7th International DOAS workshop: 6 - 8 July 2015

Pandora profile algorithms: DISCOVER-AQ preliminary results

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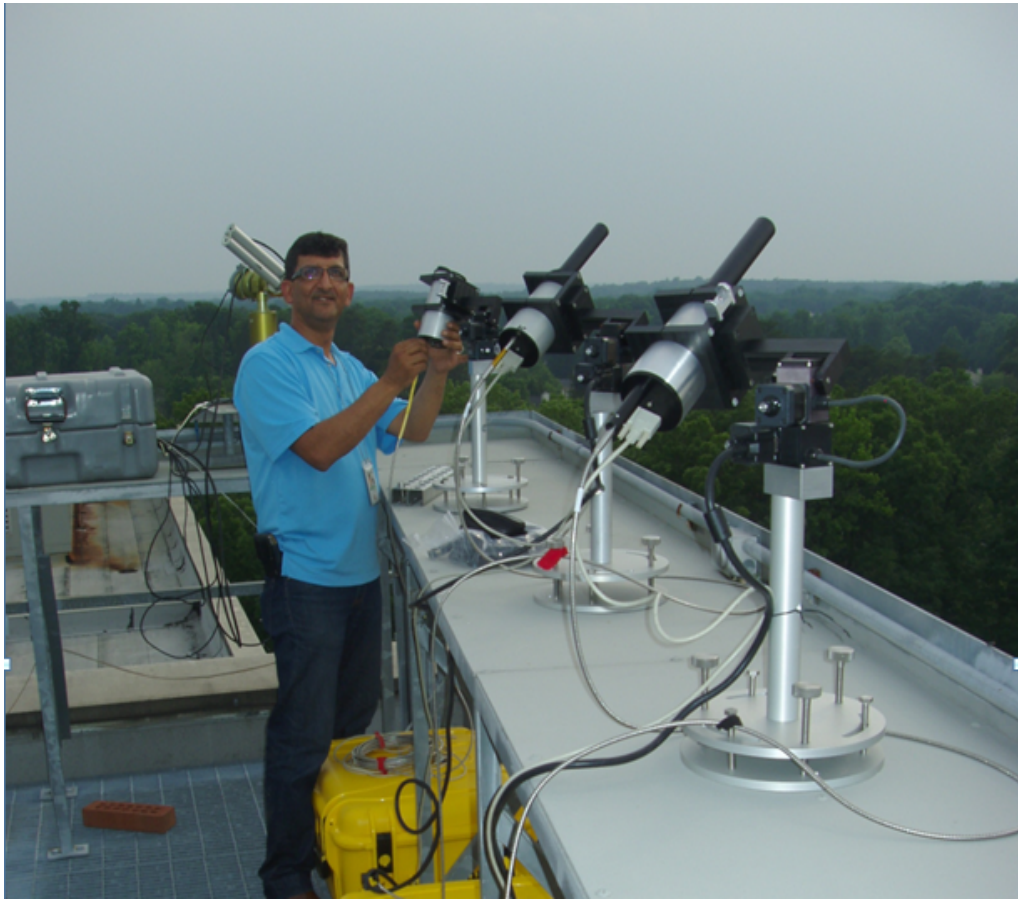
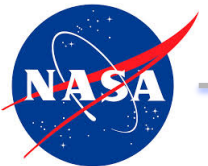


Motivation

- Pandora instruments are multi-axis and direct sun/moon systems
- Over 20 Pandoras are currently in operation and over 47 built
- Routine direct sun measurements and analysis of NO_2 and O_3 total columns at a centralized location.
- Improvements in optics and analysis will allow for separation of stratospheric and tropospheric columns of NO_2 and potentially O_3 from direct sun data
- MAX-DOAS operation has been mainly performed on a campaign basis but will be part of a normal schedule
- Need operational algorithms for multi instrument analysis with minimal "oversight"



Pandora profiling algorithms

Aerosols/clouds impact light path ⇨ retrieval of trace gases depends on "correct" aerosol/cloud representation

