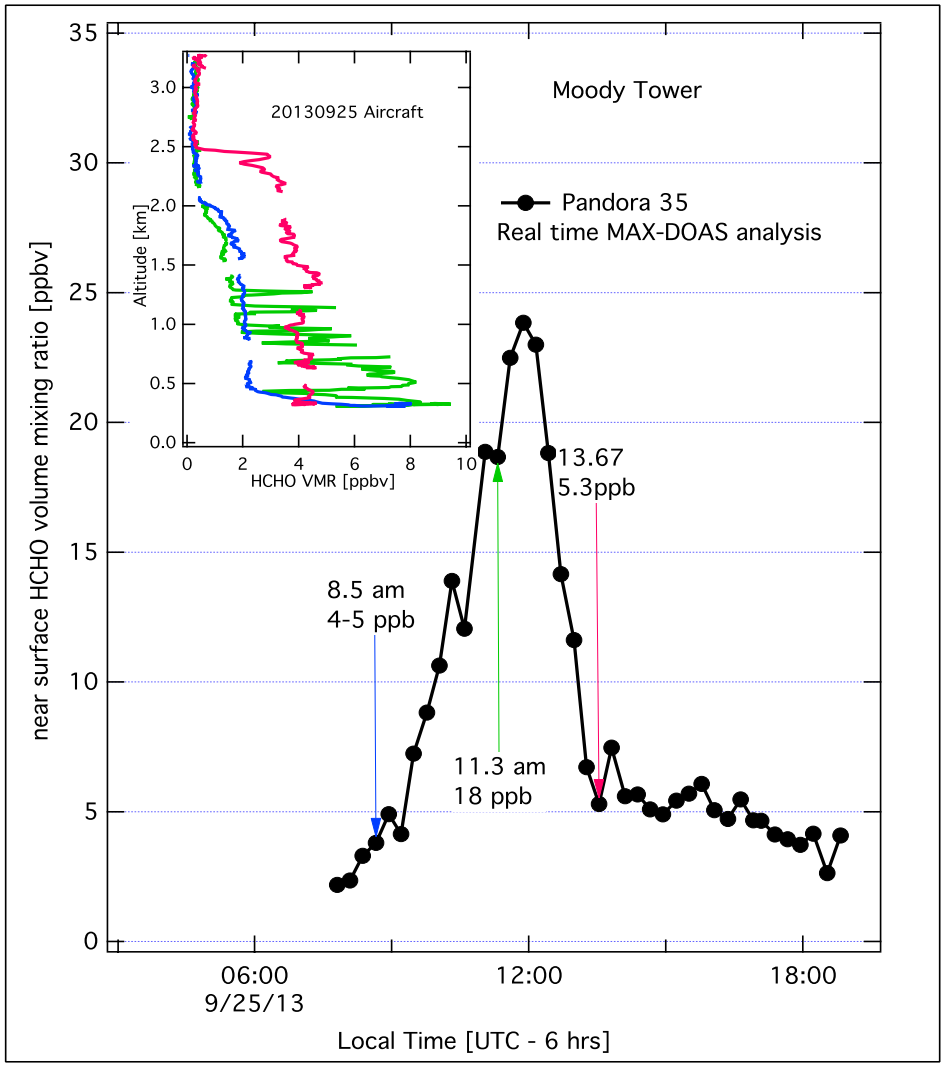
NO_2 vertical columns: Golden, CO (2014)

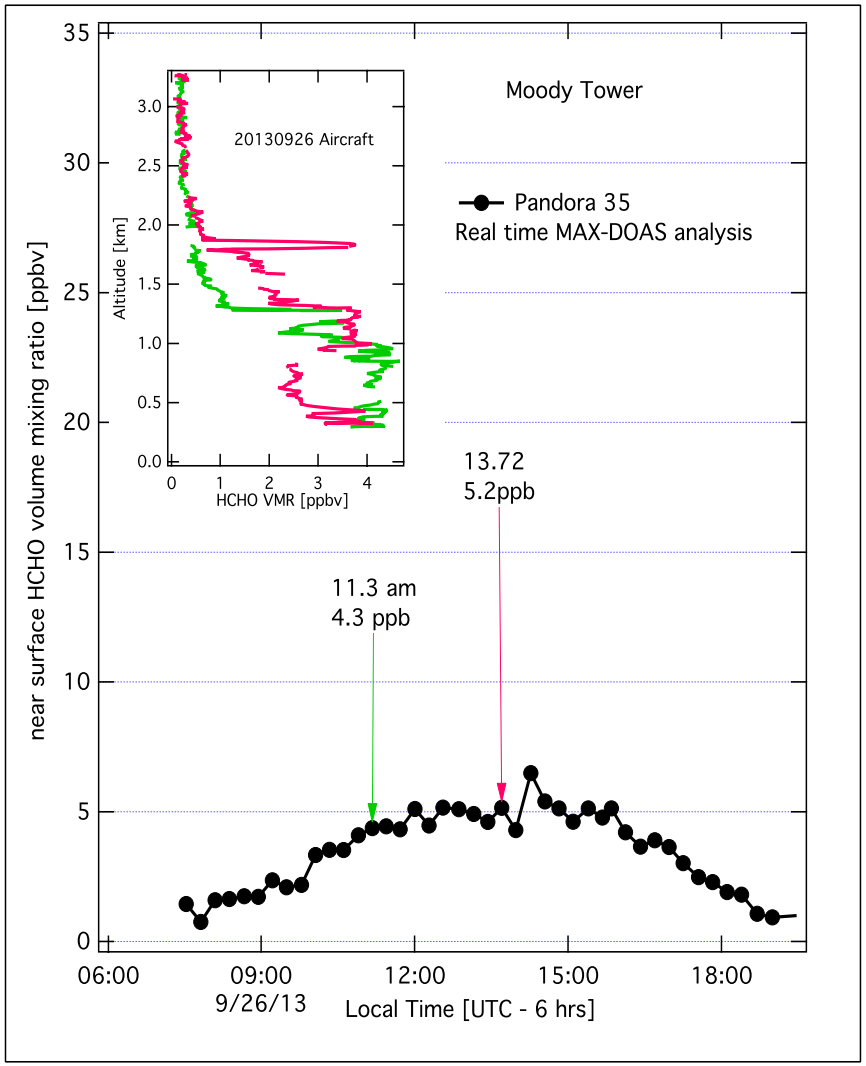


H_2O surface vmr: Golden, CO (2014)

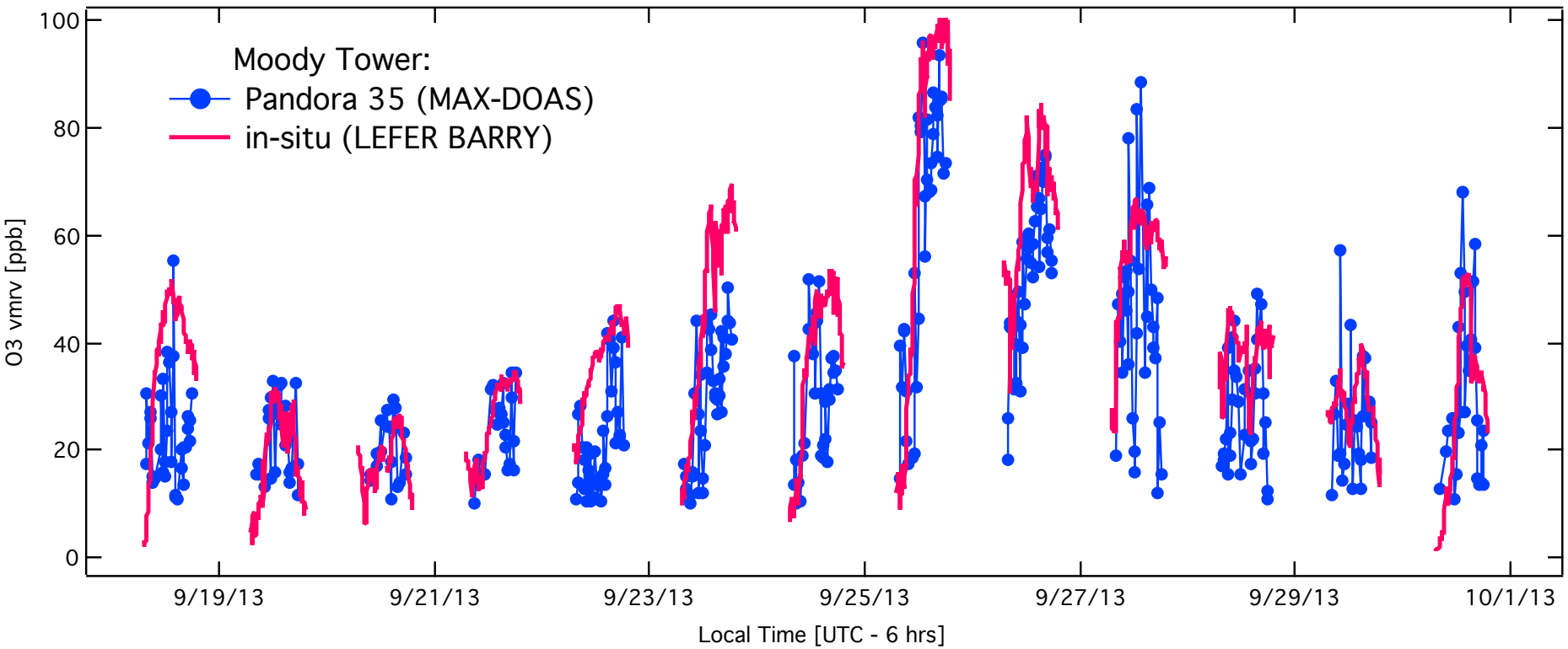


HCHO near-surface vmr: Houston, TX





O_3 near-surface vmr: Houston, TX



Extra products: H2O, HCHO, O3

Will be provided on demand by contacting elena.spinei@nasa.gov

Thank you!

