Building the Pathway from TEMPO to GeoXO

Joint Science Meeting for TEMPO, GeoXO ACX, & TOLNet

# TEMPO Validation

# (*Baseline/L2 Products*)


Xiong Liu, Luke Valin, Jim Szykman*

Steve Brown, Laura Judd

Ron Cohen, Tom Hanisco, Pawan Gupta
Michel Grutter Chris McLinden*

**virtual*


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# TEMPO Validation Components and Plans


**Xiong Liu, Luke Valin, Jim Szykman***

Steve Brown, Laura Judd

Ron Cohen, Tom Hanisco, Pawan Gupta
Michel Grutter Chris McLinden*

**virtual*


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# Large Scale Multi-Agency / Platform Sub-Orbital Activities


Xiong Liu, Luke Valin, Jim Szykman*

**Steve Brown, Laura Judd**

Ron Cohen, Tom Hanisco, Pawan Gupta
Michel Grutter Chris McLinden*

**virtual*


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## Ground-based Networks


Xiong Liu, Luke Valin, Jim Szykman*

Steve Brown, Laura Judd

**Ron Cohen, Tom Hanisco, Pawan Gupta**

Michel Grutter Chris McLinden*

*virtual


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# International Partner Activites


Xiong Liu, Luke Valin, Jim Szykman*

Steve Brown, Laura Judd

Ron Cohen, Tom Hanisco, Pawan Gupta

**Michel Grutter Chris McLinden***

**virtual*


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# TEMPO Validation Components and Plans


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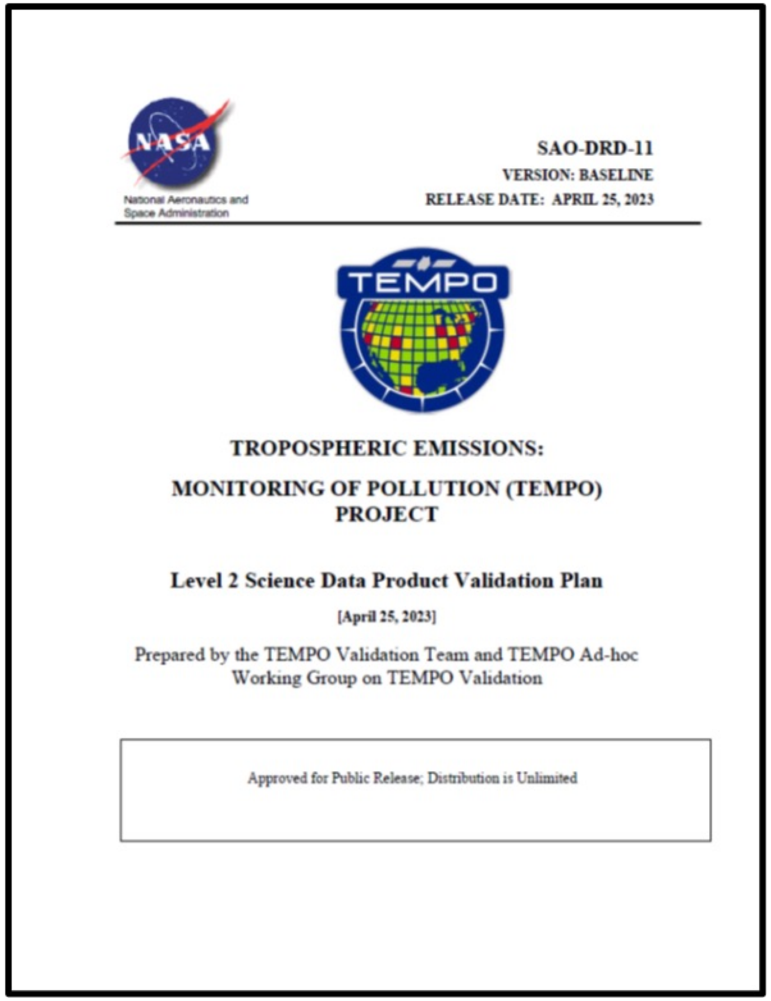
*virtual


# TEMPO (Tropospheric Emissions: Monitoring Pollution) mission Validation Plan


NASA

National Aeronautics and Space Administration

SAO-DRD-11

VERSION: BASELINE

RELEASE DATE: APRIL 25, 2023

TEMPO

TROPOSPHERIC EMISSIONS:

MONITORING OF POLLUTION (TEMPO) PROJECT

Level 2 Science Data Product Validation Plan

[April 25, 2023]

Prepared by the TEMPO Validation Team and TEMPO Ad-hoc Working Group on TEMPO Validation

Approved for Public Release; Distribution is Unlimited

- Outlines a best-efforts validation approach for the **ozone, nitrogen dioxide, and formaldehyde** data products.

- Leverages a comprehensive set of existing measurements (ground-based and satellite) for routine validation enhanced by episodic field mission and modeling efforts.

- Describes a structure for the geophysical data product maturity progression and discusses specific metrics to be generated to provide a ‘fit for purpose’ applications framework.

# What are the fundamental validation metrics/needs and plans?

## *TEMPO mission Level 2 data product (variable) requirements*

| Product Name | Product Horizontal Resolution N/S x E/W @ center of FOR | Product Precision | Frequency |
|---|---|---|---|
| Total Column $O_3$ | 2.0 x 4.75 $km^2$ | 3% | 1 hour |
| Tropospheric Column $O_3$ | 8.0 x 4.75 $km^2$ (4 N/S across-track pixels coadded) | 10 ppbv | 1 hour |
| 0-2 km $O_3$ selected scenes | 8.0 x 4.75 $km^2$ (4 N/S across-track pixels coadded) | 10 ppbv | 2 hours |
| Total Column $NO_2$ | 2.0 x 4.75 $km^2$ | $1.0 \times 10^{15}$ molecules $cm^{-2}$ | 1 hour |
| Tropospheric Column $NO_2$ | 2.0 x 4.75 $km^2$ | $1.0 \times 10^{15}$ molecules $cm^{-2}$ | 1 hour |
| Tropospheric column $CH_2O$ | 2.0 x 4.75 $km^2$ | $1.0 \times 10^{16}$ molecules $cm^{-2}$ | 3 hours |

*Note that the spatial resolution for the precision requirement is with 4 native pixels coadded, not the actual product resolution listed below.*

# What are the fundamental validation metrics/needs and plans?

Validation maturity of TEMPO Level 2 products is described by three levels: Beta, Provisional, and Full validation.

**Beta:** the product is minimally validated but may still contain significant errors; based on product quick looks using the initial calibration parameters. Publication of research based on Beta maturity products is not recommended and highly discouraged.

**Provisional:** product performance has been demonstrated through a large, but still (seasonally or otherwise) limited number of independent measurements. The analysis is sufficient for limited qualitative determinations of product fitness-for-purpose, and the product is potentially ready for testing by operational users and may be suitable for scientific publication.

**Full:** product performance has been demonstrated over a large and wide range of representative conditions, with comprehensive documentation of product performance, including known anomalies and their remediation strategies. Products are ready for systematic use and covering the full range of scientific and application use and publication.

# Product Specific Performance Indicators (PSPIs)

## L2 Geophysical Data
## Beta Maturity Level -Product Specific Performance Indicators

| $NO_2$ | $CH_2O$ | $O_3$ |
|---|---|---|
| **$NO_2$-01**: Distinguish high $NO_2$ urban areas from nearby rural areas for three select urban-rural scene combinations.<br>**$NO_2$-02**: Assess bias and precision for at least one month of retrievals in comparison to independent correlative measurements to convey an initial characterization to the user community. The assessment should evaluate TEMPO's capability to observe diurnal variations.<br>**$NO_2$-03**: Identify two radiatively homogenous, cloud-clear, low tropospheric $NO_2$ background scenes over a dark surface (e.g., water) and over a bright surface (e.g., snow, desert) under different solar zenith angles and compute point-to-point variability (1-σ) as an empirical estimate for fitting uncertainty. Compare and communicate empirical estimates with those derived from the spectral fitting process. | **$CH_2O$-01**: Distinguish high $CH_2O$ concentrations from background concentrations. Given $CH_2O$ retrieval noise levels, these qualitative evaluations may use spatial or temporal averaging.<br>**$CH_2O$-02**: Assess bias for at least one month of retrievals, including the diurnal cycle, of comparison to independent correlative measurements to convey an initial characterization to the user community. The assessment should evaluate TEMPO's capability to observe diurnal variations.<br>**$CH_2O$ -03**: Identify two radiatively homogenous, cloud-clear, low $CH_2O$ scenes over a dark (e.g., water) and over a bright surface (e.g., snow, desert) under different solar zenith angles and compute point-to-point variability (1-σ) as an empirical estimate for fitting uncertainty. Compare and communicate empirical estimates with those derived from the spectral fitting process. | **$O_3$-01:** Distinguish high tropospheric $O_3$ areas resulting from stratospheric intrusion or pollution transport or pollution from nearby normal or low $O_3$ areas for three select high-low O3 scene combinations.<br>**$O_3$-02**: Assess bias and precision for at least one month of retrievals in comparison to independent correlative measurements to convey an initial characterization to the user community. The assessment should evaluate TEMPO's capability to observe diurnal variations.<br>**$O_3$-03**: Identify two homogenous, cloud-clear, normal tropospheric $O_3$ background scenes over a dark (e.g., water) and over a bright surface (e.g., snow, desert) under different solar zenith angles and compute point-to-point variability (1-σ) as an empirical estimate for retrieval uncertainty. Compare and communicate empirical estimates with those derived from the spectral fitting process. |

# Product Specific Performance Indicators (PSPIs)

| L2 Geophysical Data<br>Provisional Maturity Level -Product Specific Performance Indicators | | |
|---|---|---|
| $NO_2$ | $CH_2O$ | $O_3$ |
| **$NO_2$-04**: Assess performance metrics (bias/precision/uncertainty) of the tropospheric $NO_2$ product across the CONUS for 1 month period in two seasons, preferably summer and winter, that includes a range of column densities.<br>**$NO_2$-05**: Conduct deep-dive analyses for an episode with relatively poor product performance, identify the root cause and recommend algorithm improvements. | **$CH_2O$-04**: Assess performance metrics (bias/precision/uncertainty) of $CH_2O$ product across the CONUS for 1 month period in two seasons, preferably winter and summer, including a range of column densities. This assessment must evaluate the capability of TEMPO to observe diurnal variations of $CH_2O$.<br>**$CH_2O$-05:** Conduct deep-dive analyses for an episode with relatively poor product performance, identify the root cause of the discrepancy and recommend algorithm improvements. | **$O_3$-04:** Assess performance metrics (bias/precision/uncertainty) of $O_3$ products across the CONUS for 1 month period in two seasons, preferably winter and summer, that includes a range of column densities. This assessment must evaluate the capability of TEMPO to observe diurnal variations of O3 products.<br>**$O_3$-05:** Conduct deep-dive analyses for several episodes with relatively poor product performance, identify the root cause of the discrepancy and recommend algorithm improvements. |

# Product Specific Performance Indicators (PSPIs)

| L2 Geophysical Data<br>Full Maturity Level -Product Specific Performance Indicators | | |
|---|---|---|
| $NO_2$ | $CH_2O$ | $O_3$ |
| **$NO_2$-06**: Assess bias, precision, and uncertainty of the tropospheric NO2 product across the CONUS for a wide range of representative conditions over a period of at least one year.<br>**$NO_2$-07**: Assess bias, precision, and uncertainty of the tropospheric NO2 product over areas of interest using data gathered during targeted field campaigns. | **$CH_2O$-06**: Assess bias, precision, and uncertainty of the $CH_2O$ product across the CONUS for a wide range of representative conditions over a period of at least one year.<br>**$CH_2O$-07**: Assess bias, precision, and uncertainty of the $CH_2O$ product over areas of interest using data gathered during targeted field campaigns. | **$O_3$-06**: Assess bias, precision, and uncertainty of the $O_3$ product across the CONUS for a wide range of representative conditions over a period of at least one year.<br>**$O_3$-07:** Assess bias, precision, and uncertainty of the tropospheric product over areas of interest using data gathered during targeted field campaigns. |

