EPA United States Environmental Protection Agency

Moving towards routine and systematic validation of Tropospheric Emissions: Monitoring of Pollution (TEMPO) Level 2 Data Products

18 October 2023

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U.S. EPA Office of Research and Development

w/ contributions from others, including Kelly Chance ,Xiong Liu, Caroline Nowlan, and Gonzalo Gonzalez Abad, CfA-Haravard-Smithsonian, Alexander Cede & Martin Tiefengraber, Luftblick, Mike Newchurch (UAH), Ron Cohen (UCB), Laura Judd (NASA-LaRC), Tom Hanisco, John Sullivan, & Nader Abuhassan (NASA-GSFC), etc.

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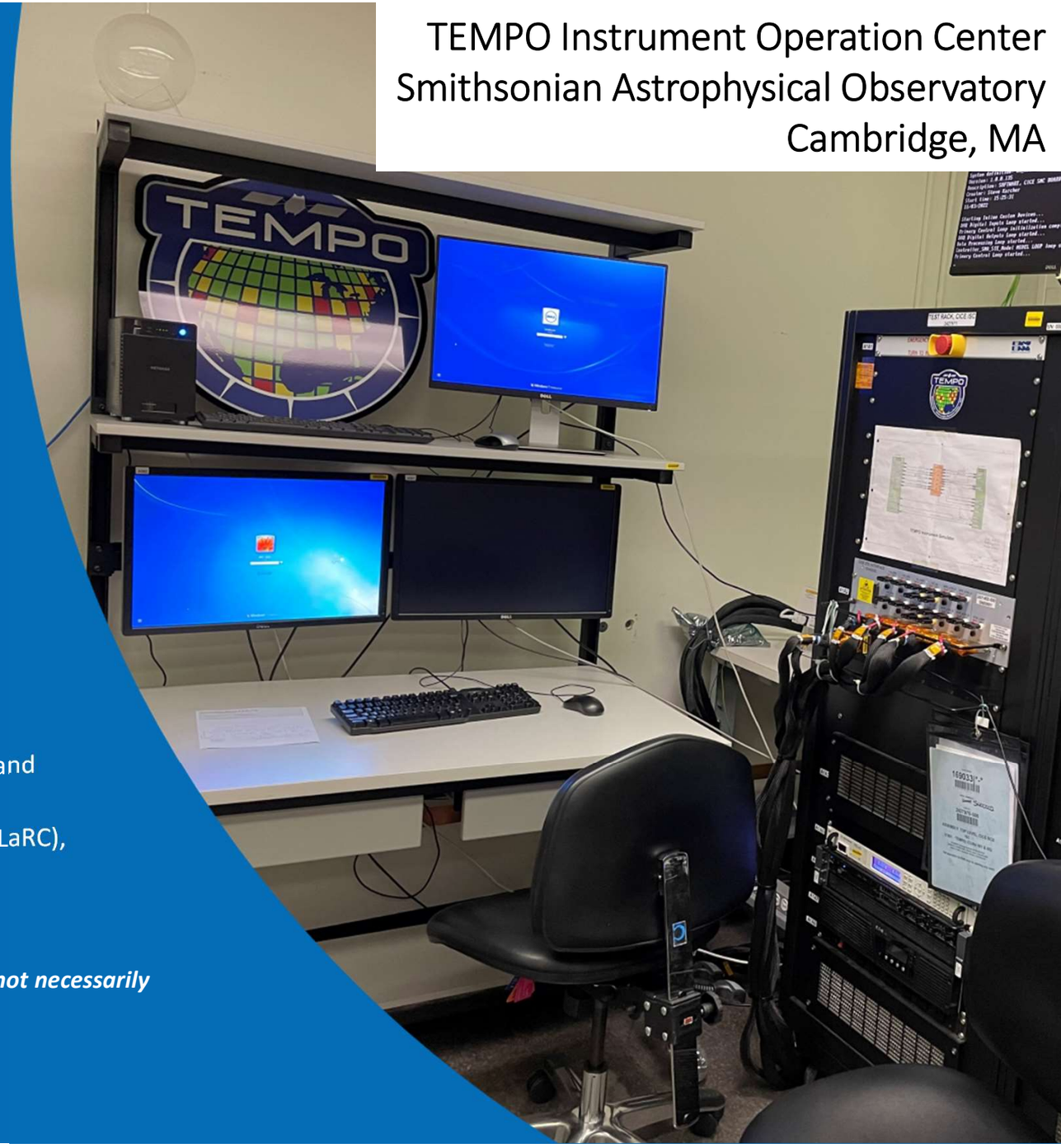
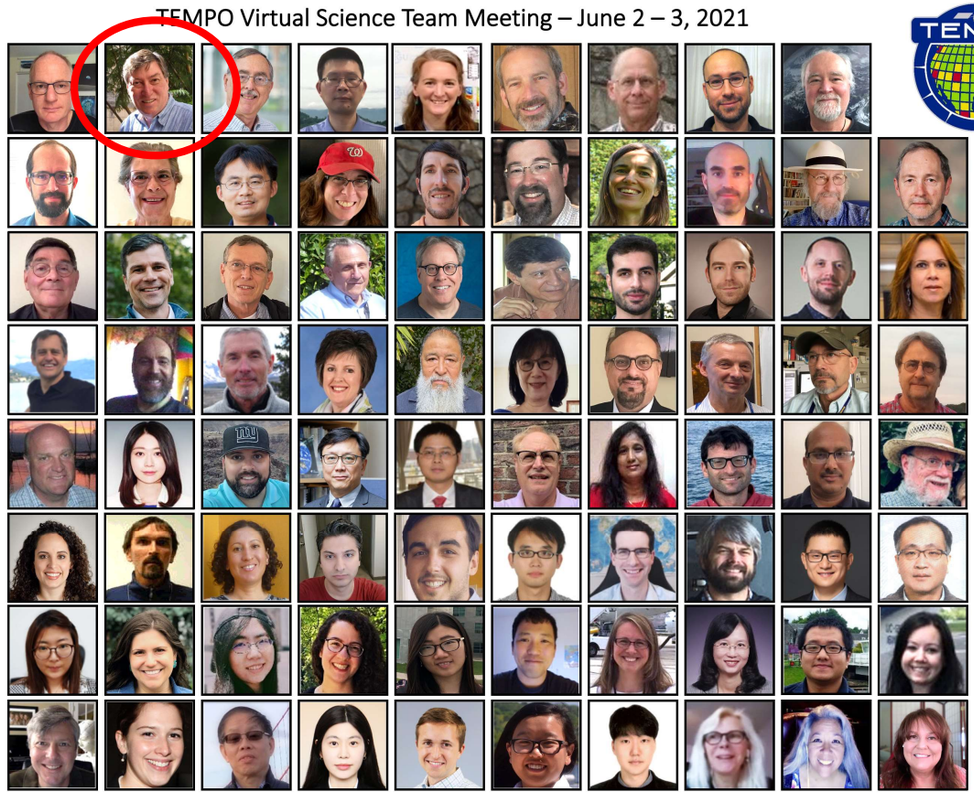