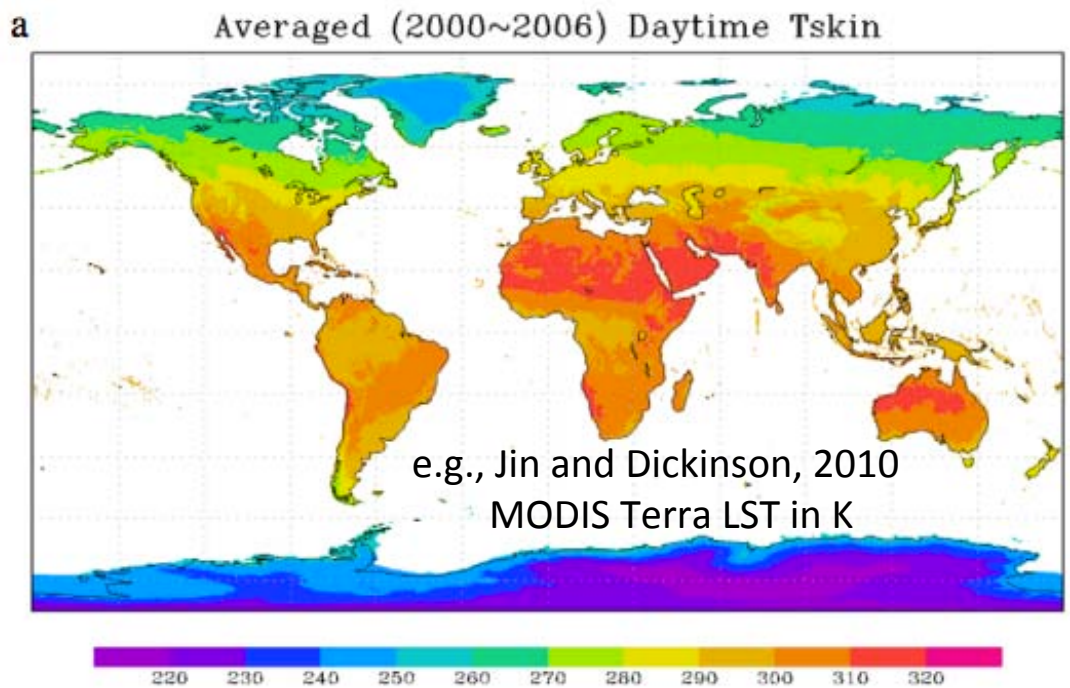
Land surface temperature (LST)

Broadly used for:

- studying climate variability
- detecting changes in land cover and urban environments
- monitoring drought conditions
- monitoring crop conditions
- indicating wildfire severity
- …

Highly variable in space and time, depending on:

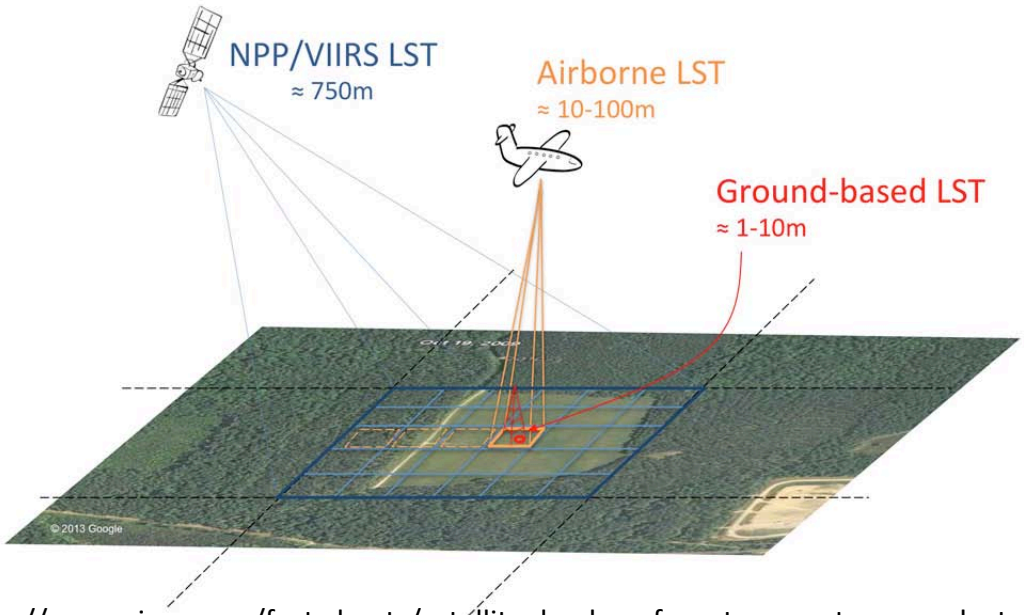
- solar radiation
- land surface properties
- atmospheric conditions



e.g., Jin and Dickinson, 2010
MODIS Terra LST in K

Current available LST observations on different scales

- Surface Climate Reference Network and Surface Radiation networks: mostly at thermally homogenous locations in the US; very sparse
- Satellites (Terra/Aqua MODIS, GOES, NPP/VIIRS, etc): of various spatial and temporal resolutions; broad coverage; IR measurements affected by clouds; need careful validation
- Aircraft: scale and uncertainty in-between; also affected by clouds; useful for model and satellite validation, especially for areas lacking surface observations



https://www.cicsnc.org/fact-sheets/satellite_land_surface_temperature_product_validation

Deriving LSTs in Houston using DISCOVER-AQ P-3B aircraft data on Sept 25, 2013 (the least cloudy day in this month)

A diurnal cycle model was used to derive LST time series at multiple locations in Houston that DISCOVER-AQ focused on, following the method in Duan et al., 2014:

$$T_s^d(t) = T_0 + T_a \cos\left(\frac{\pi}{\omega}(t - t_m)\right), t < t_s \quad (1a)$$

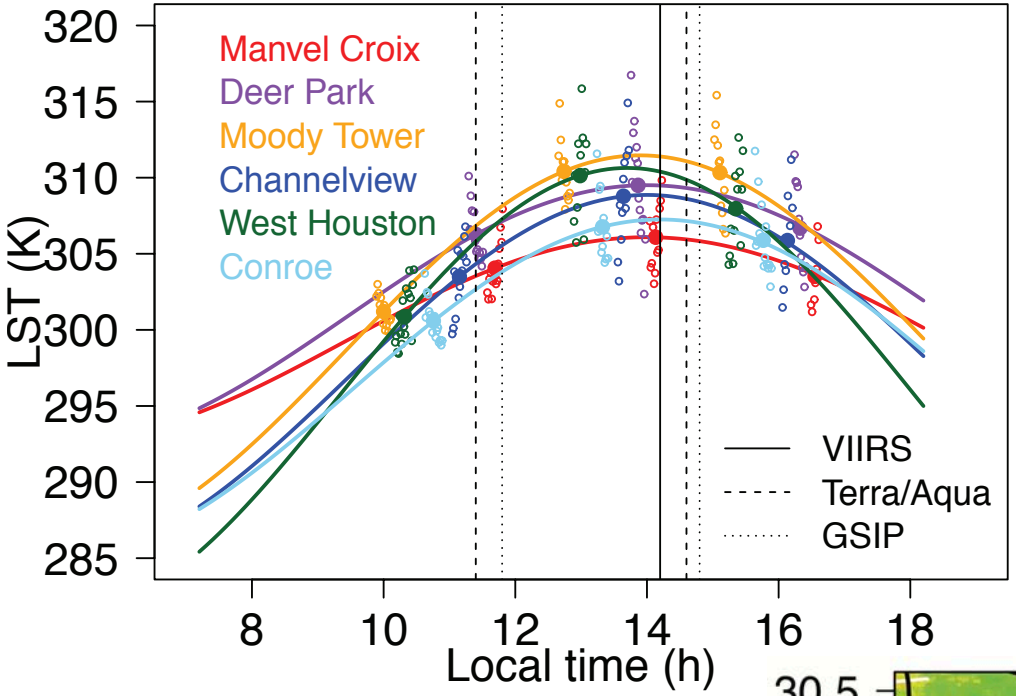
$$\omega = \frac{4}{3}(t_m - t_{sr}) \quad (1b)$$

$T_s^d(t)$, T_0, T_a, t_m, t_{sr} and t_s represent daytime LST at hour t, the residual temperature, temperature amplitude, time at which LST reaches its daily maximum, the time of sunrise, and the starting time of free attenuation (here: 1 hour before the sunset), respectively.