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Michel Grutter Chris McLinden*

**virtual*


# AEROMMA: Atmospheric Emissions and Reactivity Observed from Megacities to Marine Areas

## Principal Investigators

### Urban Flights

Rebecca Schwantes

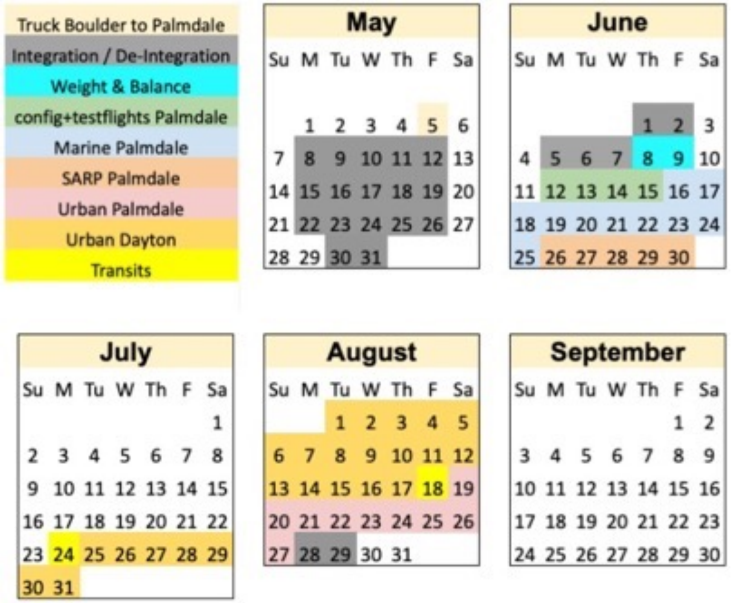
Carsten Warneke

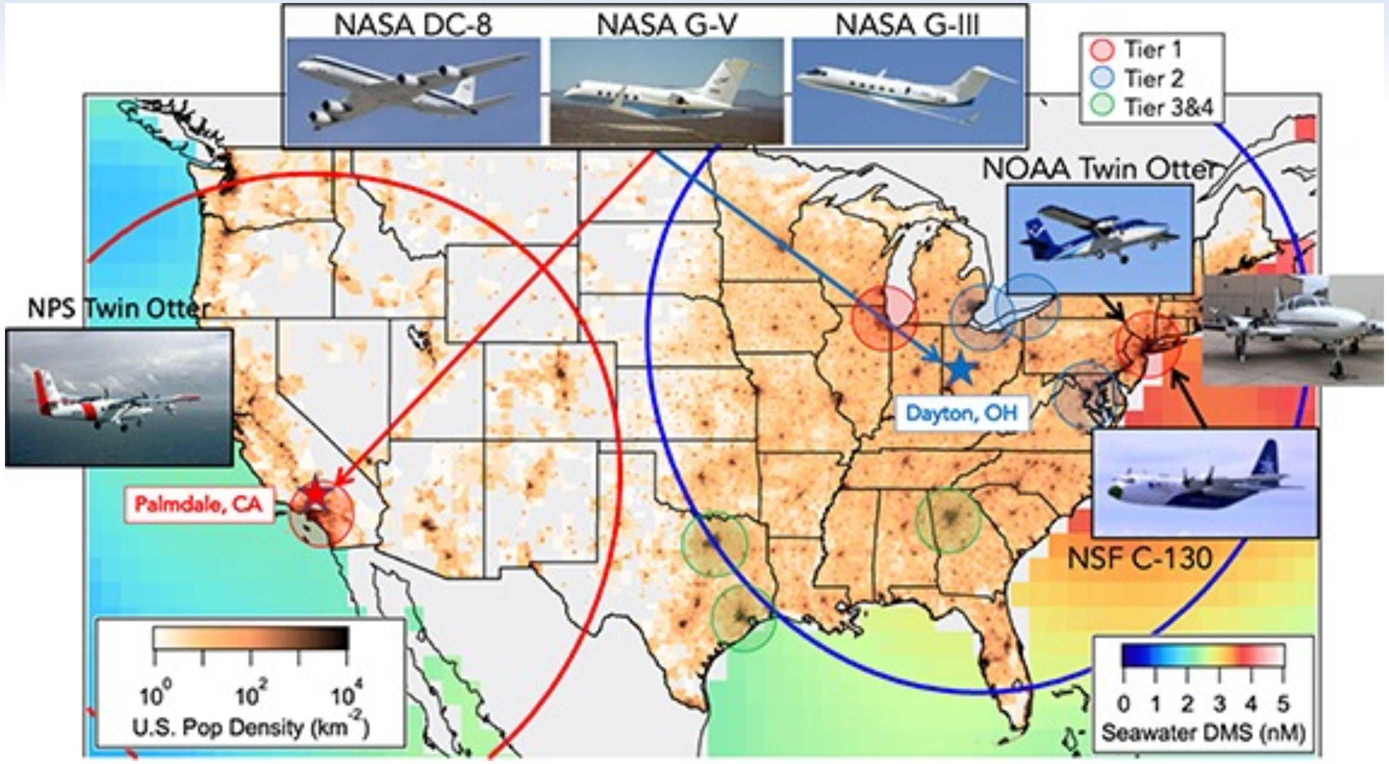
### Marine Flights

Patrick Veres

Andrew Rollins

## DC-8 Schedule



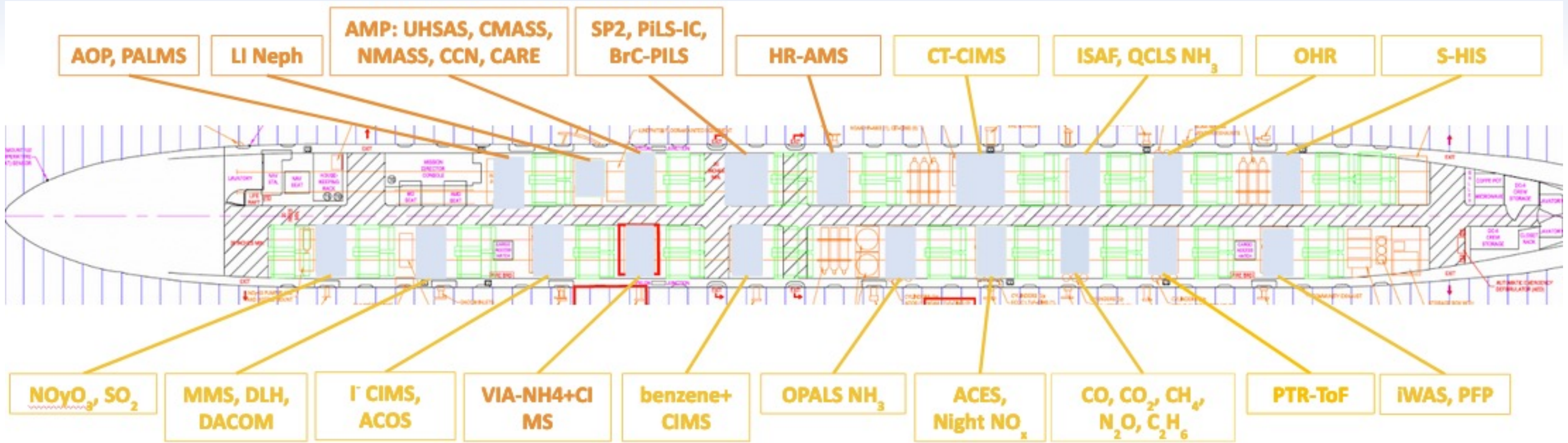

Marine Flights, Palmdale CA, June 16-25
- Remote marine atmosphere, sulfur cycle and feedbacks on climate

Urban Flights, Palmdale CA (Jun 26-30; Aug 19-27), Dayton OH (Jul 25-Aug17)
- New paradigms in emissions and the future of urban air quality
- Validation and new science with geostationary remote sensing

NOAA Chemical Sciences Laboratory Deployment on NASA DC-8 Supported by NESDIS through GeoXO Program

# AEROMMA: Atmospheric Emissions and Reactivity Observed from Megacities to Marine Areas

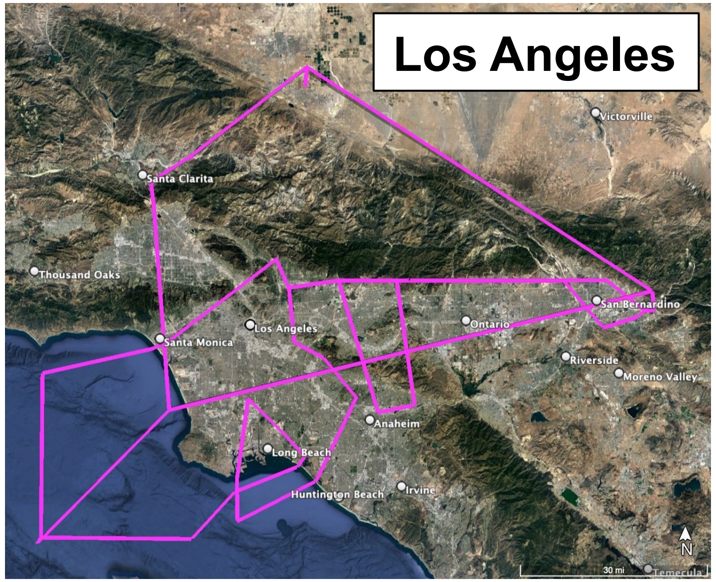
## NASA DC-8 Instrumentation

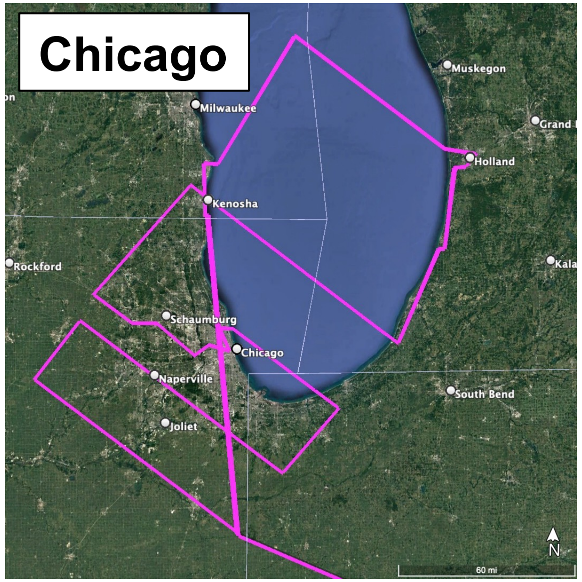


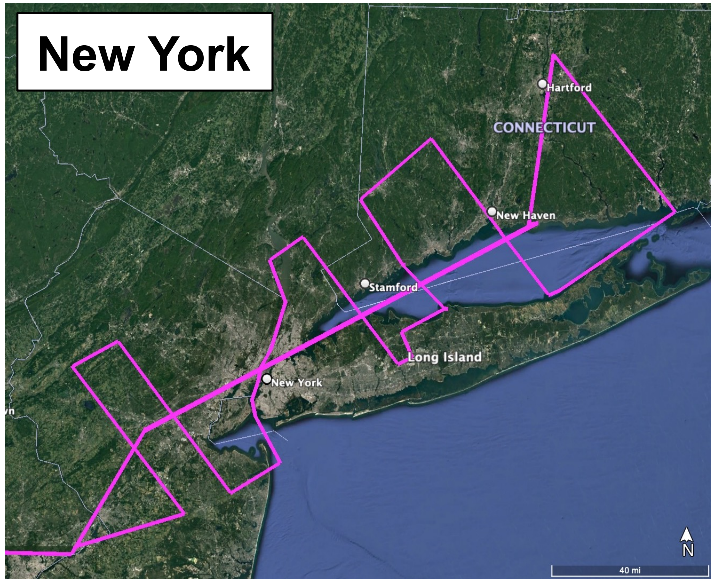

Comprehensive suite for VOCs, $NO_x$, GHG, aerosols (composition, size, optics), radiation, remote sensing, etc.