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

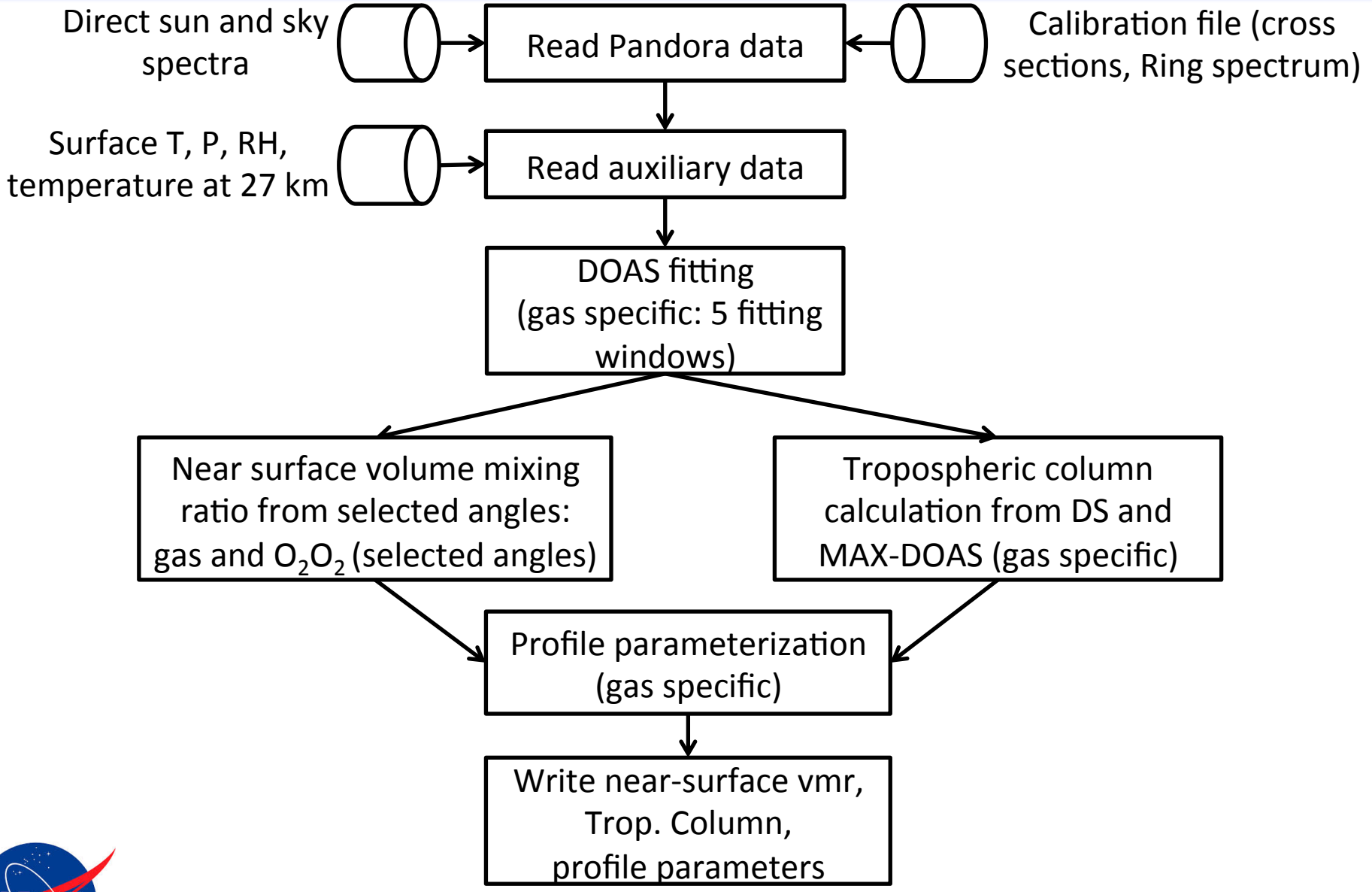
2. Direct Intensity fitting

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

➔

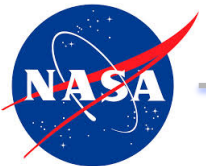
Aerosol Ext. Coef. Profile, SSA, ASY factor, Surface Albedo Trace gas profiles

Real-time analysis: no inversion



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

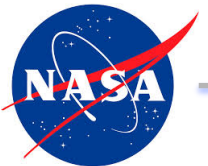


Real-time analysis: NO_2 surface VMR

- Spectra collected at 1, 2, 15, 30, 90° viewing elevation angles (VEA)
- 435 – 490 nm and 345 – 390 nm fitting windows
- Fitting constant and linear terms of $\sigma(NO_2)$
- At low VEA stratospheric NO_2 is removed using DOAS fit results of constant/linear terms and 0/27km T
- At high AOD MAX sensitivity is close to the ground. NO_2 and O_2O_2 profiles are assumed similar within a shallow layer
- At low AOD MAX sensitivity to NO_2 and O_2O_2 profiles is significantly different -> two wavelength windows are used to decrease the sensitivity of NO_2 and O_2O_2 to aloft absorption

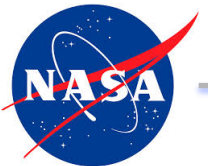
Real-time analysis: tropospheric NO_2

- Total column from DS data
- Separation of stratospheric and tropospheric columns based on T-sensitivity (low residuals and high pollution level, 75° SZA)
- Linear interpolation between morning and evening stratospheric columns at 75° SZA to estimate stratospheric column at SZA < 75°
- Adding tropospheric column from DS at reference time to ΔSCD at 30° VEA and dividing by geometric AMF = 2
- Averaging tropospheric columns from DS and 30° VEA

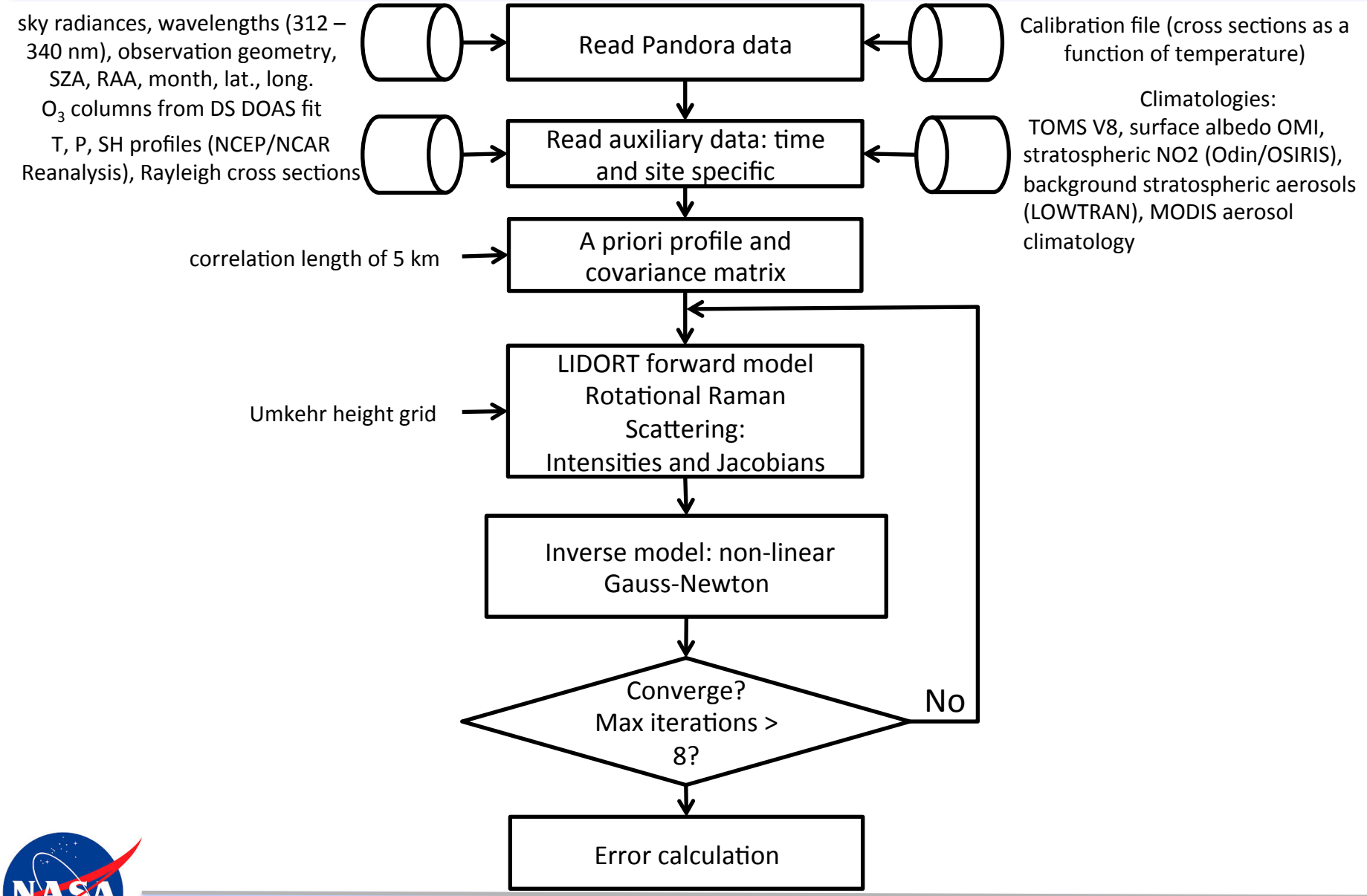


Real-time tropospheric NO_2 profile

- Tropospheric column
- Near surface VMR
- Comparing diurnal variation of tropospheric column and near surface VMR. If profiles are constant the normalized columns and VMR values "track" within corresponding errors
- Comparing normalized $\Delta SCD(NO_2)$ and $\Delta SCD(O_2O_2)$ at VEA < 30°
- Estimating parameters of several profiles (box, exponential, Gaussian) and assigning profile probabilities (high, med, low)