TEMPO Instrument Operation Center
Smithsonian Astrophysical Observatory
Cambridge, MA

The TEMPO Science Team

Kelly Chance, Smithsonian Astrophysical Observatory – PI

Demonstrated the ability to rederive formaldehyde from space using European Global Ozone Monitoring Experiment instrument over two decades ago.

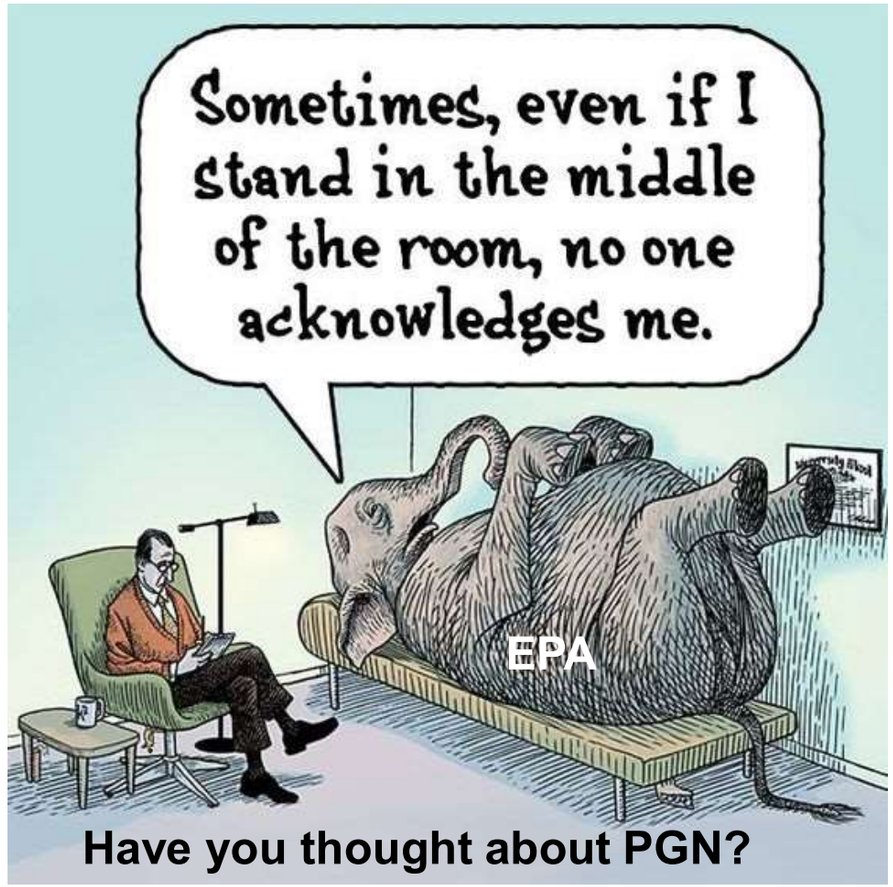


Satellite Data Product Validation

- Quantifying the quality of these products by decomposing the inherent uncertainty components is often a very challenging task and limited by appropriate independent geophysical measurements with appropriate levels of traceability.

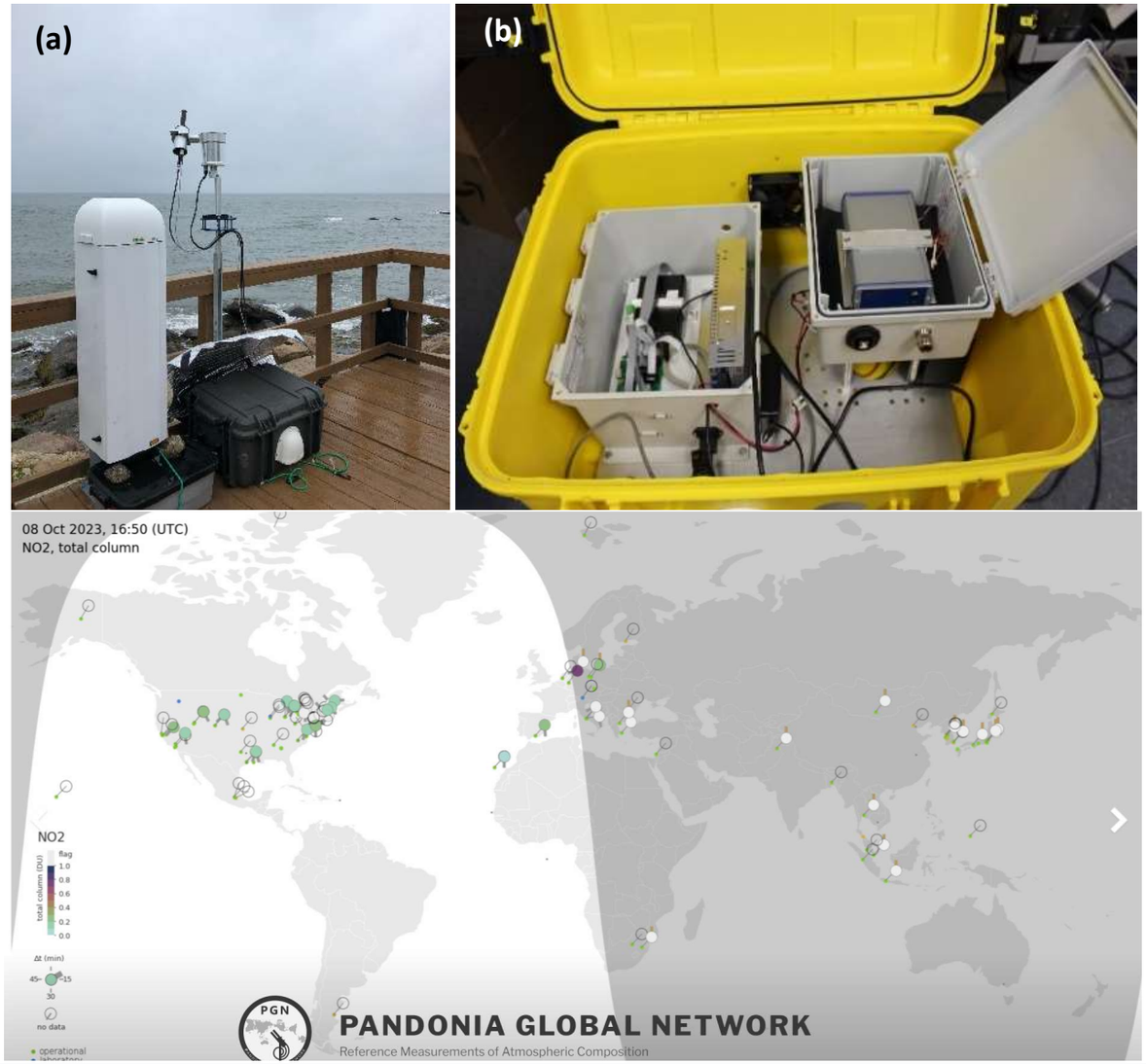
- Historically validation for non-operational satellite science missions such as TEMPO have relied on episodic field campaigns and research measurements to assess data quality.