Instruments from NOAA CSL, NASA, external collaborators (NOAA AC4)

## Urban Flight Plans – Los Angeles, Chicago, New York




Repeated flight patters over each major target city

Boundary layer legs < 1 km AGL

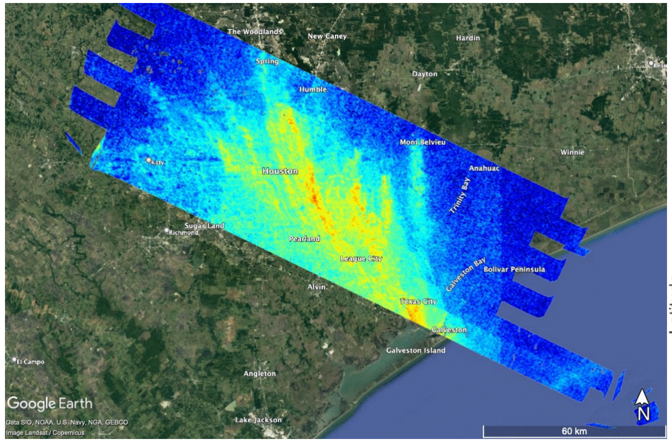
3-7 spirals per flight leg to ~ 6 km

Transits at 10-11 km

# Synergistic TEMPO Air Quality Science (STAQS)

**In Summer 2023, STAQS seeks to integrate TEMPO observations with traditional and enhanced air quality monitoring to improve the understanding of air quality science for increased societal benefit.**

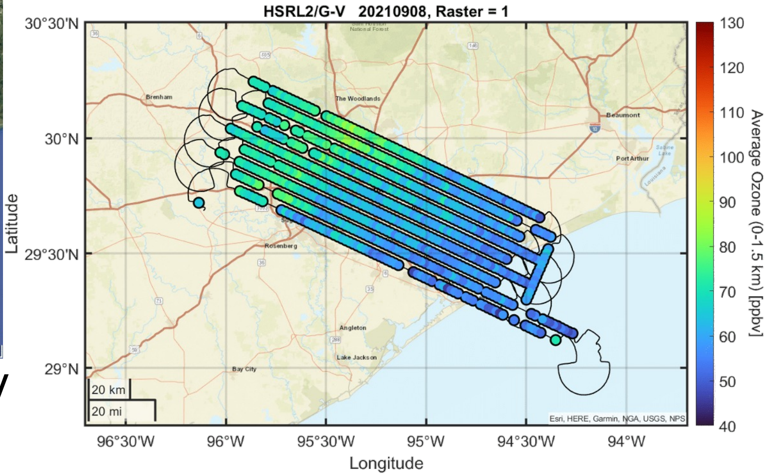



Aiming for ~4 flight days in each city (+1 Toronto flight)

Laura Judd
airborne lead

John Sullivan
ground lead



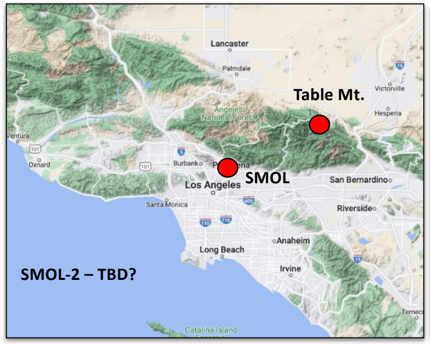

| Platform | Instrument | Data Products | Sampling Strategy |
|---|---|---|---|
| NASA JSC G-V | GCAS | $NO_2$ Column (250 x 560 m)<br>HCHO Column (750 x 1680 m) | Systematic sampling of a ~ 50 x 140 km area 3x per day (morning-midday-afternoon) |
| | HSRL2/DIAL | Ozone profiles, aerosol profiles, mixed layer height | |
| NASA LaRC G-III | AVIRIS-NG | $CH_4$ (> 10 kg/hr) and $CO_2$ (large point sources) emissions | Systematic sampling of a ~ 50 x 140 km area 2x per day (morning-afternoon) |
| | HALO | $CH_4$ columns, aerosol profiles, mixed layer height | |

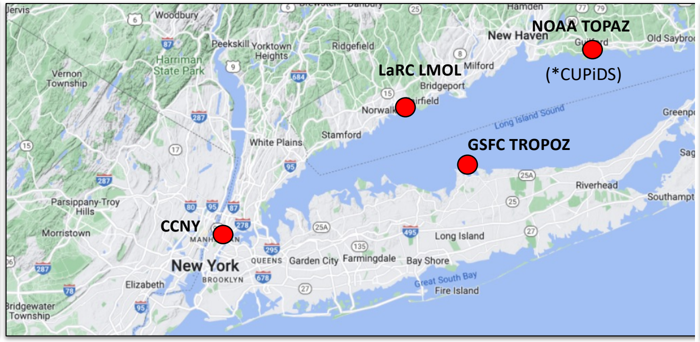
# Synergistic TEMPO Air Quality Science (STAQS)

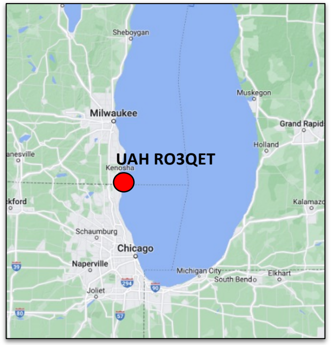
**In Summer 2023, STAQS seeks to integrate TEMPO observations with traditional and enhanced air quality monitoring to improve the understanding of air quality science for increased societal benefit.**

Laura Judd
airborne lead

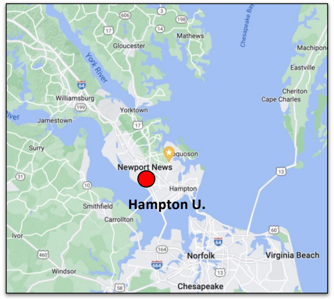
John Sullivan
ground lead

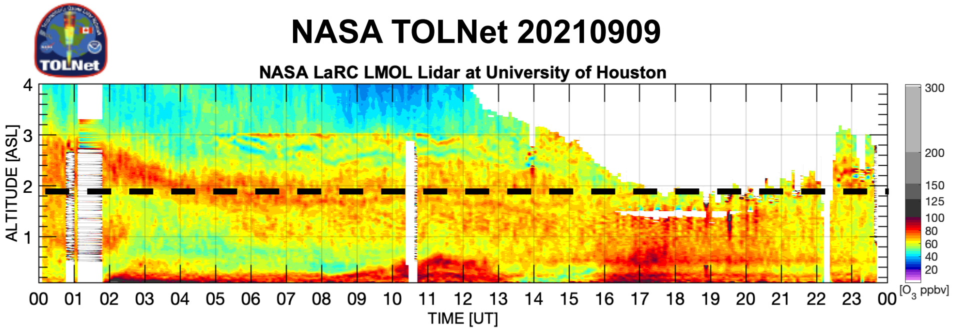






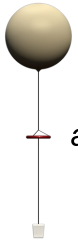




66+ in TEMPO FOR

*2 in Chicago*

*2 in LA*

*13 in NYC/Philly/CT*



*Ozonesondes will also be available in some locations*

| Platform | Instrument | Data Products | Sampling Strategy |
|---|---|---|---|
| Ground-based | TOLNet | Lower tropospheric ozone profiles | Routine sampling with enhanced measurements during flight days within the domain |
| | Pandora | $NO_2$ and HCHO columns and profiles | |

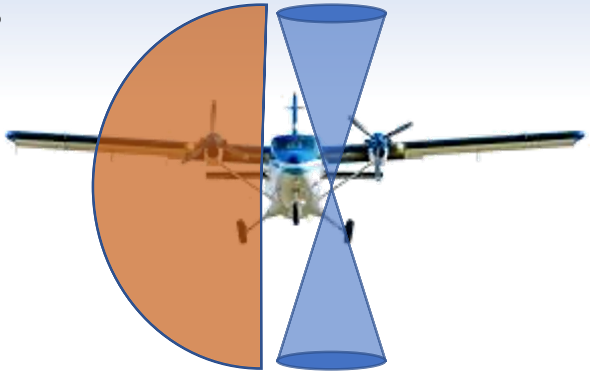
# CUPiDS: Coastal Urban Plume Dynamics Study

## Principal Investigators


Sunil Baidar


Alan Brewer

NOAA Twin Otter

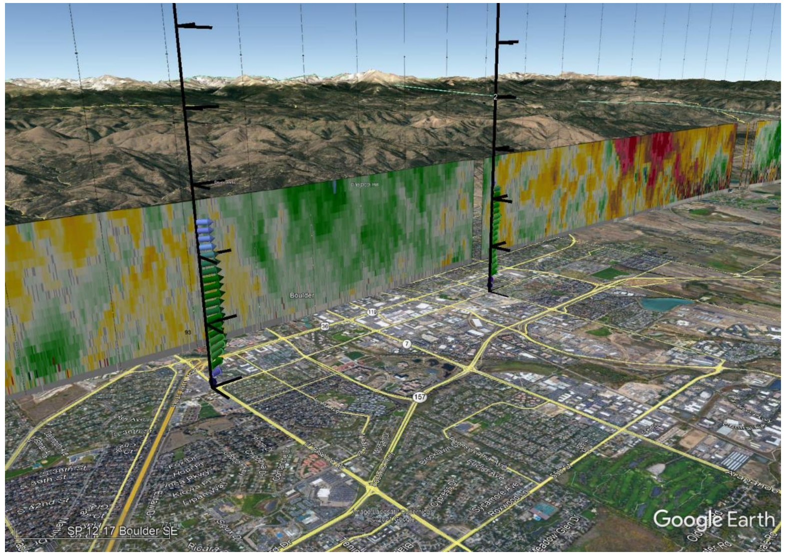


July 5 – August 15, 2023, Long Island MacArthur Airport, 175 total flight hours

Emissions and chemistry within complex coastal transport environment

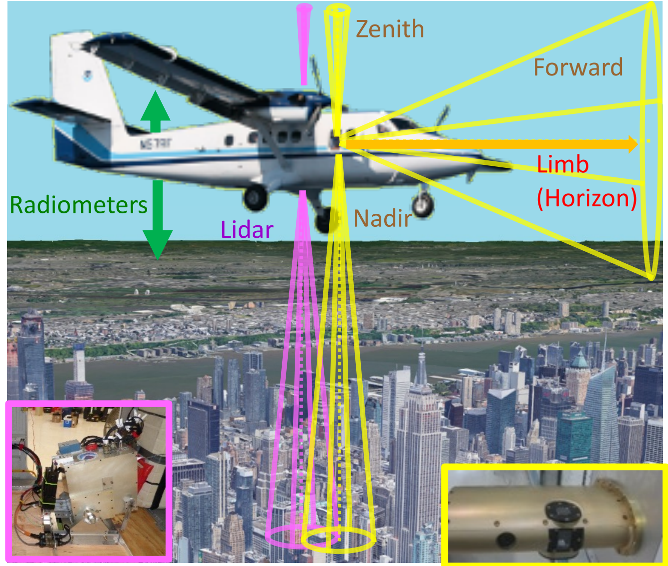
### Scanning Doppler Lidar (CSL)