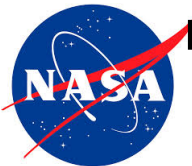
Direct intensity fitting: nonlinear MAP



Acknowledgement: Rob Spurr wrote a good portion of the code

Direct Fitting Algorithm: O_3

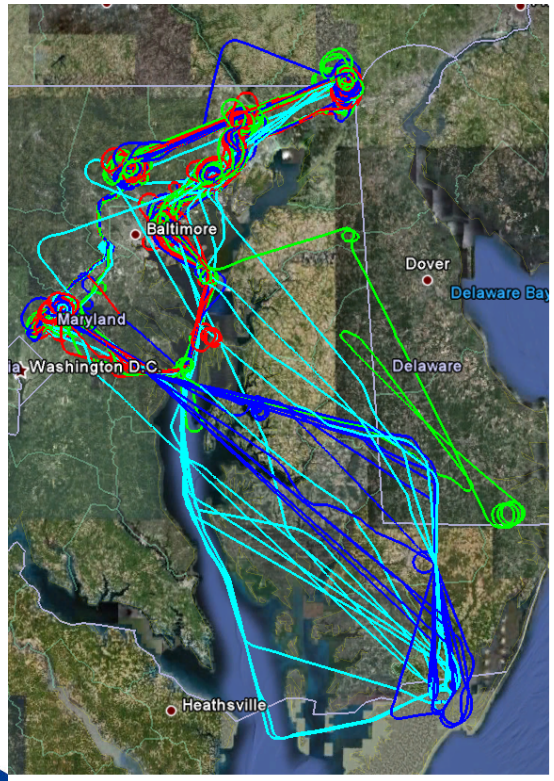
- Spectra are normalized with respect to zenith noon reference spectrum
- Zenith and multi-axis from 87 to 65deg SZA full profile inversion
- Retrieved profile (10 km and up) assumed constant at SZA < 65deg
- Aerosol profile shape is assumed exponential: total AOD as a function of wavelength – low order polynomial
- Heney-Greenstein phase function is fitted
- Aerosol SSA is fitted
- Trace gases currently are not fitted – profiles are taken from stratospheric climatology and real time DOAS retrievals



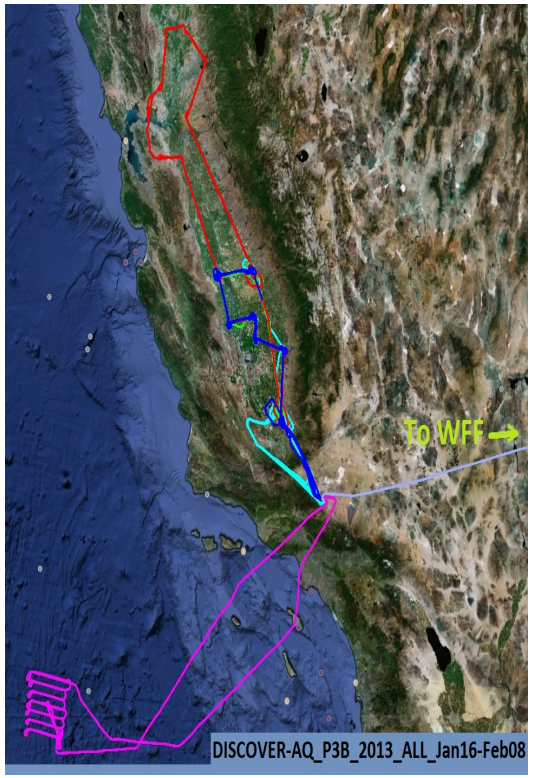
DISCOVER-AQ campaigns

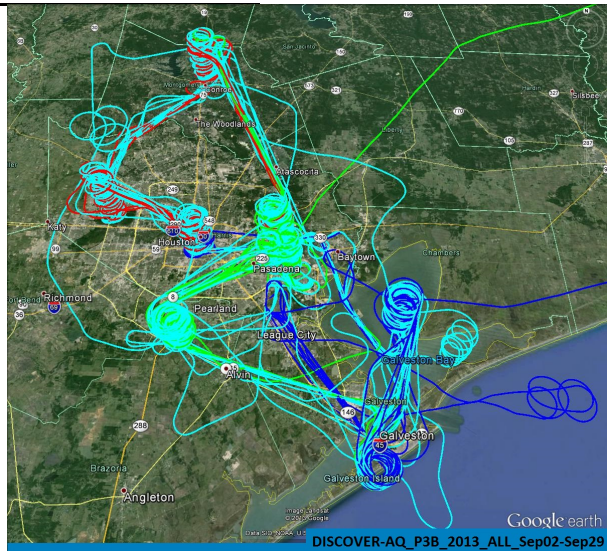
Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality – NASA sponsored mission

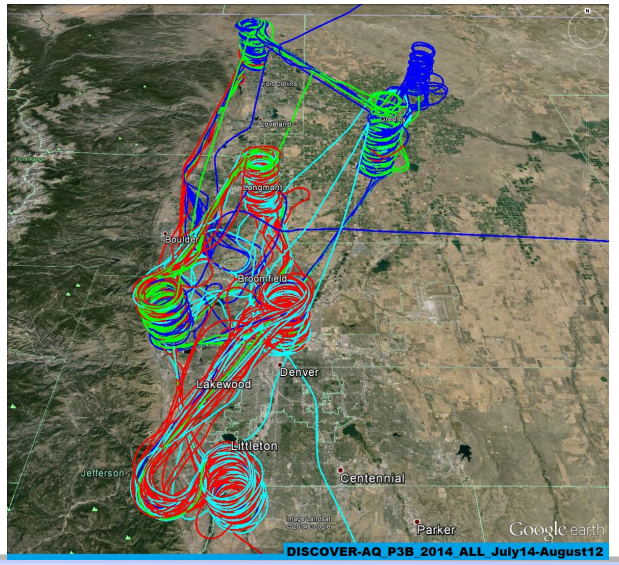
- **Baltimore-Washington, D.C. 2011**
- **California 2013**
- **Texas 2013**
- **Colorado 2014**