The three P-3B circuit-wide mean LST values at each location were used to derive the three free parameters of T_0, T_a, t_m in equation (1a). LSTs at other day times on September 25, 2013 at each location were then calculated.

Huang et al., in revision

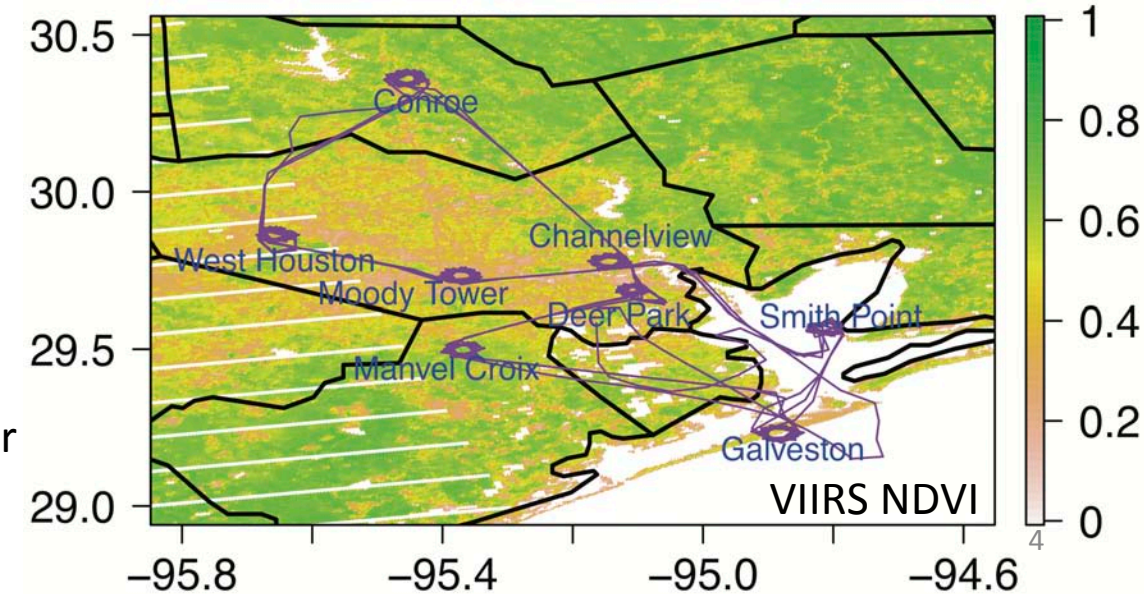
Aircraft-derived LSTs using a diurnal temperature cycle model



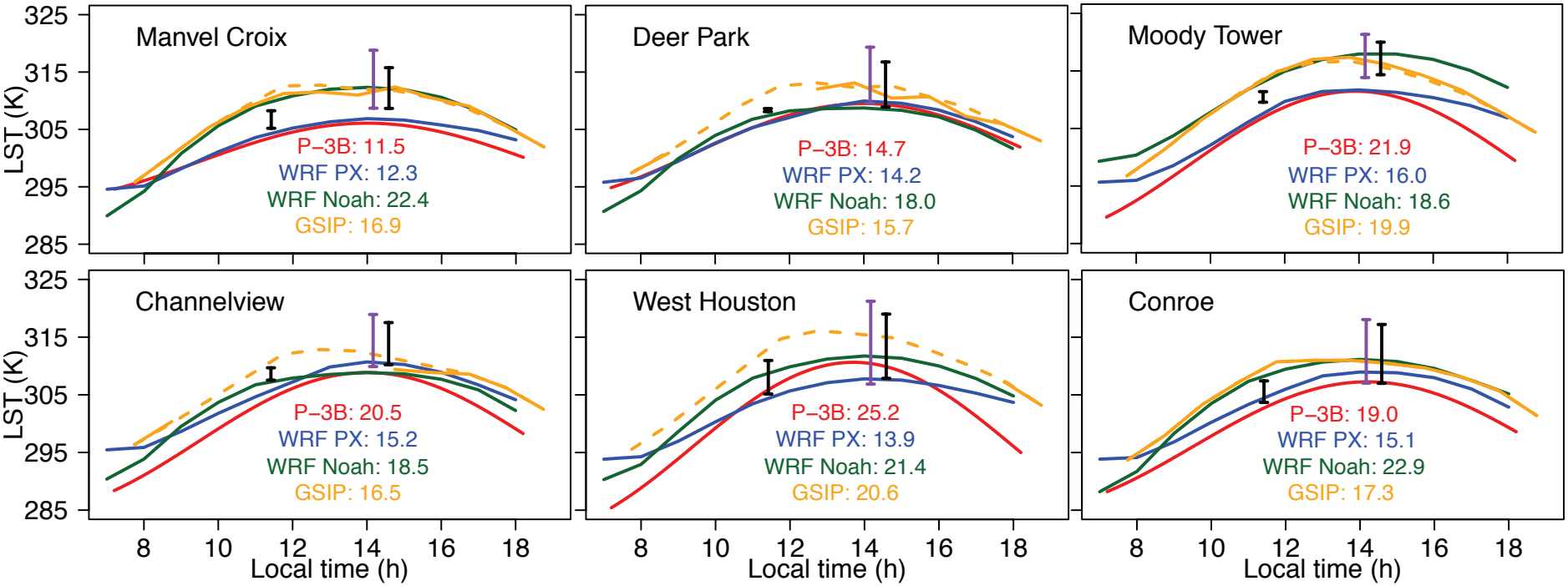
- At each site, the vegetation indexes and LSTs around/within the spirals were highly variable.
- The aircraft-derived daytime LSTs show ranges of 11-25 °K varying by location, with the daily maxima occurring near 13-14 local time (near the VIIRS and Aqua overpasses).

<u>Early p.m. from high to low:</u>

Moody Tower (urban center)
West Houston
Deer Park
Channelview
Conroe
Manvel Croix } More vegetation cover



Comparing aircraft-derived LSTs with WRF simulations and satellites (MODIS, GOES, VIIRS)



- WRF performance depended on its configurations
- Discrepancies between the model and the observations from various platforms (aircraft, satellites) differed by location and time.