- Wind, Turbulence and Aerosol profiles
- Boundary Layer Depth



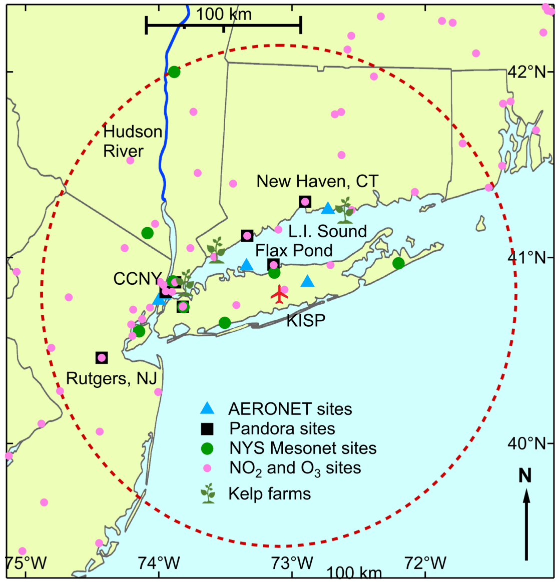

### MAX-DOAS (CU – AC4 supported)

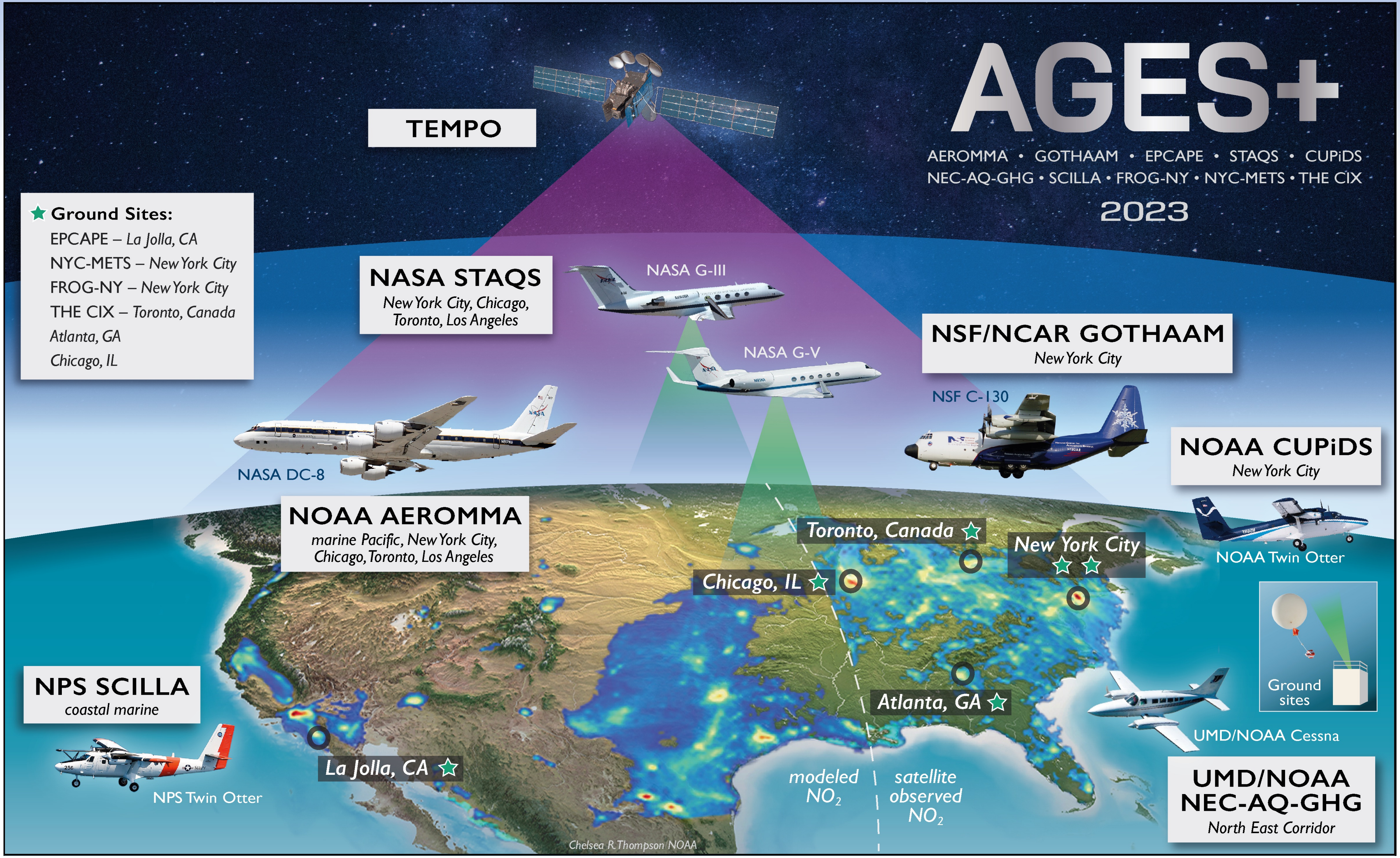
- $NO_2$, Formaldehyde, Glyoxal, IO profiles
- Surface albedo




### In-Situ Airborne (CSL,GML)

- GHG, NO2, NO, NOY, ozone
- Temp, Press, RH






https://csl.noaa.gov/projects/ages/

Image Credit: Chelsea Thompson/NOAA

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# Ground based Networks


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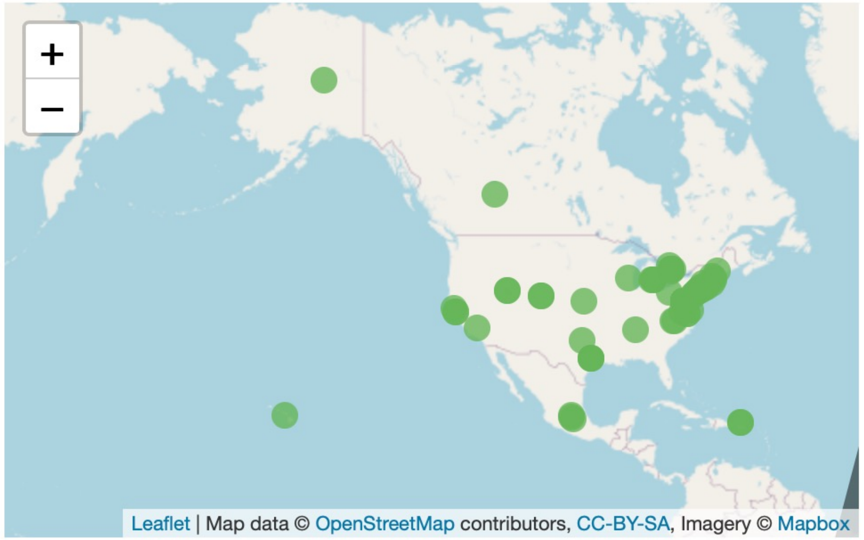
Steve Brown, Laura Judd

Ron Cohen, Tom Hanisco, Pawan Gupta

Michel Grutter Chris McLinden*

*virtual

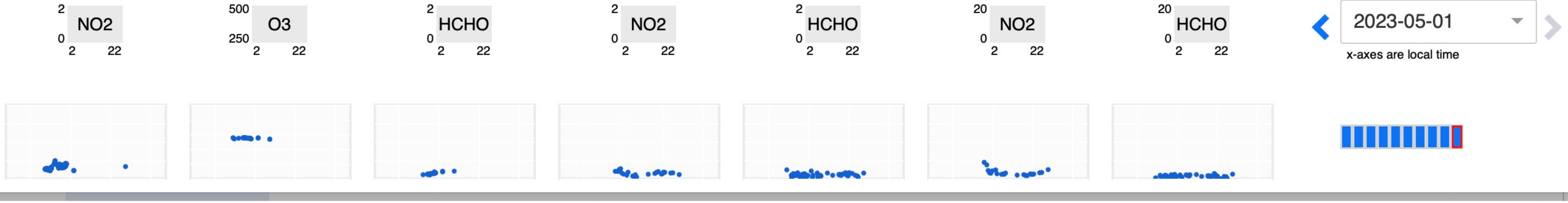

### Stations

GreenbeltMD - 2
LabGSFC - 17
Busan - 20
Bremen - 21
HoustonTX - 25
CambridgeMA - 26
LabGSFC - 27
Fajardo - 29
Juelich - 30
CharlesCityVA - 31
GreenbeltMD - 32
MountainViewCA - 34
Dakar - 36
HamptonVA - 37
BayonneNJ - 38
DearbornMI - 39
WallopsIslandVA - 40
HoustonTX - 49
OldFieldNY - 51
RichmondCA - 52
Potchefstroom-METSI - 53
Seoul - 54
QueensNY - 55
MaunaLoaHI - 56
BoulderCO - 57
GreenbeltMD - 58
GreenbeltMD - 59
Fajardo - 60
AldineTX - 61
LabSciGlob - 63
NewHavenCT - 64
Altzomoni - 65
HuntsvilleAL - 66
Cologne - 67
LabSciGlob - 68
NewBrunswickNJ - 69
ChapelHillNC - 70
SaltLakeCityUT-Hawthorne - 72
Islamabad-NUST - 73
EdwardsCA - 74
Dhaka - 76
ColumbiaMD - 101
LabGSFC - 103
Downsview - 104
Helsinki - 105
Innsbruck - 106
Toronto-West - 108
StGeorge - 109
LabLuftBlick - 110
Bucharest - 111
Broadmeadows - 112
LabGSFC - 114
Rome-ISAC - 115
Rome-SAP - 117
Cabauw - 118
Athens-NOA - 119
Innsbruck-FKS - 120
Downsview - 122
StonyPlain - 123
ComodoroRivadavia - 124
BuenosAiresSMN - 125
ColumbiaMD - 127
GreenbeltMD - 128
LabSciGlob - 129
Lindenberg - 130
Berlin - 132
BristolPA - 134
ManhattanNY-CCNY - 135
Rome-IIA - 138
WashingtonDC - 140
MexicoCity-UNAM - 142
LabSciGlob - 143
Eureka-PEARL - 144
Toronto-Scarborough - 145
Yokosuka - 146
SWDetroitMI - 147
Seoul-SNU - 149
Ulsan - 150
NyAlesund - 152
LynnMA - 153
SaltLakeCityUT - 154
HamptonVA-HU - 156
MexicoCity-Vallejo - 157
Wakkerstroom - 159
Beijing - 160
Xianghe - 161
ColumbiaMD - 162
Tsukuba-NIES-West - 163
Seosan - 164
Durham - 165
PhiladelphiaPA - 166
KenoshaWI - 167
Egbert - 169
Downsview - 170
Beijing-RADI - 171
FairbanksAK - 174
Tsukuba-NIES - 176
WestportCT - 177
ManhattanKS - 178
CornwallCT - 179
BronxNY - 180
SanJoseCA - 181
Tel-Aviv - 182
LondonderryNH - 183
CapeElizabethME - 184
EastProvidenceRI - 185
MadisonCT - 186
PittsburghPA - 187
Bangkok - 190
Tsukuba - 193
Sapporo - 196
Kobe - 198
BoulderCO-NCAR - 204
ArlingtonTX - 207
Windsor-West - 208
Izana - 209
Dalanzadgad - 217
Thessaloniki - 240