- Use of satellite data for air quality applications often lack the appropriate validation metrics to inform fitness for purpose, a more routine and systematic approach can help fill this void.



Pandonia Global Network is a network of Ground-Based Spectrometers for Satellite Validation

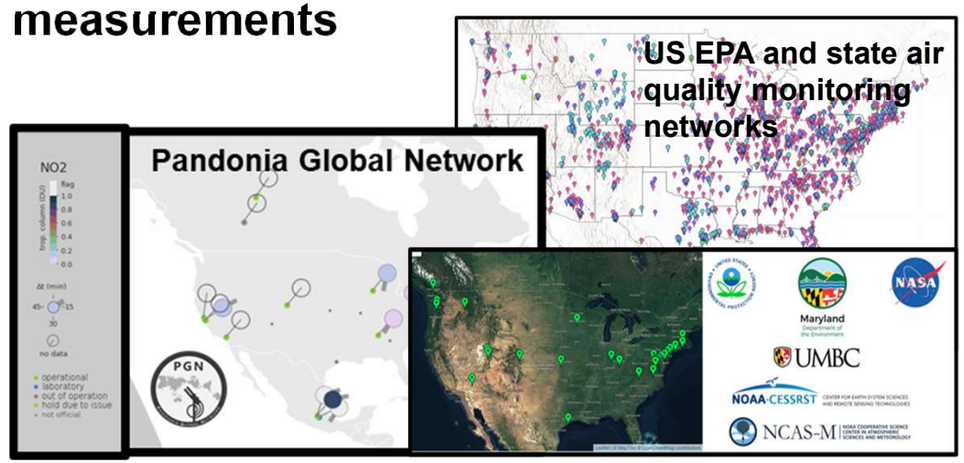
- System originally developed by NASA at Goddard Space Flight Center for satellite validation. Now supported by NASA and European Space Agency and customers like EPA
- Ground-based direct sun/moon & sky scanning remote sensing for air quality and atmospheric composition (1S - ~270 – 530 nm, 0.6 nm; 2S – 400 – 900 nm, 1 nm)
- **Because the instrument collects direct un-scattered sunlight, its measurements are extremely precise and have well-understood biases.**
- Operational Products: Total Column Ozone (+/-15 DU, ~5%); Total Column NO2 (+/-0.05 DU) HCHO column, SO2 column & near surface NO2 and HCHO