DISCOVER-AQ_2011_ALL_P3B_July1-July29

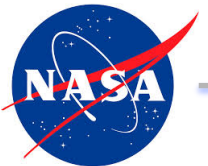




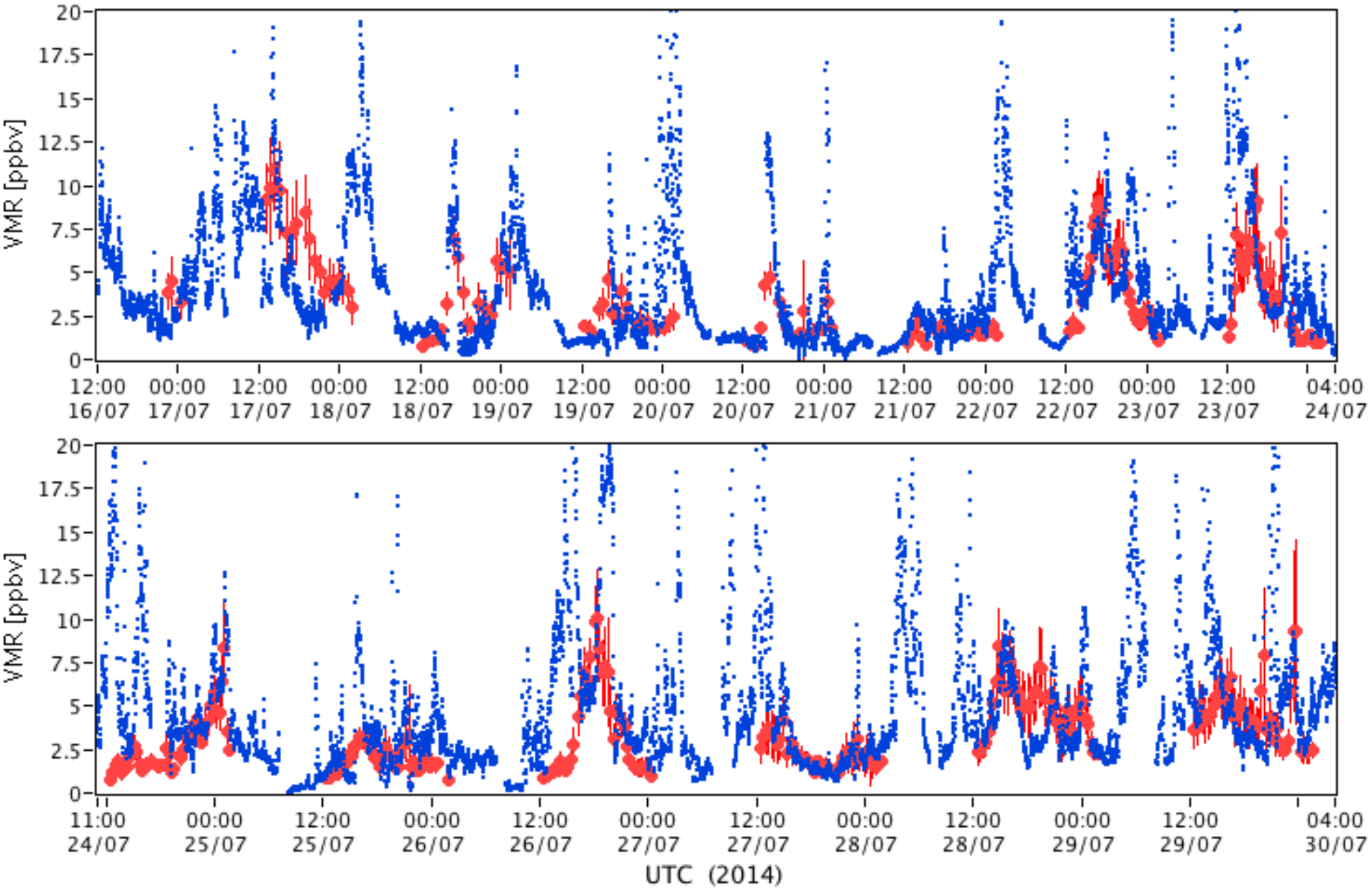


DISCOVER-AQ Pandora participation

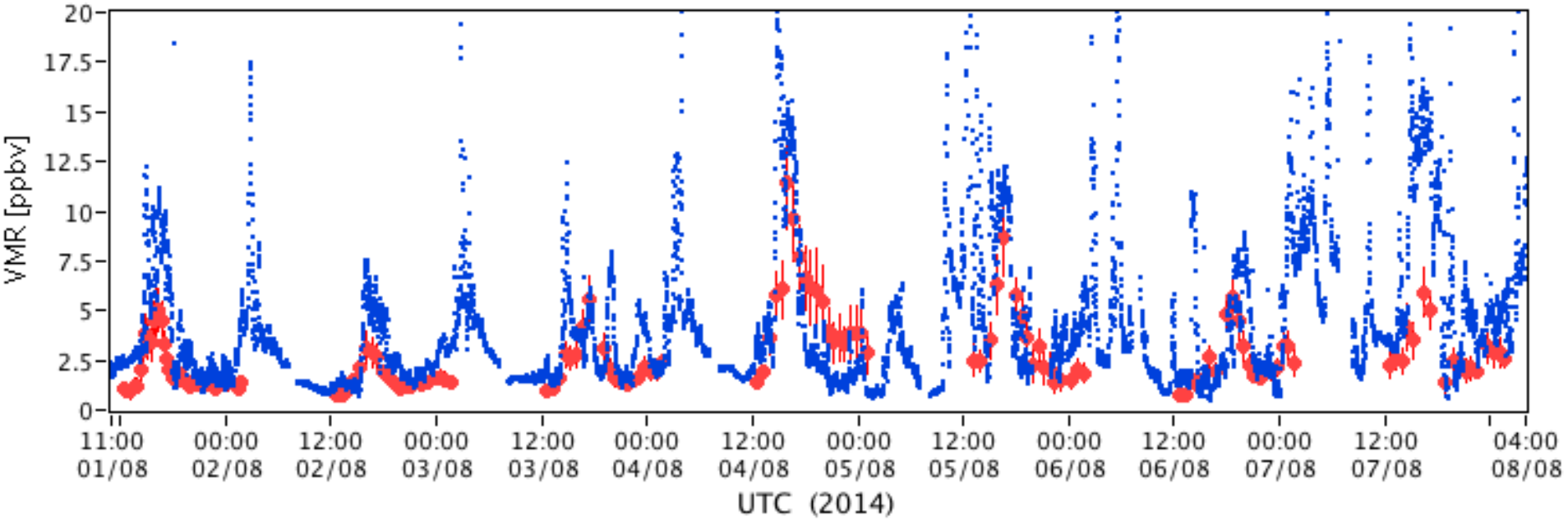
- **Baltimore-Washington, D.C. 2011: only direct sun data (total NO_2 and O_3 columns)**
- **California 2013: direct sun and 2 profiling sites**
- **Texas 2013: direct sun and 2 profiling sites**
- **Colorado 2014: direct sun and 2 profiling sites**



NO_2 surface vmr: Golden, CO (2014)