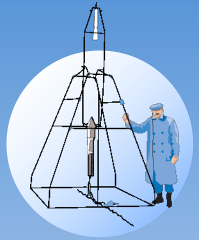
66+ instruments in TEMPO FOV
Adding 13+ in 2023 (IPMSI)
Adding 10+ in 2024 (SNWG USDA)

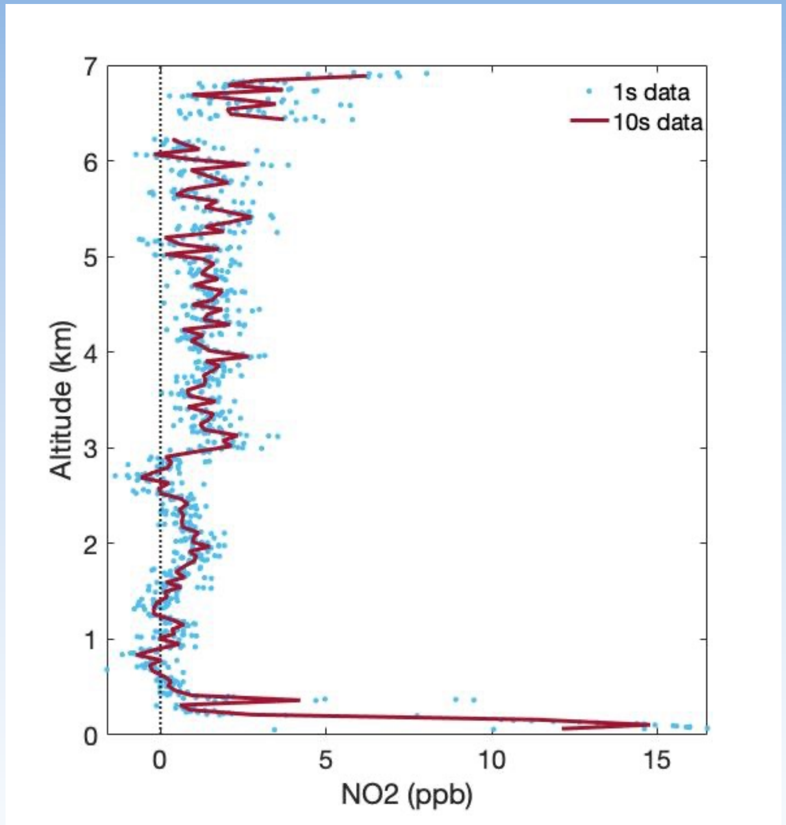
NEW "Out of the Box" data

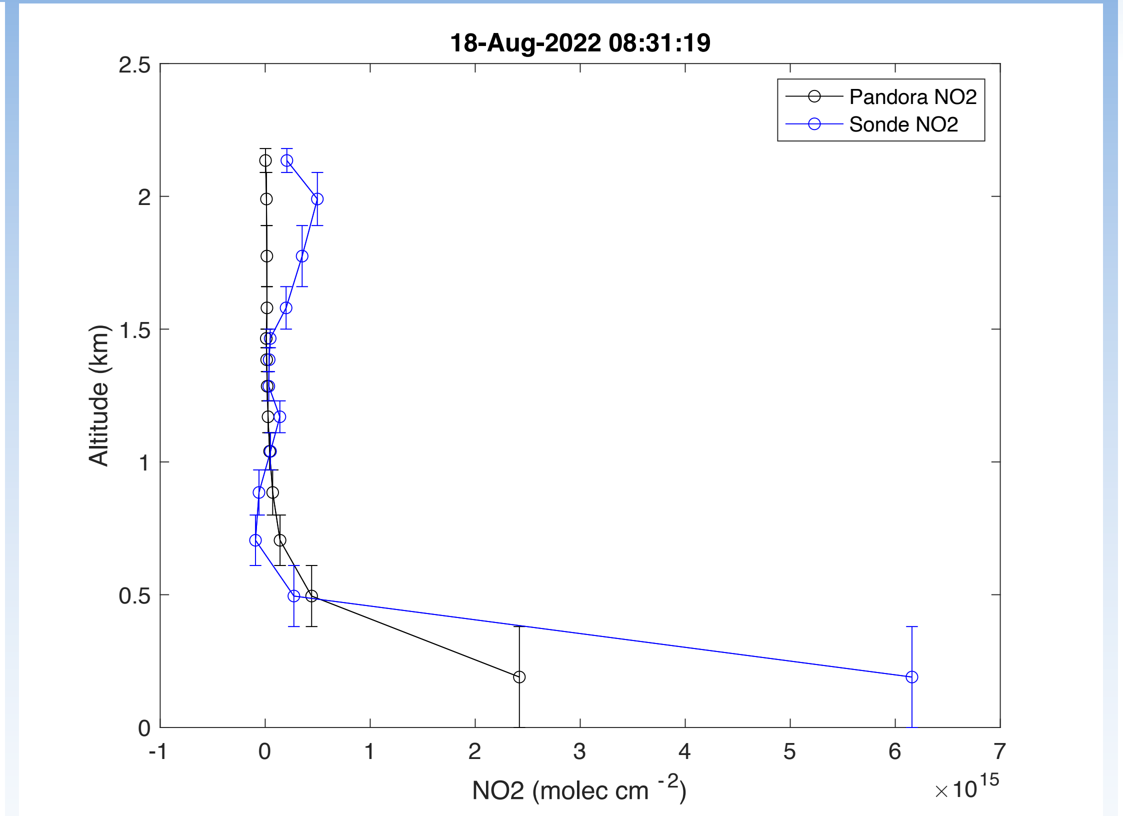
Total Column (DU) Trop Column (DU) Surface Concentration (ppb)



# $NO_2$ Sonde Instrument

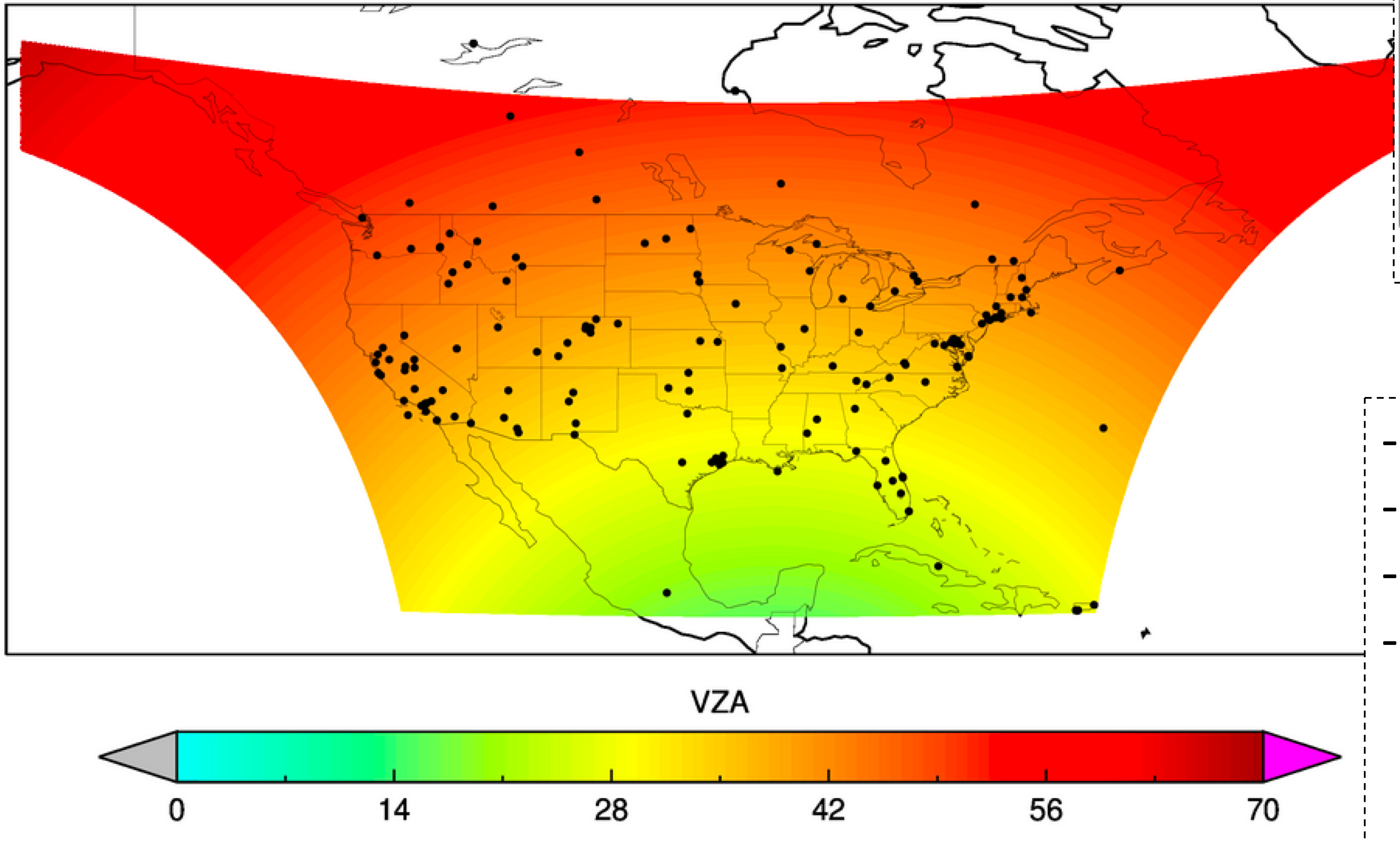


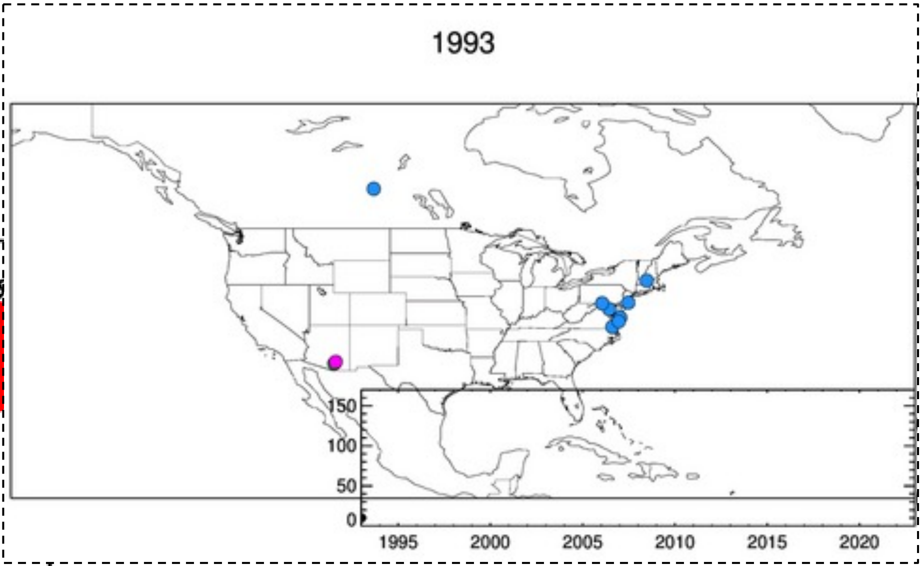



New optical NO2 sonde instrument (<5lbs) can help validate/understand Pandora $NO_2$ profiles. Howard University, Beltsville MD