Comments on future use of aircraft LSTs

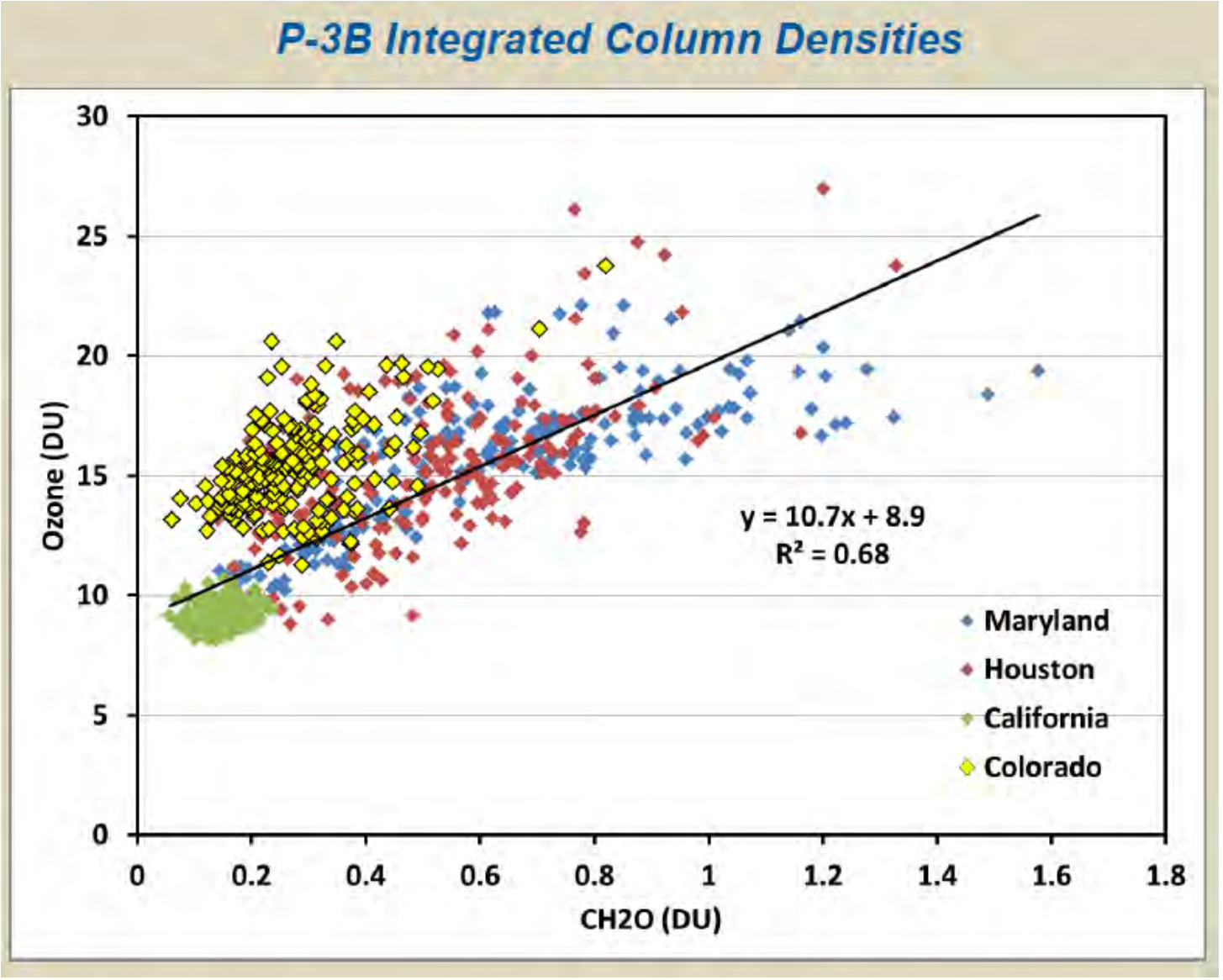
- Similar approaches applicable to other locations and times under clear conditions (e.g., to look at the drought in the US west)
- Night time data would be helpful
- Validation of the diurnal cycle model (e.g., making more observation data at each site)

Working towards understanding the drivers of variability in column ozone/formaldehyde relationships

DISCOVER-AQ telecon – September 24, 2015

Jason Schroeder
Jim Crawford
Al Fried
Armin Wisthaler
Don Blake

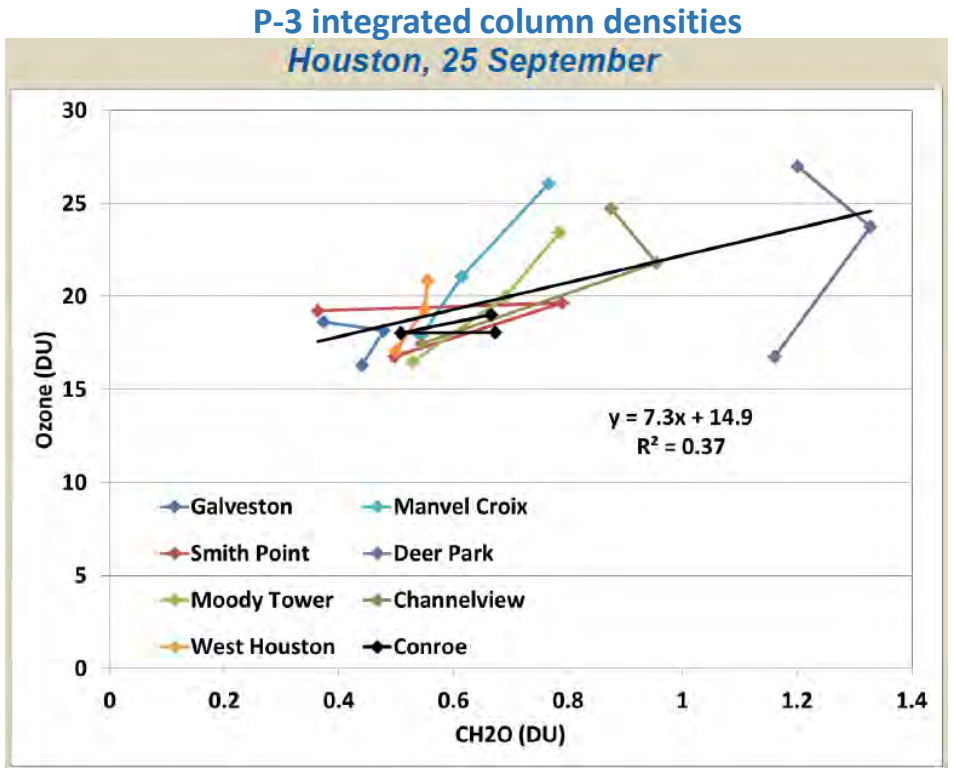
Relatively strong relationship between column formaldehyde and ozone

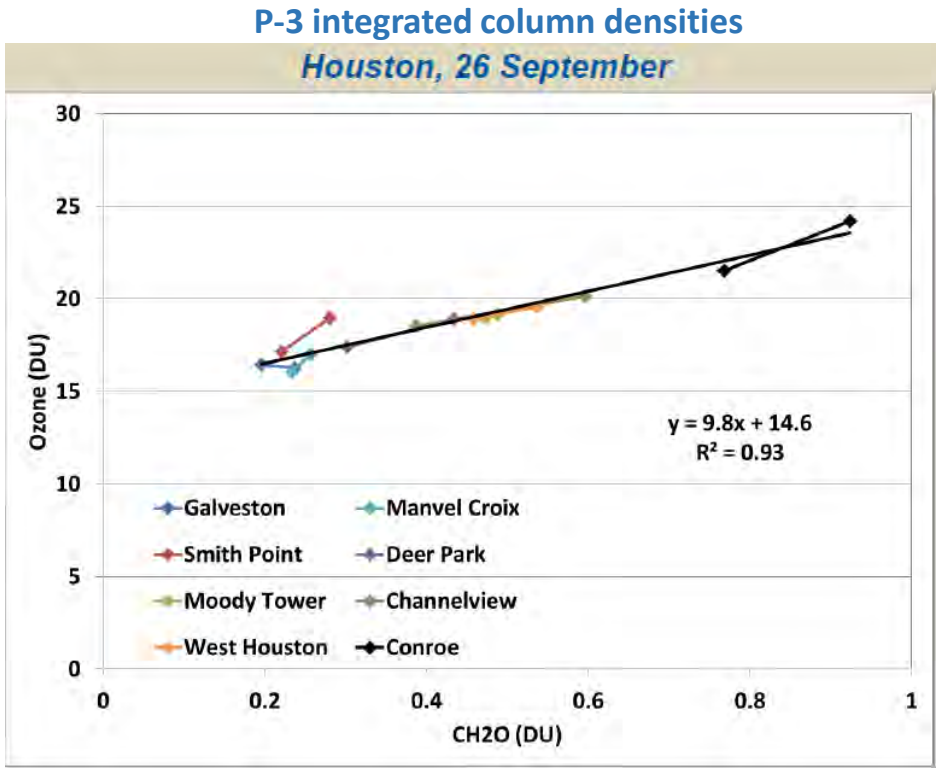


Advantage: Most of the CH2O vertical column is likely to be found in the boundary layer

- Possible to use space-based CH2O measurements to learn about O3 in the boundary layer
- Need to understand drivers of variability in this relationship

Case study: back-to-back days in Houston with different slopes, different coefficients of determination





What was happening on the 25th, specifically at Deer Park?