EPA ORD investments in TEMPO validation

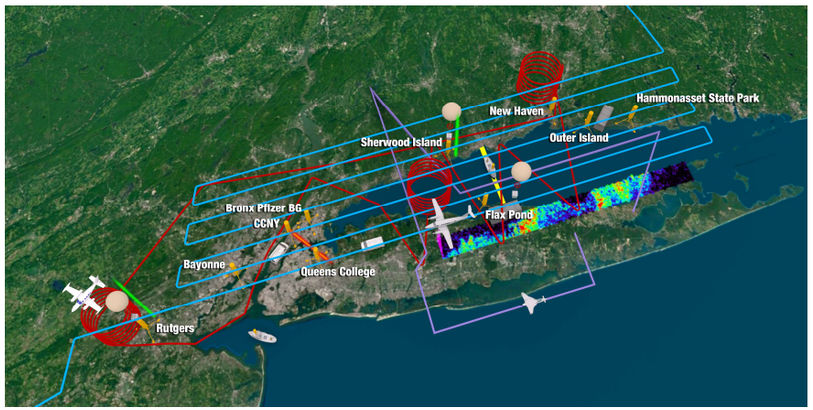
Science Team participation and capacity building

Supporting and building networks with added validation and profiling measurements

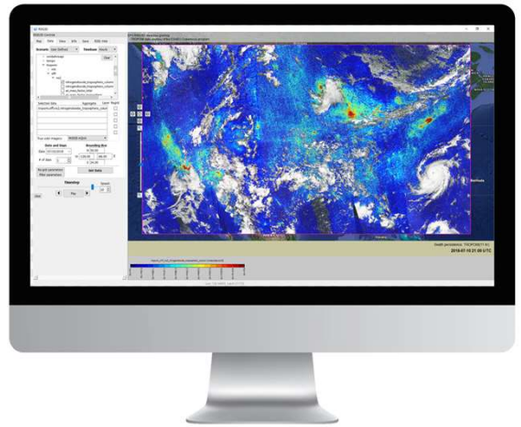


Unified Ceilometer Network

Field Campaigns to prototype TEMPO-like measurements and validation methods



Data and analysis sharing



The schematic on the right depicts the light path from the sun, through the atmosphere to the sun, and the assumptions needed to generate vertical columns, NO2 in this case.

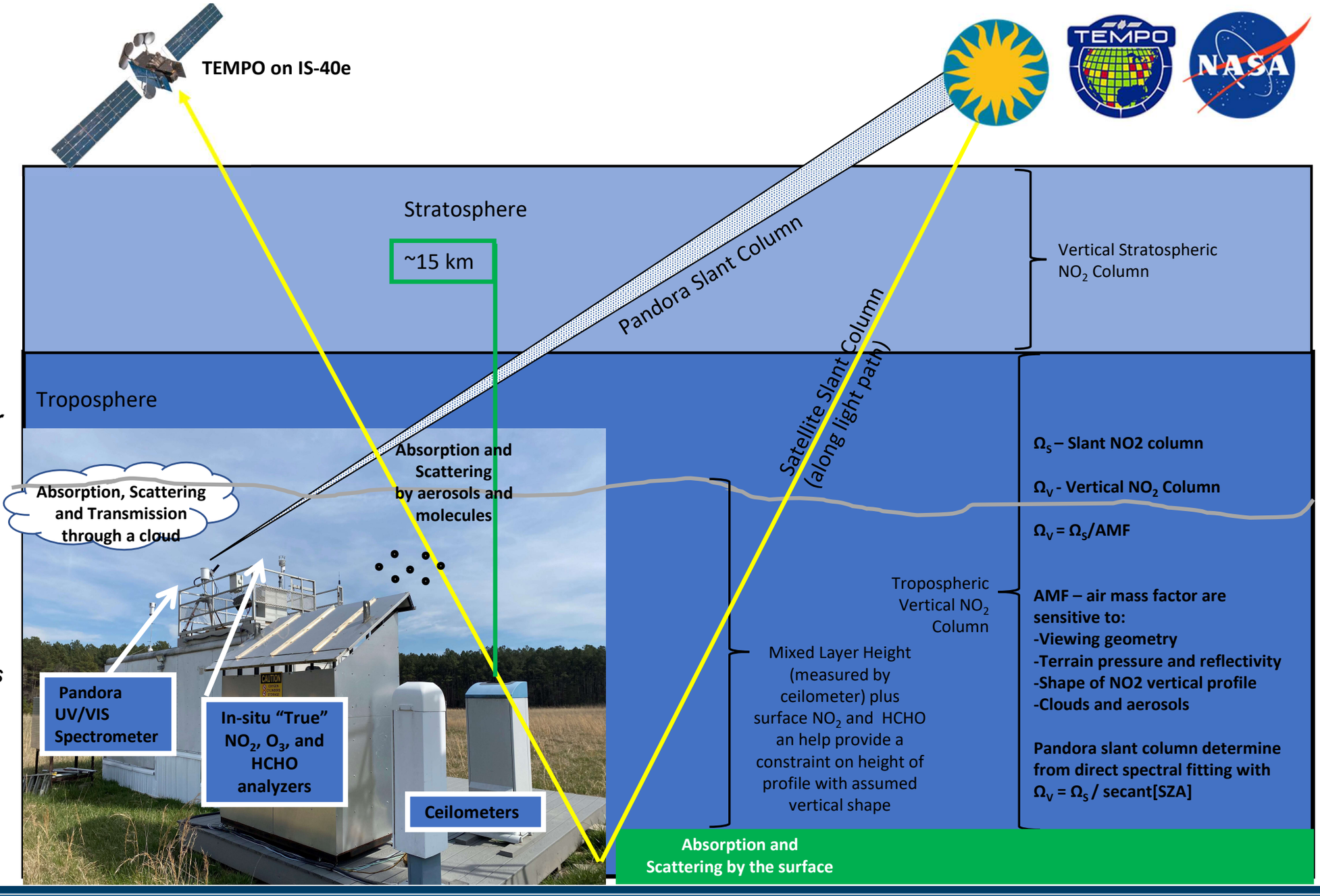
EPA is uniquely positioned to constrain some components of satellite uncertainty by combining remote sensing measurements at surface air quality monitoring locations