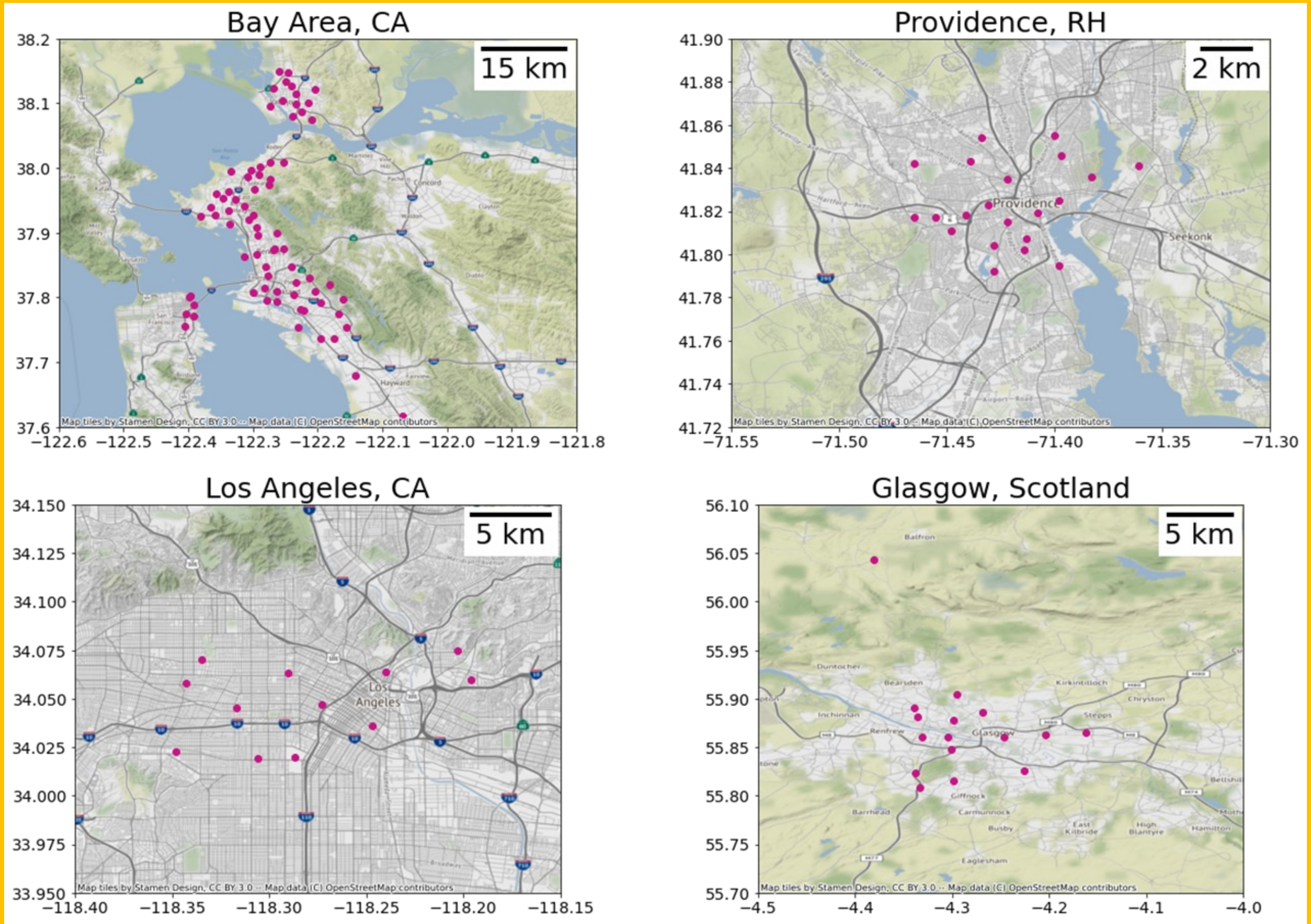
# AERONET for TEMPO




- ~160 active sites in 2022
- ~140 in US covering 37 states
- ~10 MSI sites coming up
- Multiple sites to support upcoming field campaigns (STAQS, MAGPI, SARP-East, AEROMMA, GOTHAAM)

# One example of other activities BEACO$_2$N in 3 U.S. urban centers. Many other "low cost" sensor networks are being deployed.




**NO$_2$, O$_3$, PM2.5**

**Also CO$_2$, NO, CO**

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# International Partner Activites


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Michel Grutter, Chris McLinden*

*virtual


# Validation capacities in Mexico

EM27/Sun | Pandora | FTIR Solar absorption spectrometers

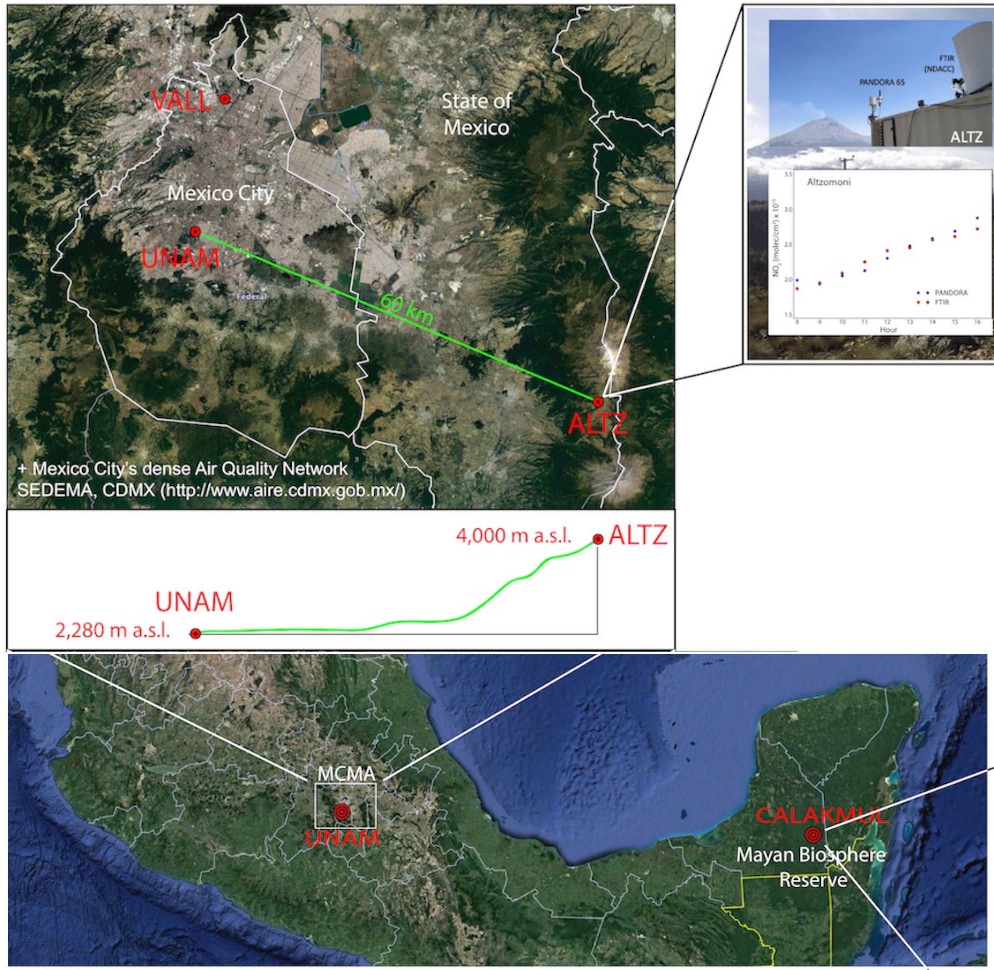
VALLEJO

UNAM

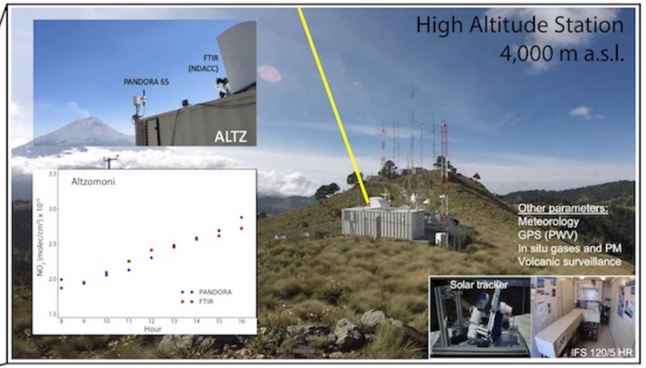
ALTZOMONI

CALAKMUL


Mexico City Metropolitan Area (MCMA)




Altzomoni Atmospheric Observatory (>2012)



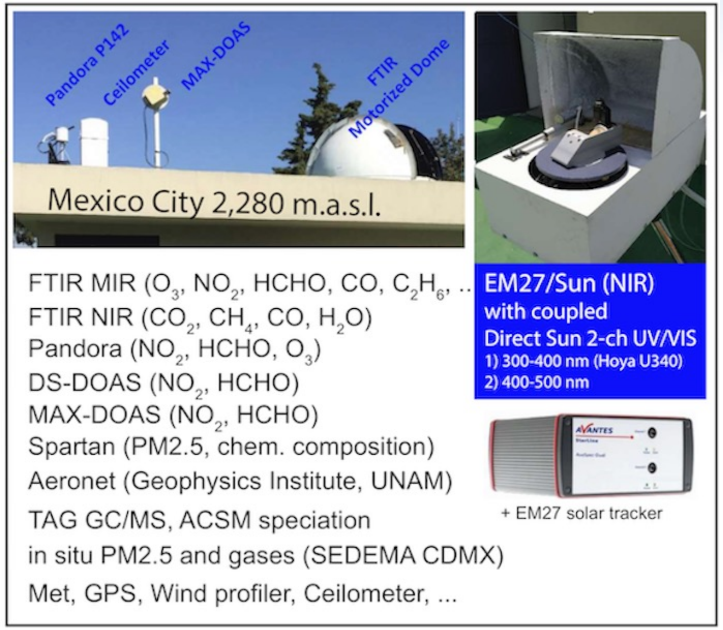

11 years of operation

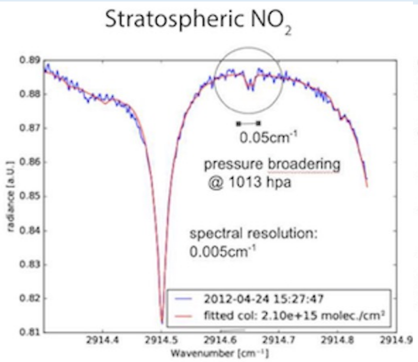
Starting > 2023

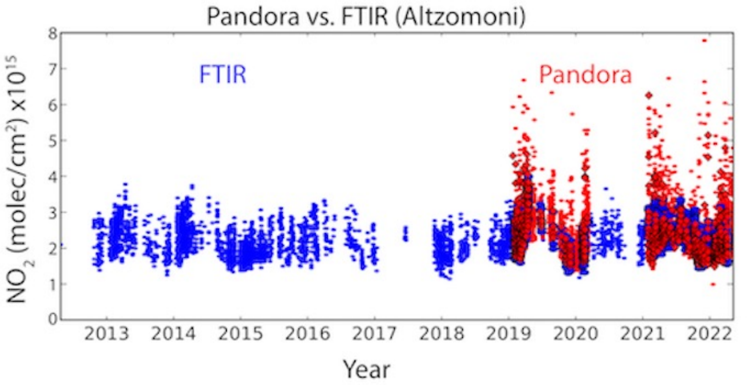
Calakmul Atmospheric Observatory (>2023)