- Use the LaRC photochemical box model to investigate the effects of chemistry on the O3/CH2O relationship in Houston

Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
CH4	X
Ethane	
Propane	
Alkanes (lumped)	
Ethene	
Alkenes (lumped)	
Aromatics (lumped)	
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	

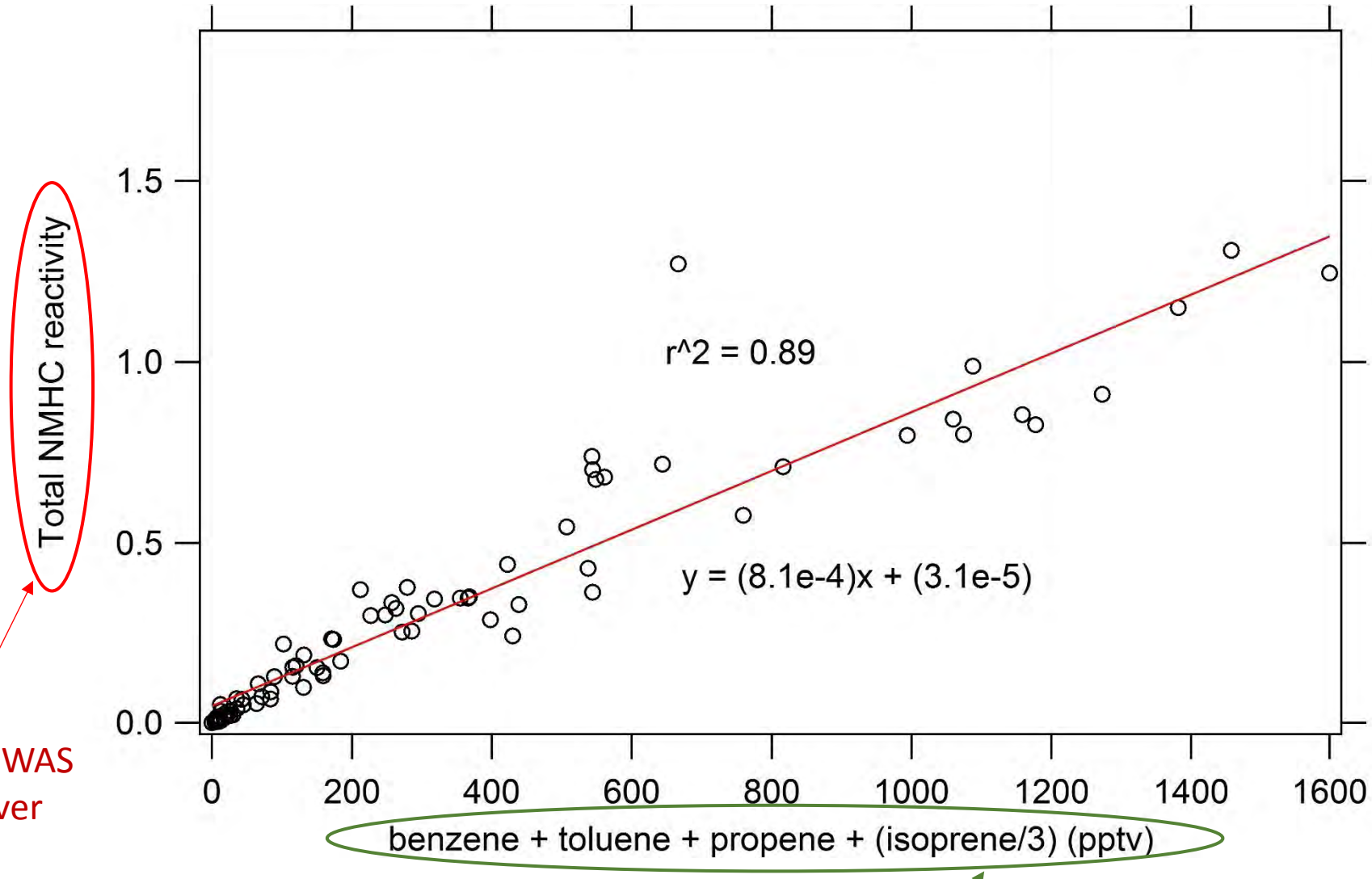
Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
CH4	X
Ethane	
Propane	
Alkanes (lumped)	
Ethene	
Alkenes (lumped)	
Aromatics (lumped)	
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	

These species *were* measured on the DC-8 by UCI during SEAC4RS.

SEAC4RS	DISCOVER-AQ
WAS	
PTrMS	PTrMS

Can we find relationships between PTrMS and WAS measurements to help fill in these blanks?

$$ROH_{NMHC} = \sum [NMHC]_i \, k_{OH,i}$$

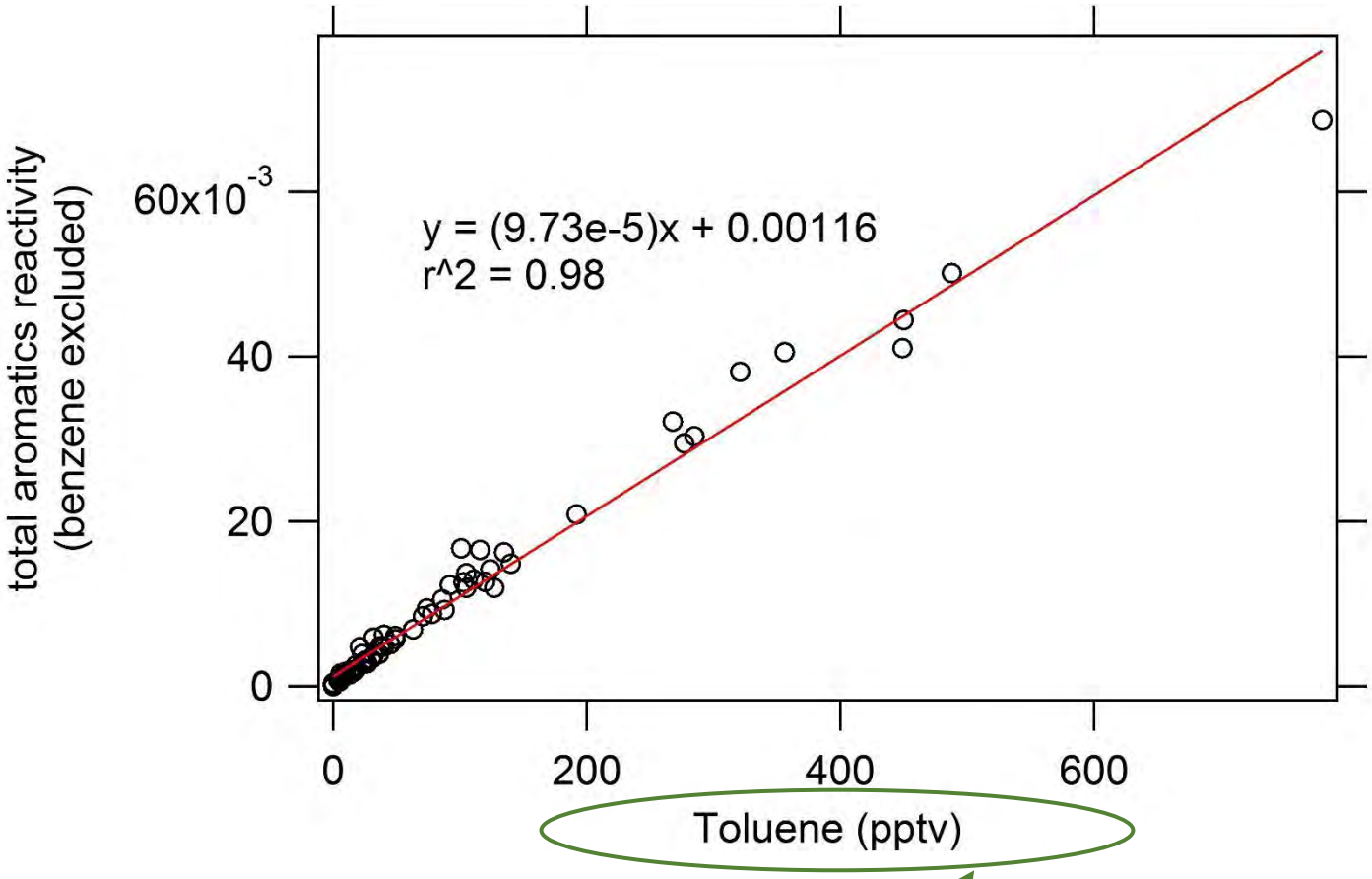


Calculated from WAS data collected over Houston during SEAC4RS

Calculated from WAS data over Houston. However, these were ALSO measured by the PTr-TOF-MS during DISCOVER-AQ