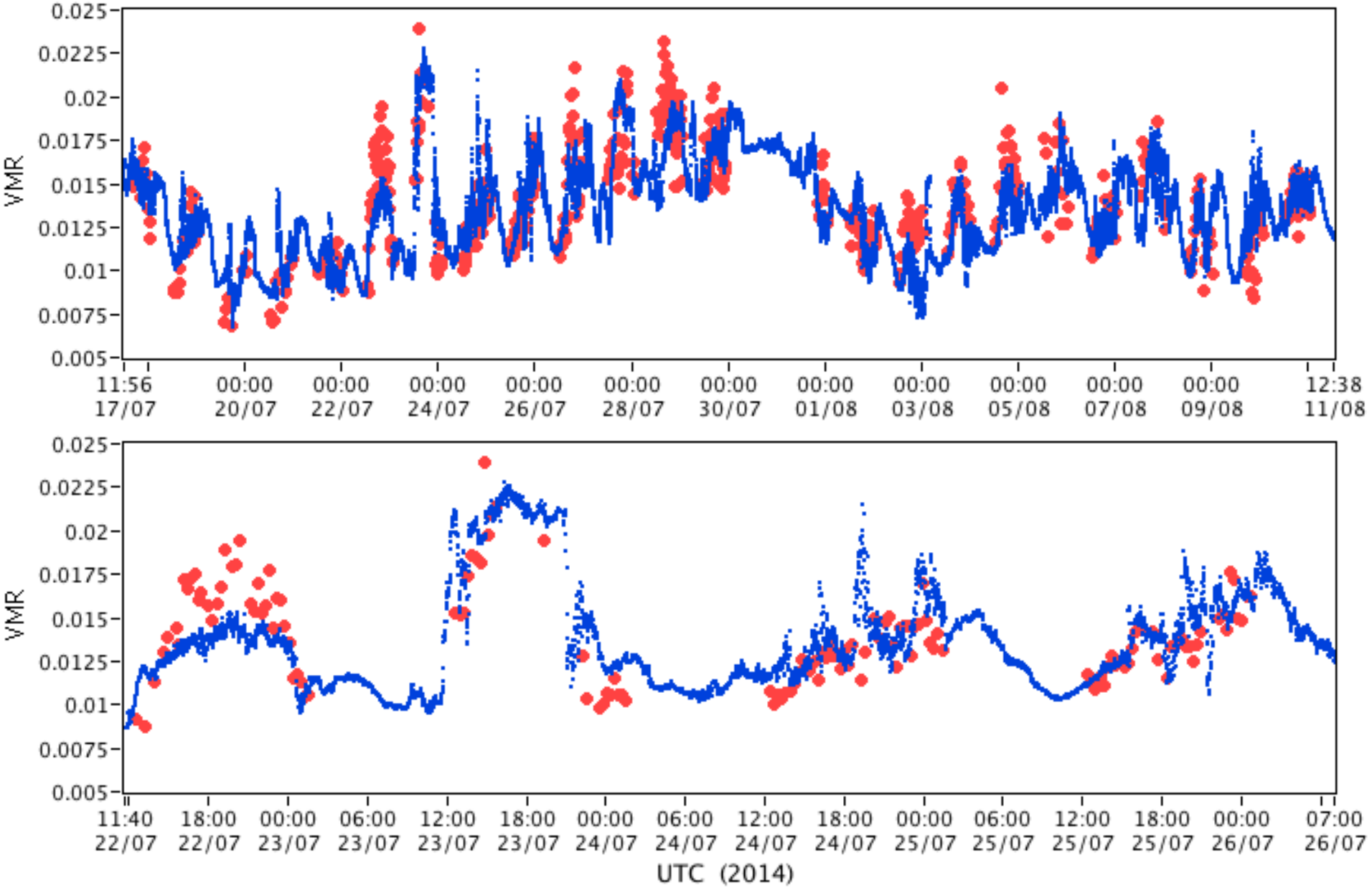


NO_2 surface vmr: Golden, CO (2014)