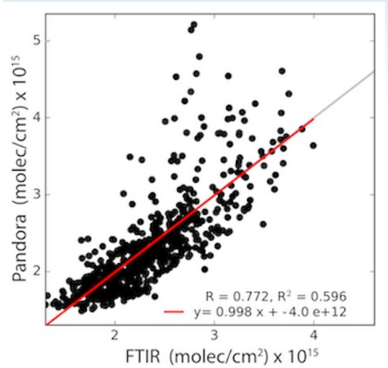
# Validation capacities in Mexico

The UNAM Atmospheric Obsertvatory

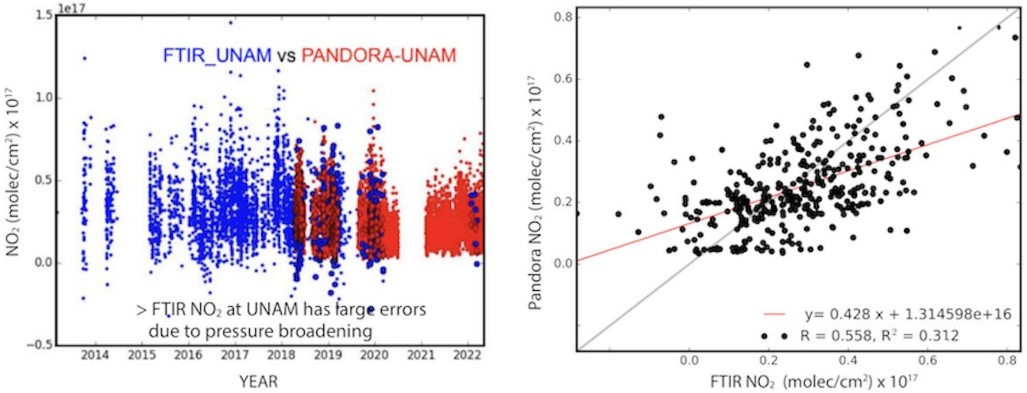


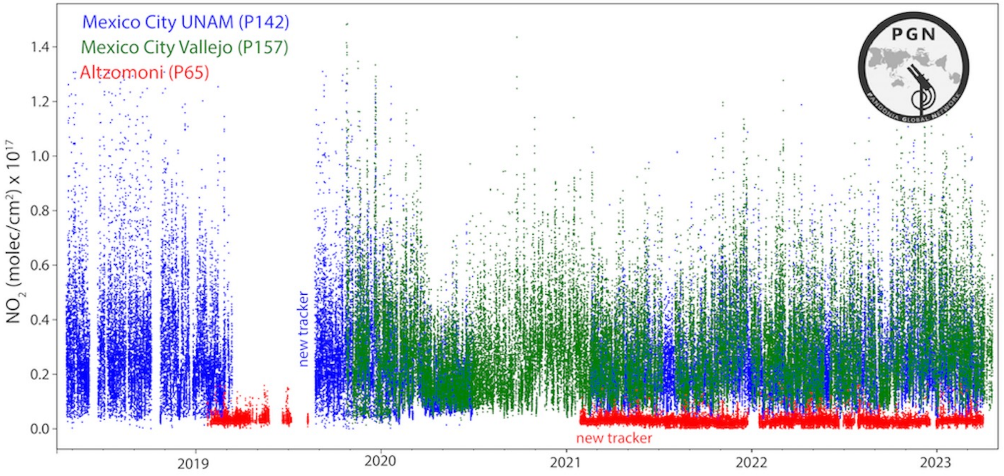



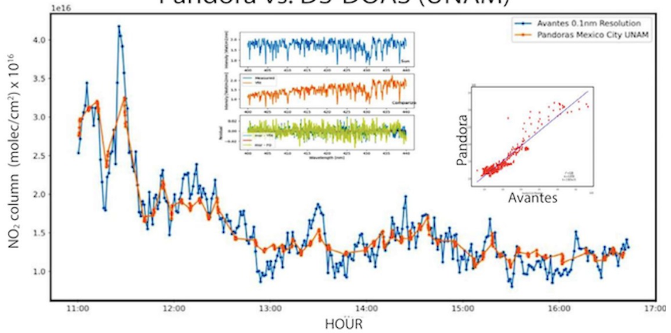

Pandora vs. FTIR (UNAM)




Pandora data




Pandora vs. DS-DOAS (UNAM)




Combining
IR and UV/Vis
Instruments

# Key messages

- Importance of longtime measurements with ground-based remote sensors through international network efforts
- Validation (high spatial resolution), trend and variability of atmospheric composition
- Proper treatment of sensitivites among different RS techniques
- Joint air pollution and GHG investigations
- Other species: CO, $NH_3$, $CH_4$, HCN, $C_2H_6$ …
- Importance to measure boundary layer evolution also from the ground (Doppler Lidar, Ceilometer)