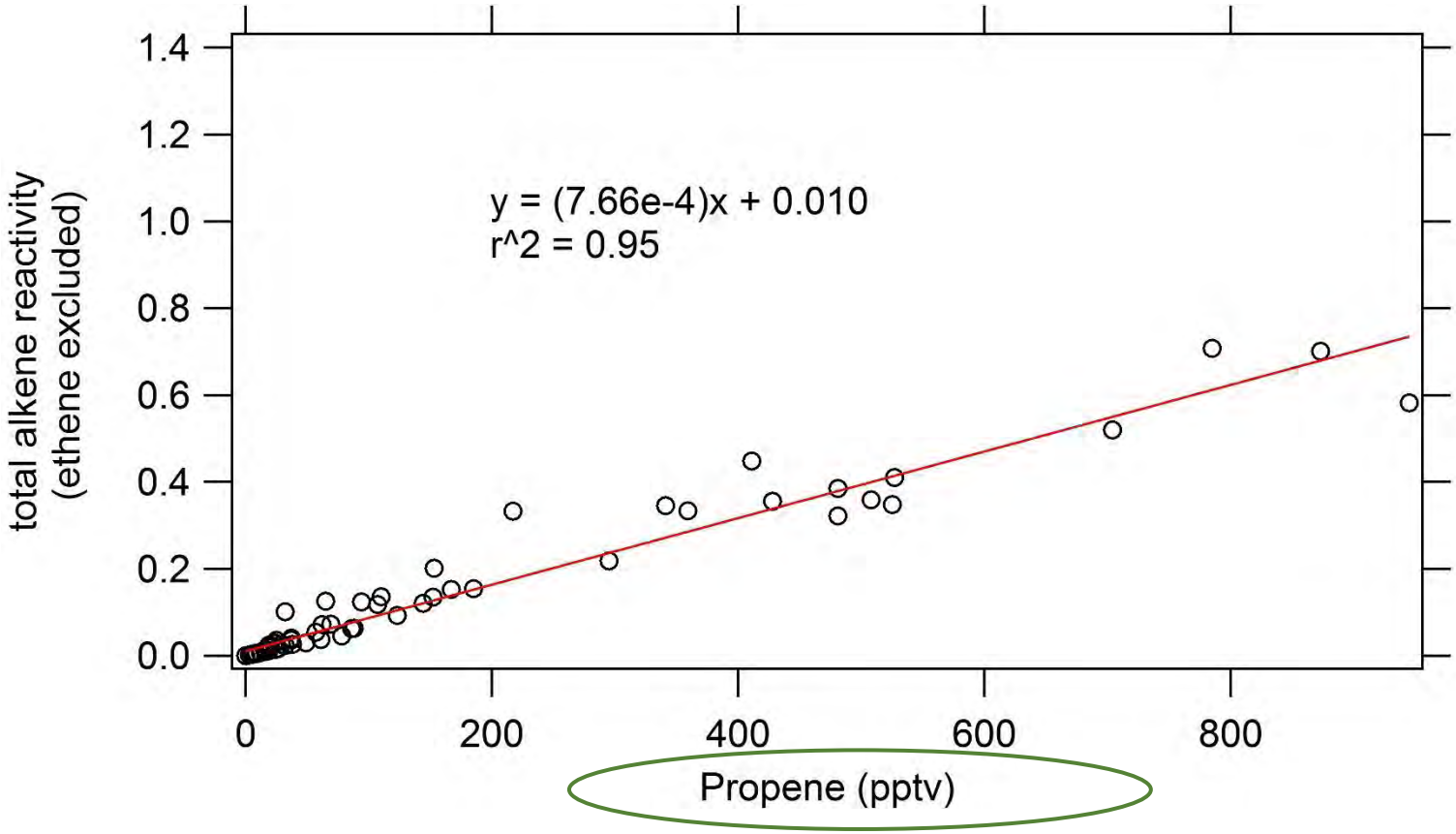
Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
Ethane	
Propane	
Alkanes (lumped)	
Ethene	
Alkenes (lumped)	
Aromatics (lumped)	
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	

$$ROH_{lumped_arom} = [aromatics]_{lumped}\ x\ k_{OH,lumped_arom}$$



WAS data over Houston. However, toluene was ALSO measured by the PTr-TOF-MS during DISCOVER-AQ

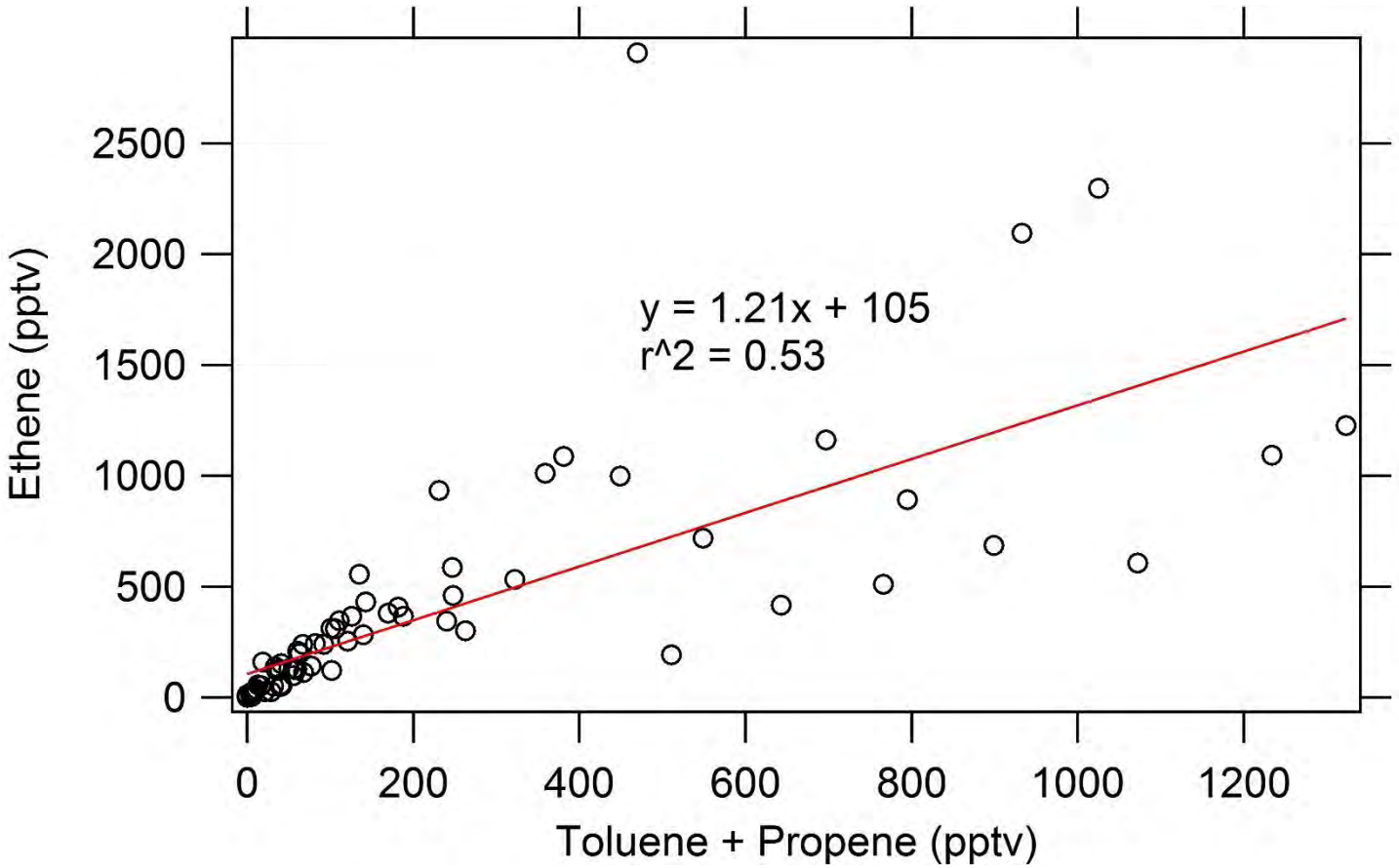
Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
Ethane	
Propane	
Alkanes (lumped)	
Ethene	
Alkenes (lumped)	
Aromatics (lumped)	X (estimated)
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	