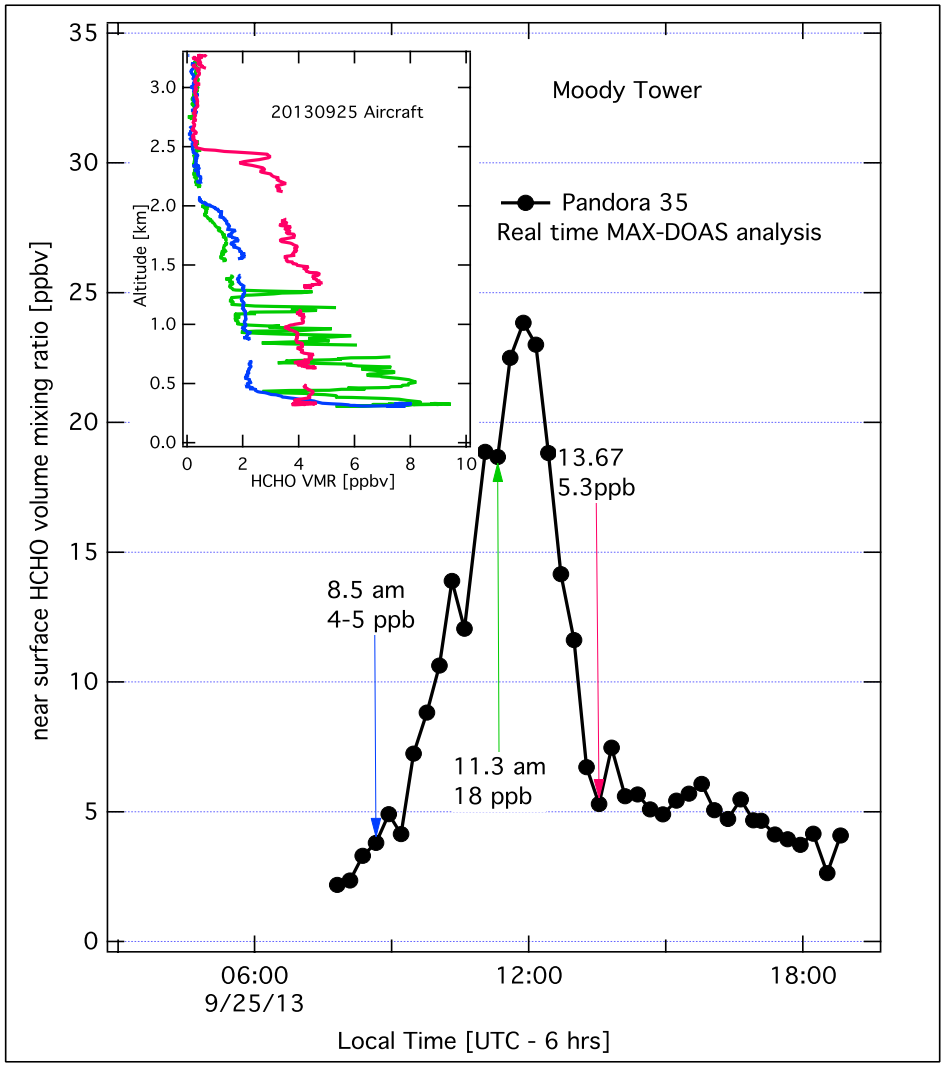


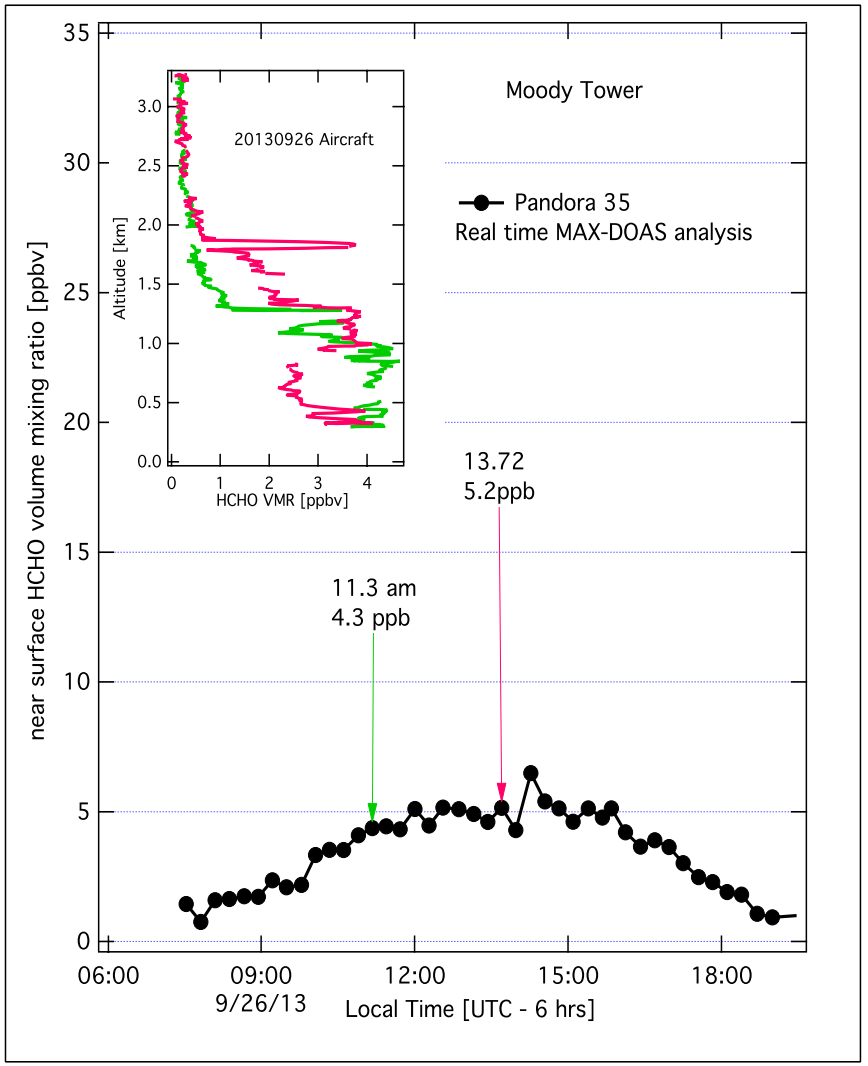
- in-situ CAPS NO2 (Russell Long)
- Pandora 38 near-surface real time

H_2O surface vmr: Golden, CO (2014)