Building the Pathway from TEMPO to GeoXO

Joint Science Meeting for TEMPO, GeoXO ACX, & TOLNet

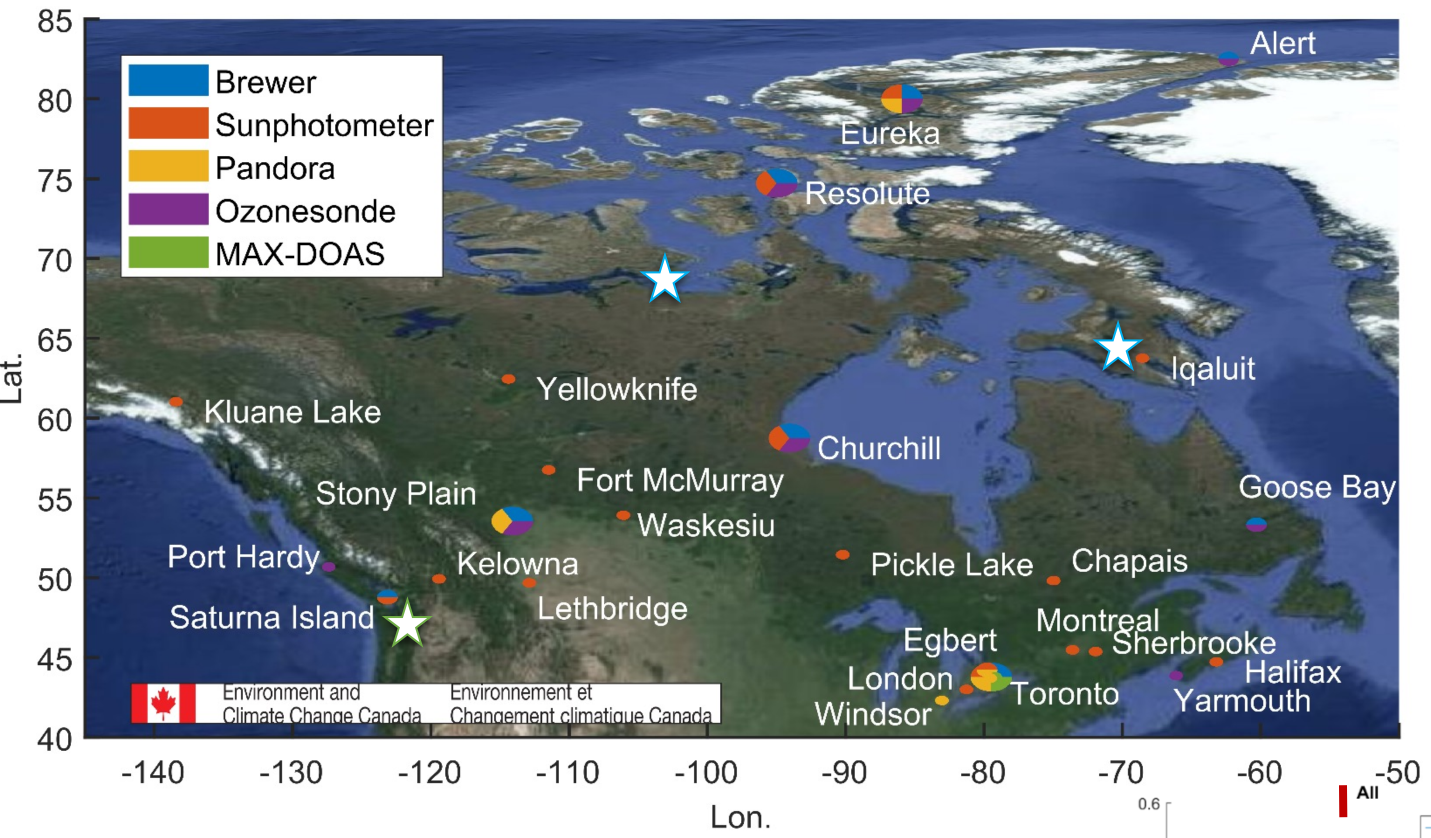
# Validation Activities at ECCC

Chris McLinden and collaborators

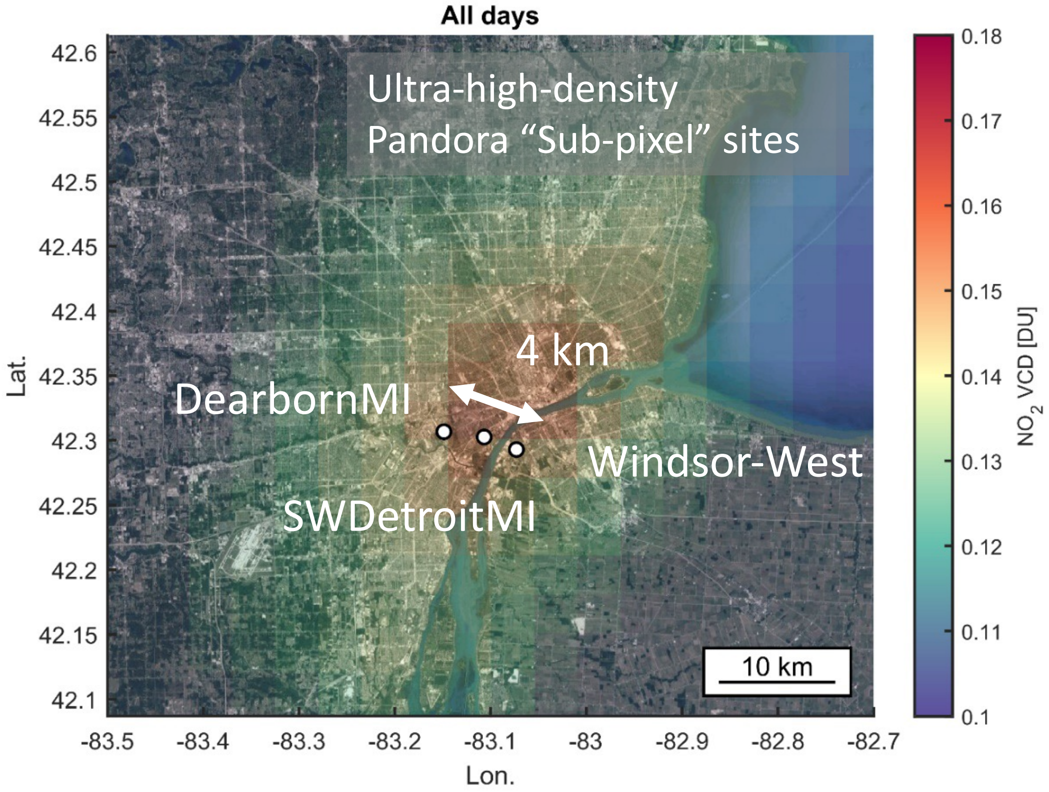
Environment and Climate Change Canada

Environnement et Changement climatique Canada

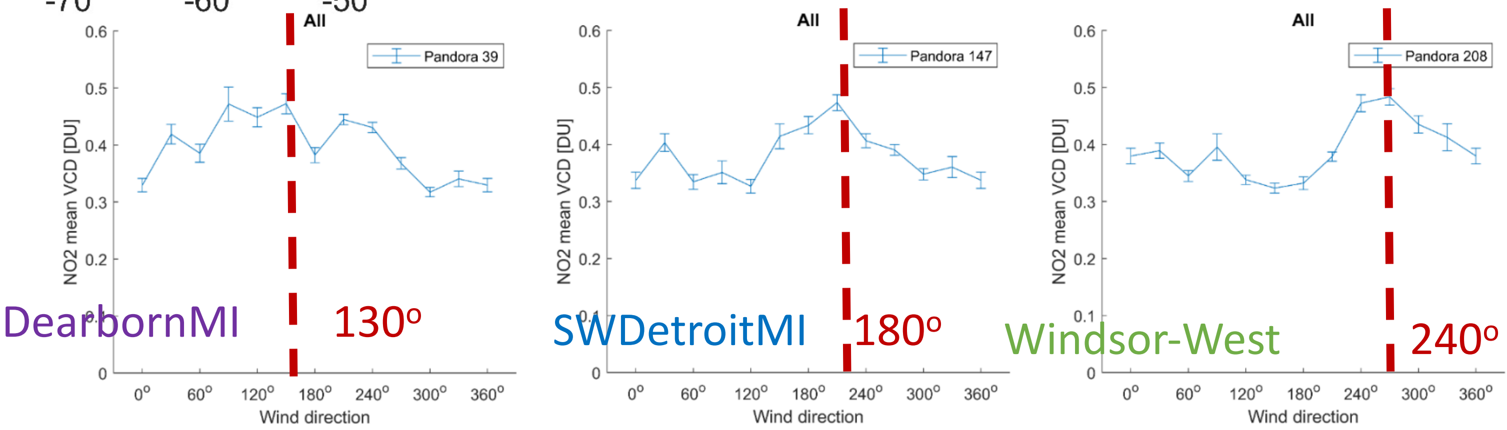
**Planned sites:**
- ❑ ECCC future site
- ❑ In collaboration with UofT



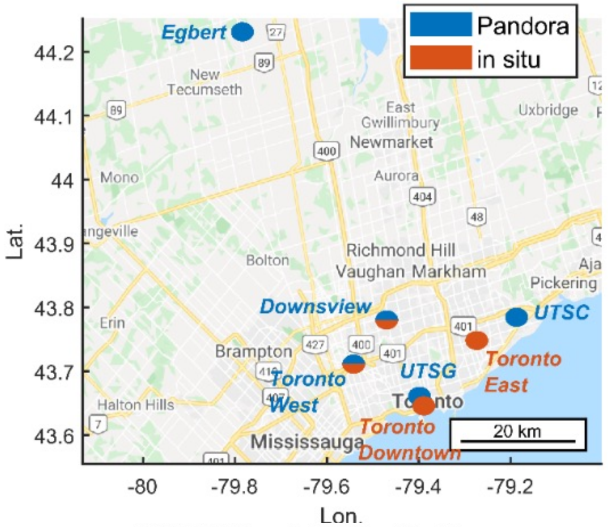

- ECCC Remote Sensing Sites

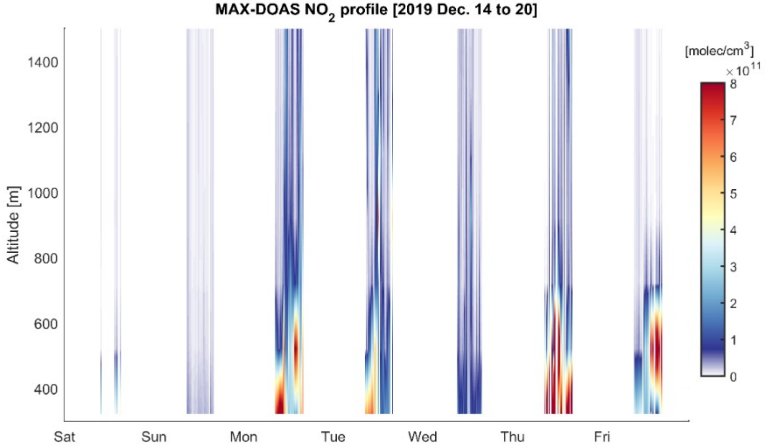



- ECCC, NASA, and US-EPA Pandora sites in Detroit-Windsor region

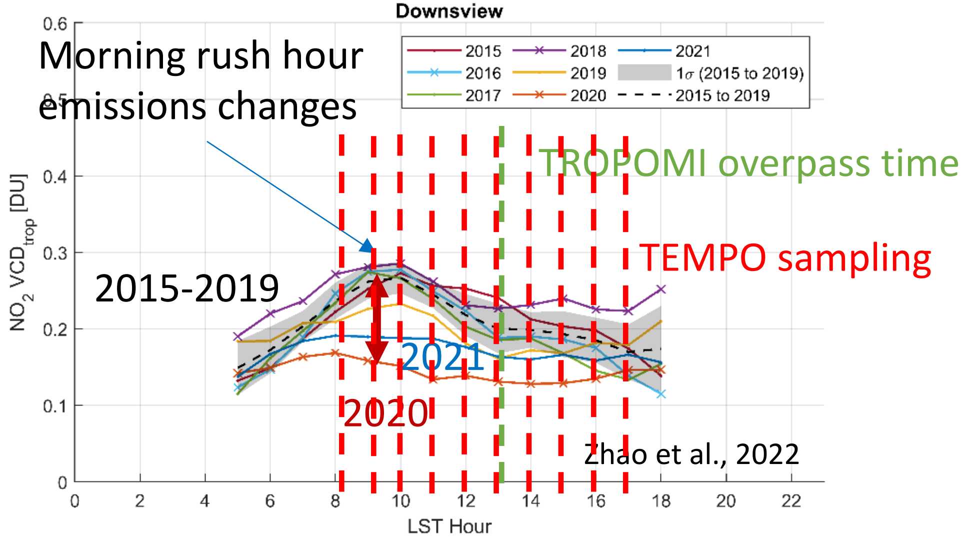


# Air quality monitoring in GTA

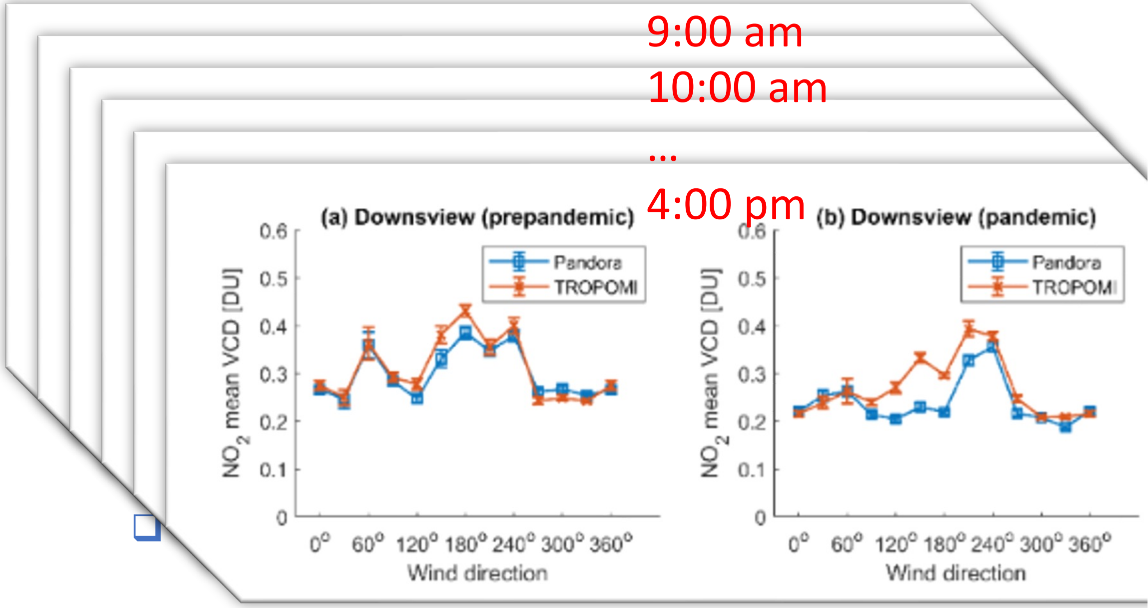




- CN Tower: New vertical profiling experimental site




- Temporal changes; data binned by LST hours

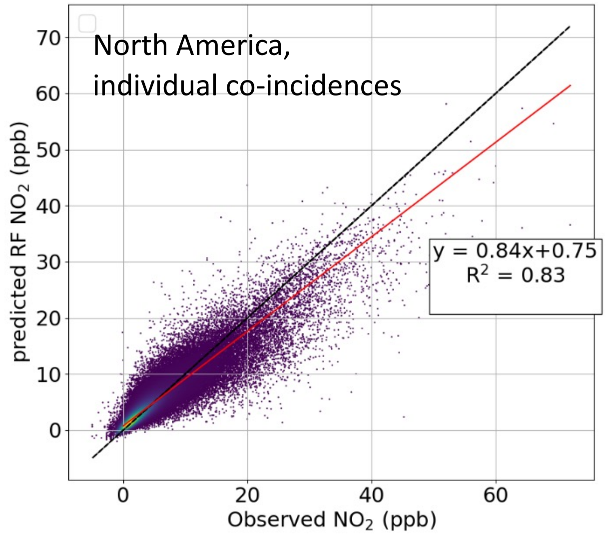



- The NO$_2$ changes are inhomogeneous in space and time
- TEMPO observations are needed to reveal such diurnal changes

# Other Validation Activities

- Calculate alternative AMFs for $NO_2$ and HCHO
  - Based on ECCC 2.5 km or 250 m model profiles; treatment of snow/albedo
  - U of Saskatchewan group has alternative 2D AMF to help with large viewing angles
- SWAPIT campaign (2024), others tbd
- Ongoing paired surface-HCHO + Pandora observations
- Evaluate TEMPO-based surface NO2 vmr product (developed using TROPOMI) from machine learning methods
- Evaluation of TEMPO's ability to capture spatial and diurnal gradients using in-situ and remote ground-based networks; mobile MAX-DOAS

Early prototype:
Surface NO2 using TROPOMI VCD & Machine learning



# Panel Questions

a) How will each of the correlative instruments assess the precision and accuracy of the TEMPO metrics?

| Product Name | Product Horizontal Resolution N/S x E/W @ center of FOR | Product Precision | Frequency |
|---|---|---|---|
| Total Column $O_3$ | 2.0 x 4.75 $km^2$ | 3% | 1 hour |
| Tropospheric Column $O_3$ | 8.0 x 4.75 $km^2$ (4 N/S across-track pixels coadded) | 10 ppbv | 1 hour |
| 0-2 km $O_3$ selected scenes | 8.0 x 4.75 $km^2$ (4 N/S across-track pixels coadded) | 10 ppbv | 2 hours |
| Total Column $NO_2$ | 2.0 x 4.75 $km^2$ | $1.0 \times 10^{15}$ molecules $cm^{-2}$ | 1 hour |
| Tropospheric Column $NO_2$ | 2.0 x 4.75 $km^2$ | $1.0 \times 10^{15}$ molecules $cm^{-2}$ | 1 hour |
| Tropospheric column $CH_2O$ | 2.0 x 4.75 $km^2$ | $1.0 \times 10^{16}$ molecules $cm^{-2}$ | 3 hours |

b) Utility of "At Home" Validation vs. Field Observations

- What is best for validation?– this summer acts as continued avenue for joint multi-agency field campaigns

c) What are the plans/ideas for for activities in 2024 and 2025?

- How can we leverage Green Paper efforts as a sounding board for next validation campaign?