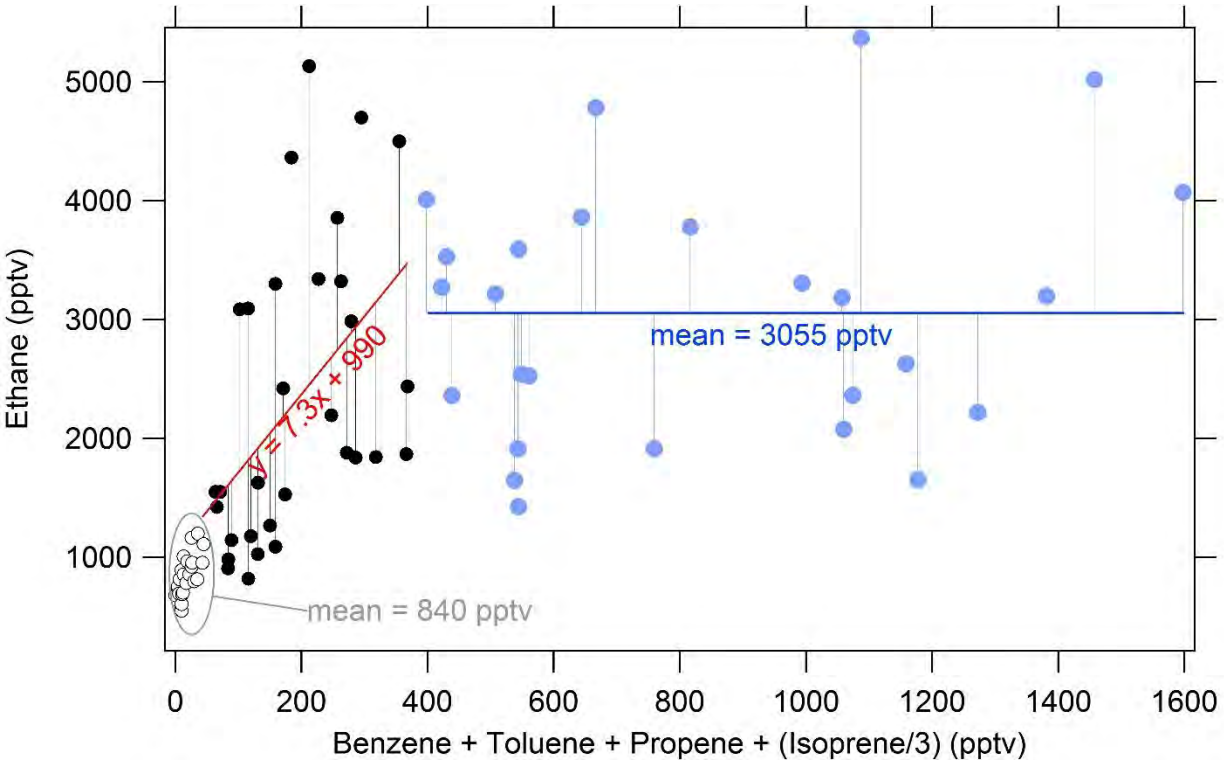
$$ROH_{alkenes,lumped} = k_{alkenes,lumped}[alkenes]_{lumped}$$

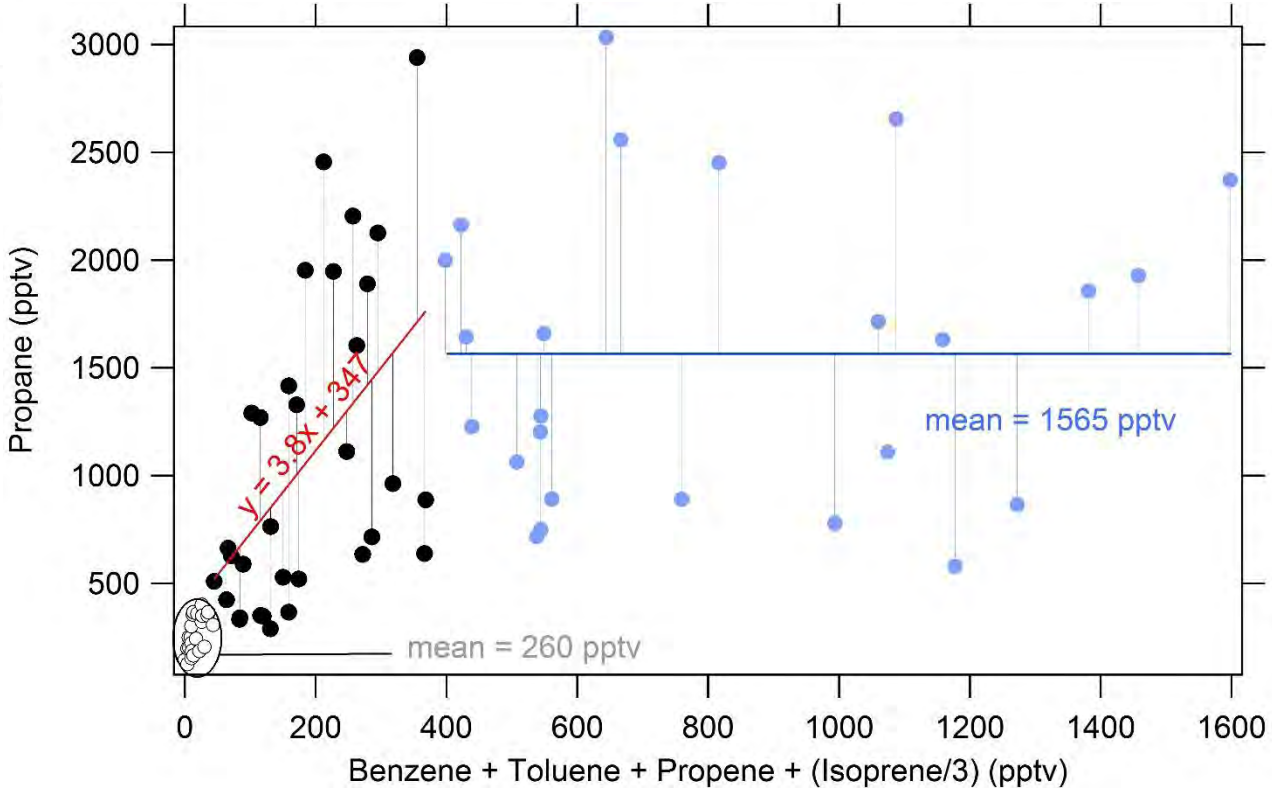
WAS data over Houston. However, propene was ALSO measured by the PTr-TOF-MS during DISCOVER-AQ

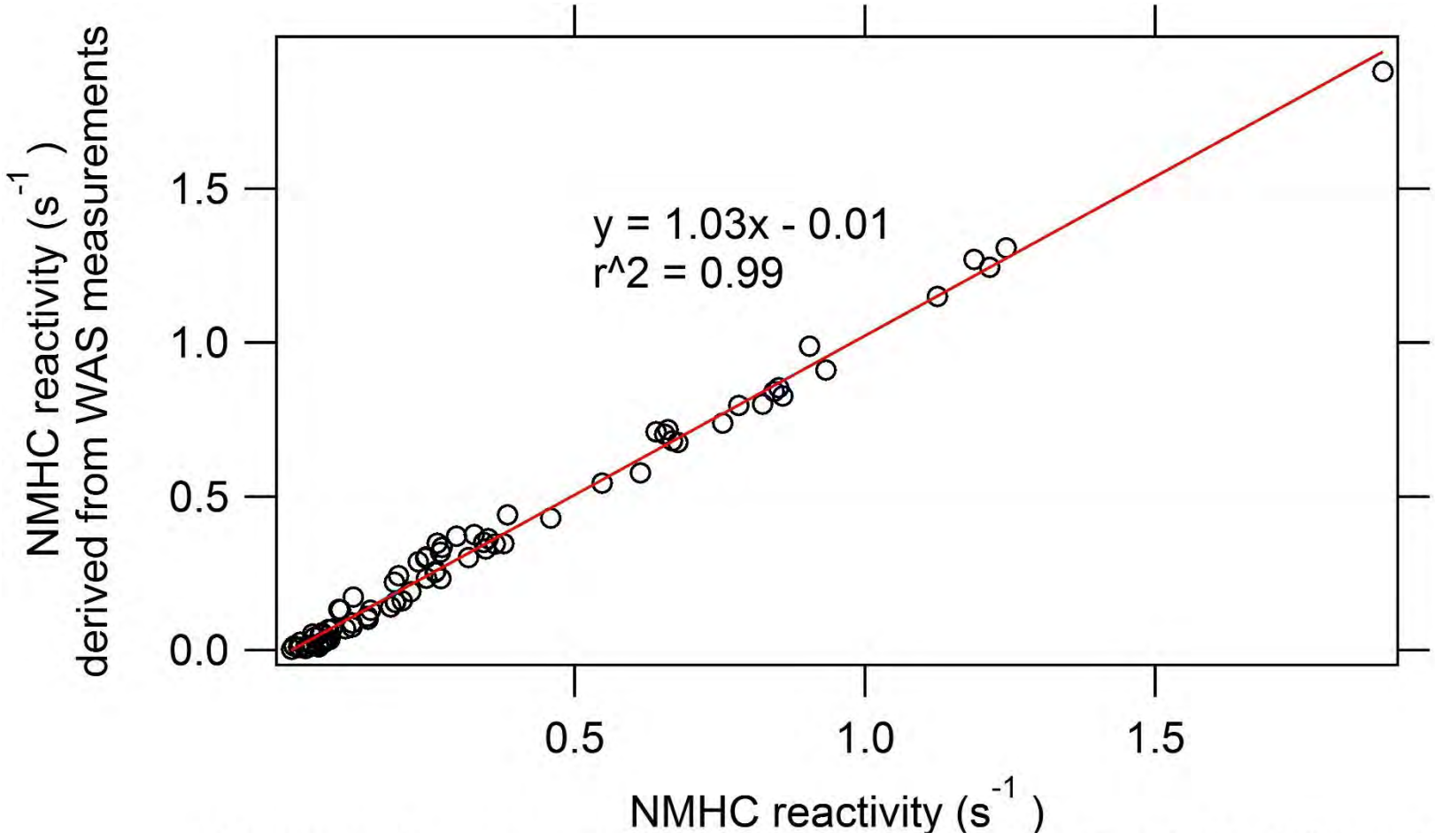
Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
CH4	X
Ethane	
Propane	
Alkanes (lumped)	
Ethene	
Alkenes (lumped)	X (estimated)
Aromatics (lumped)	X (estimated)
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	


y = 1.21x + 105
r^2 = 0.53
Ethene (pptv)
Toluene + Propene (pptv)
0
500
1000
1500
2000
2500
0
200
400
600
800
1000
1200

Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
CH4	X
Ethane	
Propane	
Alkanes (lumped)	
Ethene	X(estimated)
Alkenes (lumped)	X (estimated)
Aromatics (lumped)	X (estimated)
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	

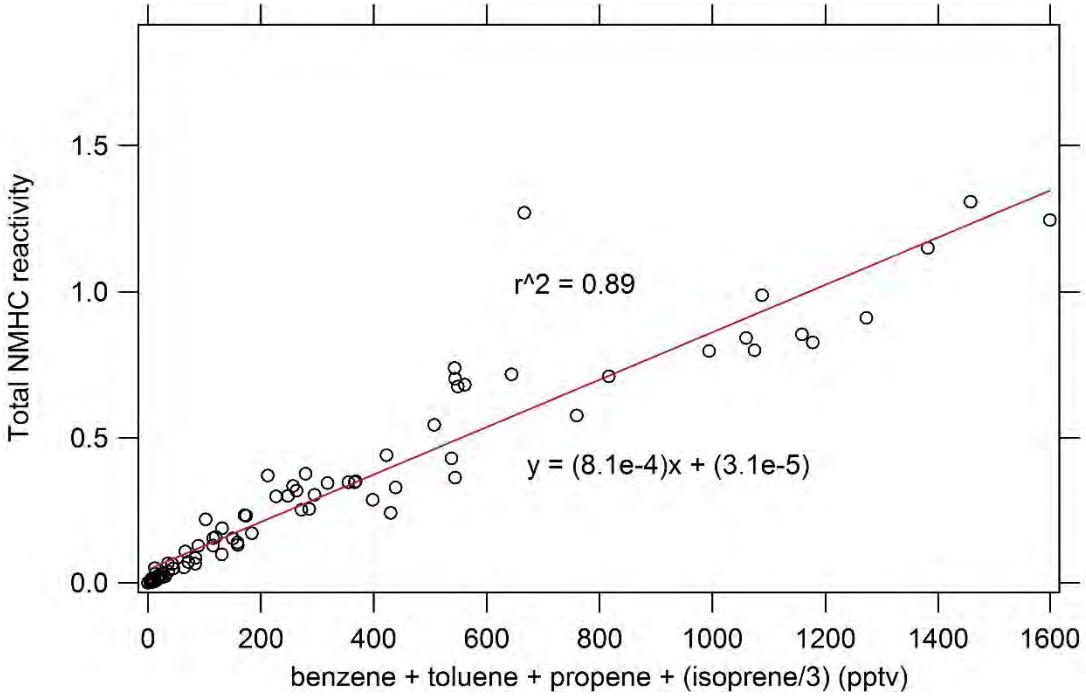

Ethane (pptv)
5000
4000
3000
2000
1000
0
200
400
600
800
1000
1200
1400
1600
Benzene + Toluene + Propene + (Isoprene/3) (pptv)
y = 7.3x + 990
mean = 3055 pptv
mean = 840 pptv


Propane (pptv)
3000
2500
2000
1500
1000
500
0
200
400
600
800
1000
1200
1400
1600
Benzene + Toluene + Propene + (Isoprene/3) (pptv)
y = 3.8x + 347
mean = 1565 pptv
mean = 260 pptv

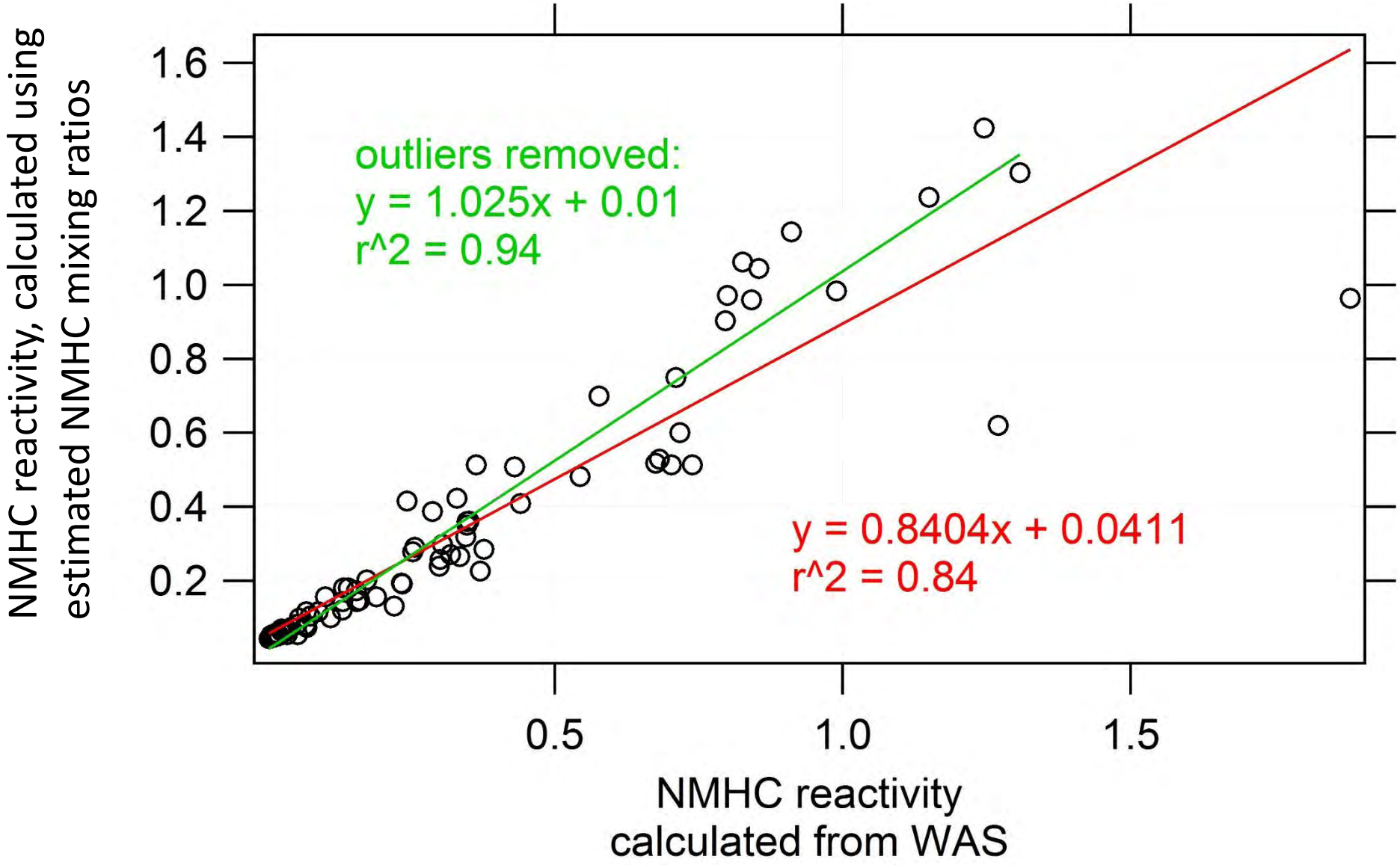


Ethane and propane substituted with estimated mixing ratios

Chemical species needed for model input	Measured during DISCOVER-AQ (texas)?
H2O	X
O3	X
CO	X
NO	X
NO2	X
CH4	X
Ethane	X (estimated)
Propane	X(estimated)
Alkanes (lumped)	
Ethene	X(estimated)
Alkenes (lumped)	X (estimated)
Aromatics (lumped)	X (estimated)
Isoprene	X
Benzene	X
CH2O	X
Acetone	X
MEK	X
Methanol	X
PAN	
HNO3	



Alkane reactivity treated as residual NMHC reactivity


NMHC reactivity, calculated using estimated NMHC mixing ratios
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
outliers removed:
y = 1.025x + 0.01
r^2 = 0.94
y = 0.8404x + 0.0411
r^2 = 0.84
0.5
1.0
1.5
NMHC reactivity calculated from WAS