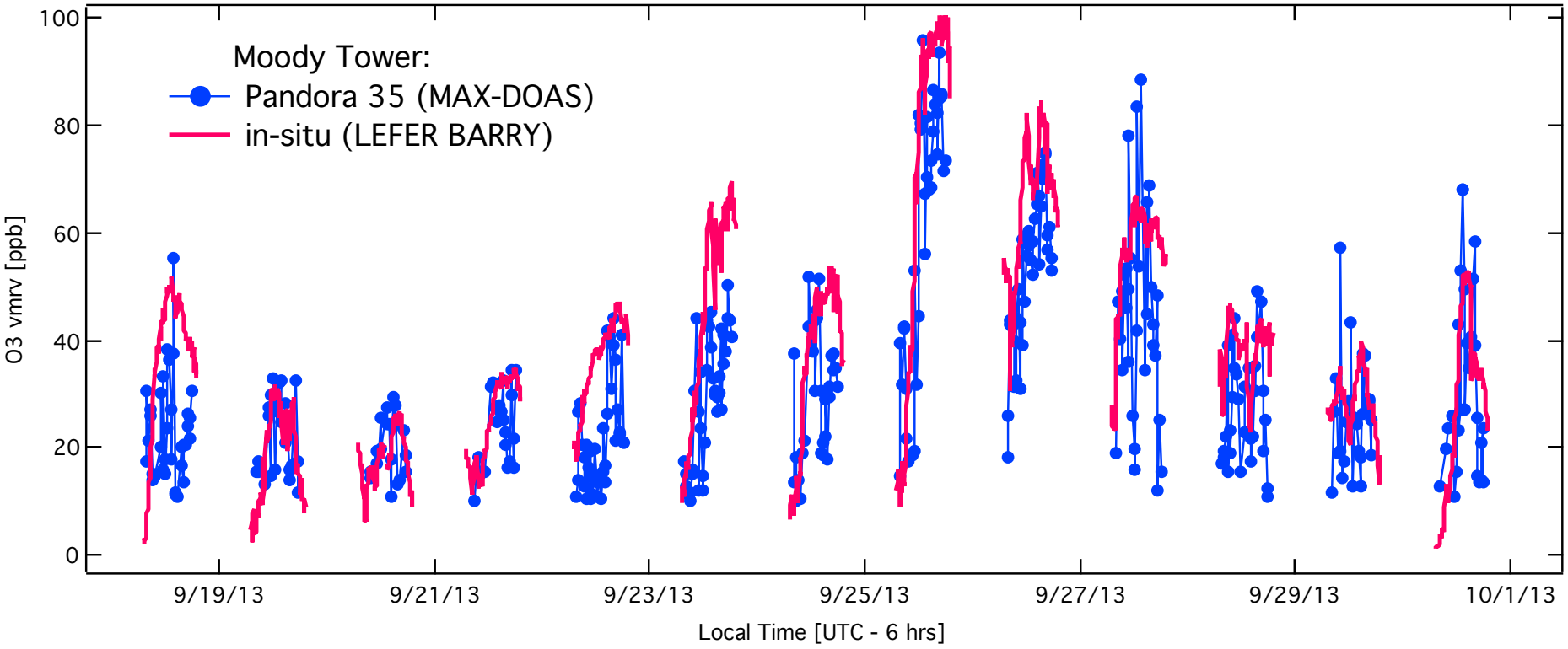


HCHO near-surface vmr: Houston, TX

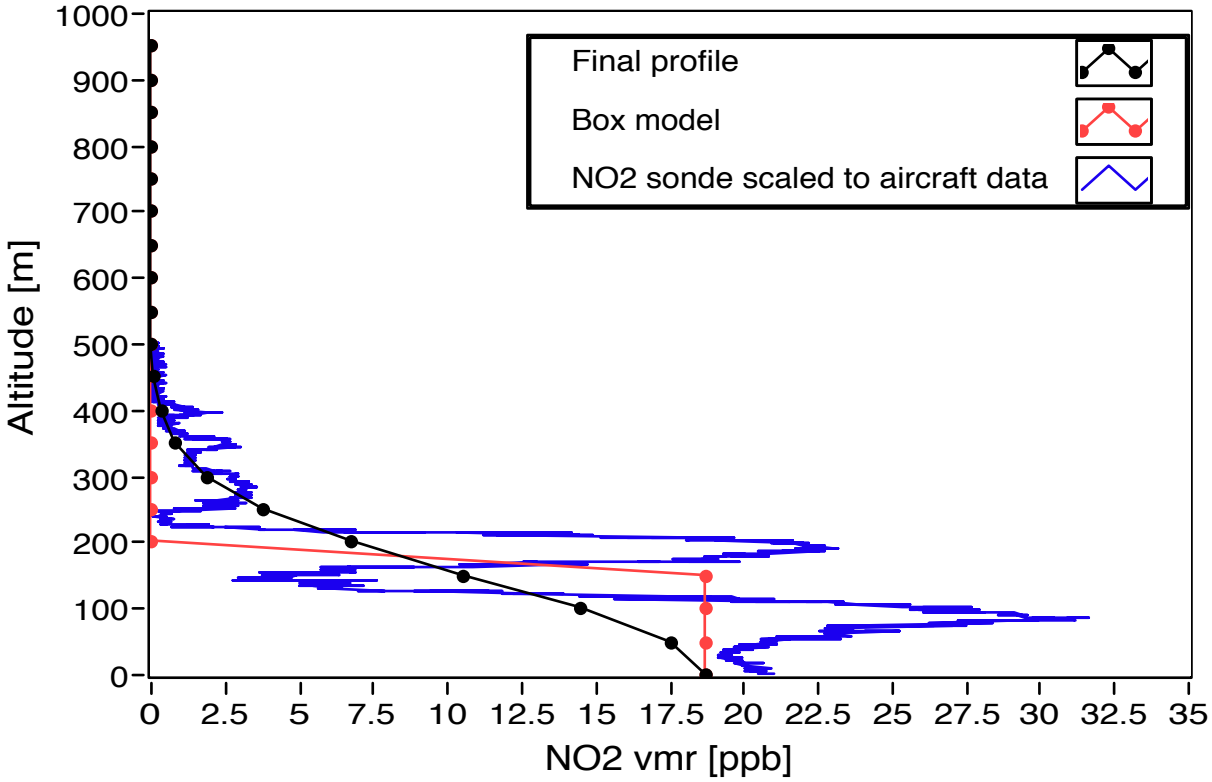




O_3 near-surface vmr: Houston, TX

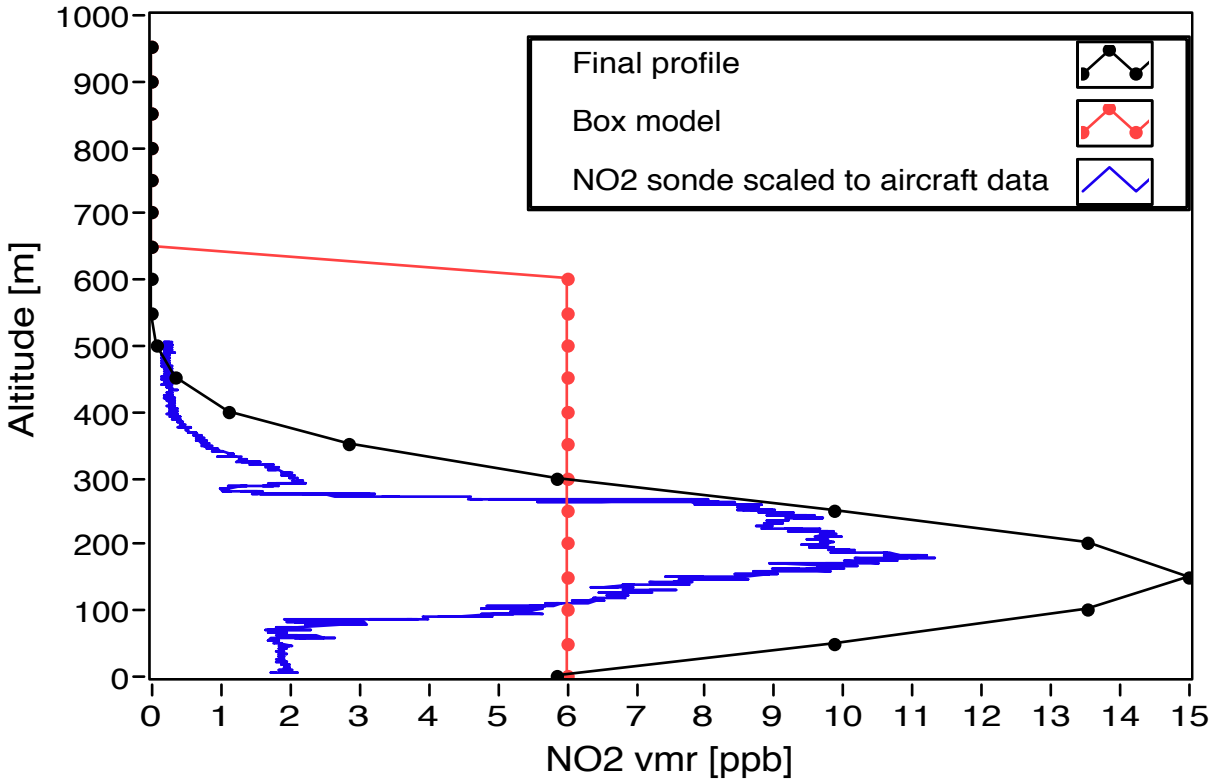


NO_2 profiles: real time (Smith Point, TX)



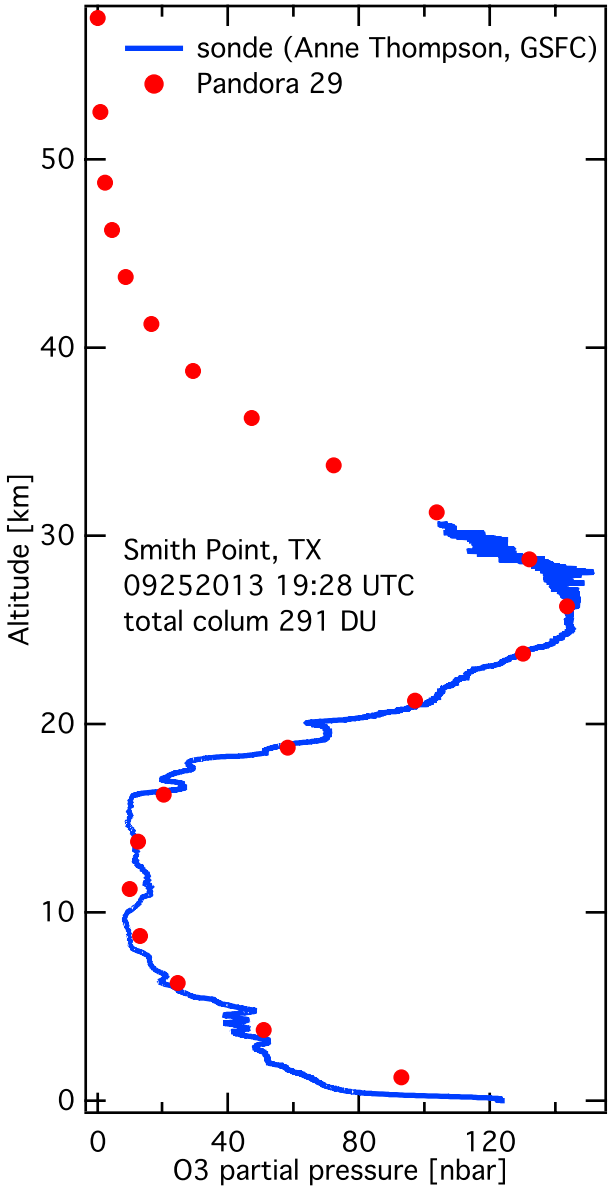
NO_2 sonde data courtesy of Deborah Stein-Zweers (KNMI)

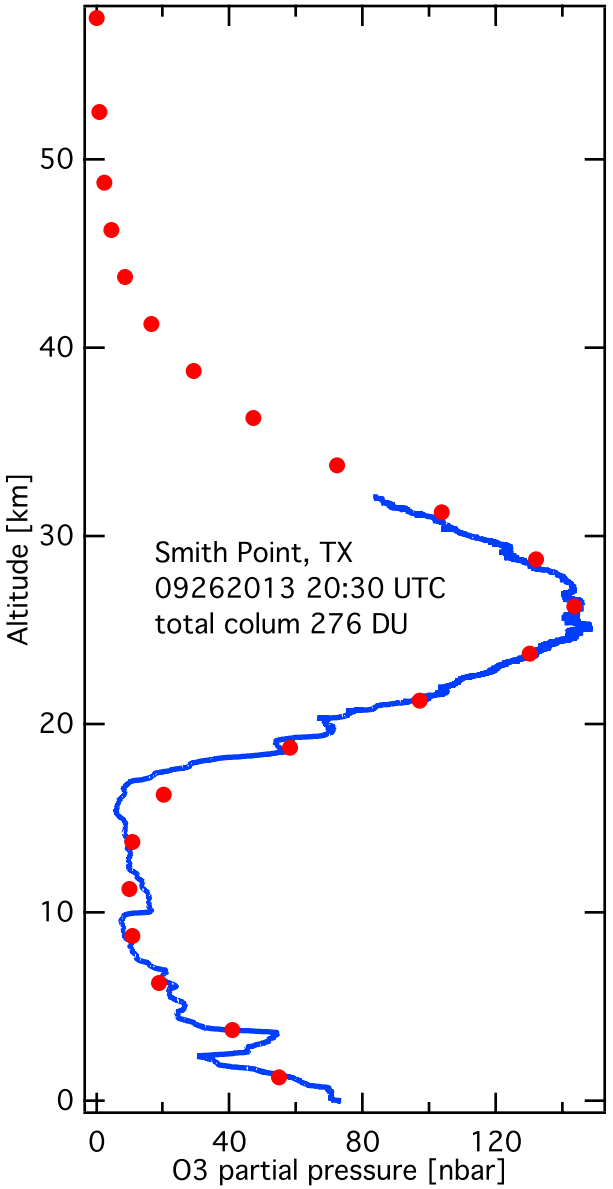
NO_2 profiles: real time (Smith Point, TX)



NO_2 sonde data courtesy of Deborah Stein-Zweers (KNMI)

O_3 profile: direct fitting (Smith Point, TX)

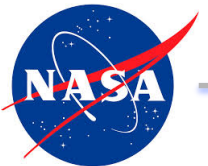
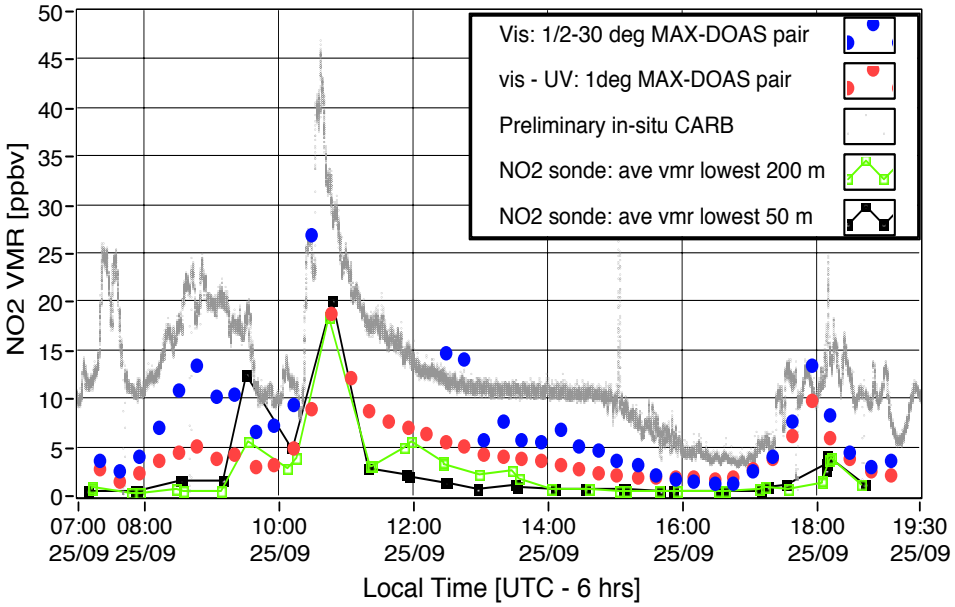
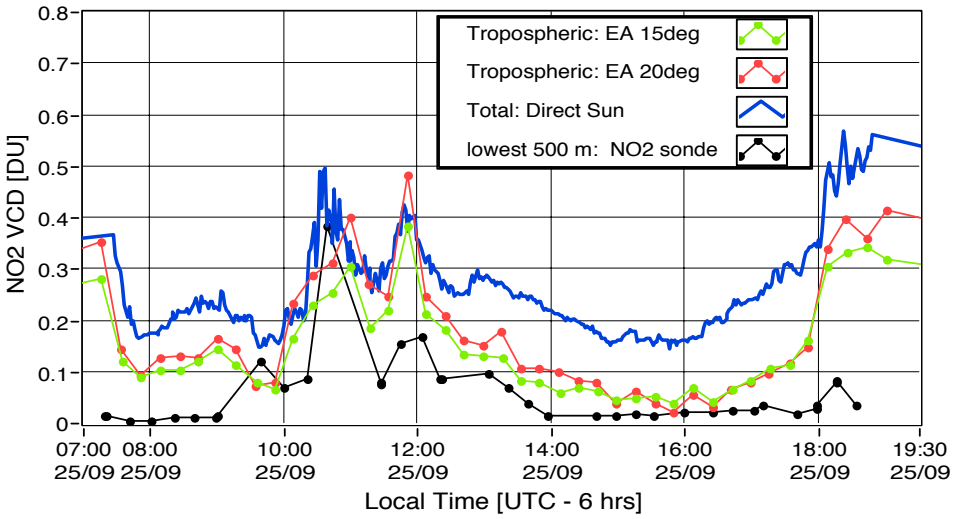




Future work

- Incorporate Mie code in Direct Fitting algorithm
- Trace gas profile fitting
- Cloud parameterization
- Error budget
- Extensive validation of results using surface and aircraft data during 3 DISCOVER-AQ campaigns

Thank you!



NO_2 profiles