Ceilometer
- *Mixed Layer Height*

Pandora
- *NO2, HCHO total column*

Surface Monitors
- *'true' NO2, PM, ozone, HCHO surface mixing ratios*

ORD has established ~24 similar measurement sites in conjunction with the PAMS network and State and Local agencies.



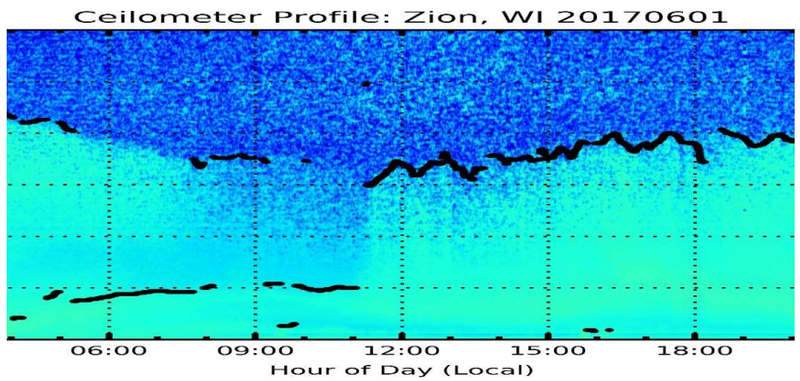
How we use ground-based data to characterize vertical profiles overhead: Case Study over Lake Michigan Shoreline with airborne profiles

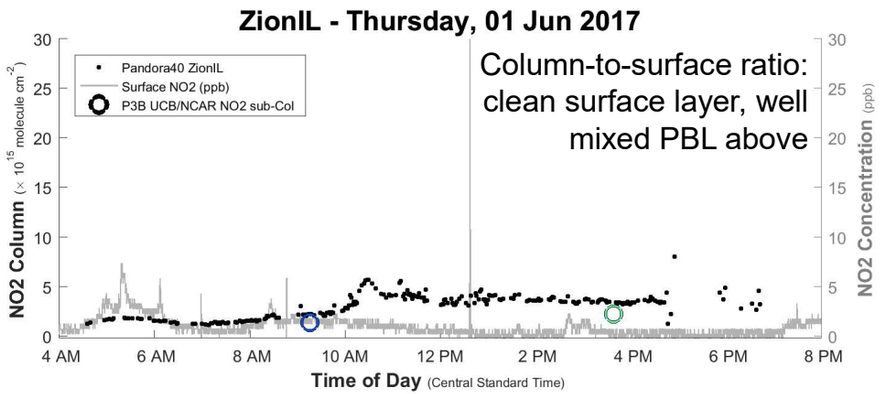
Dirunal Ceilometer (UCN) Backscatter Profile

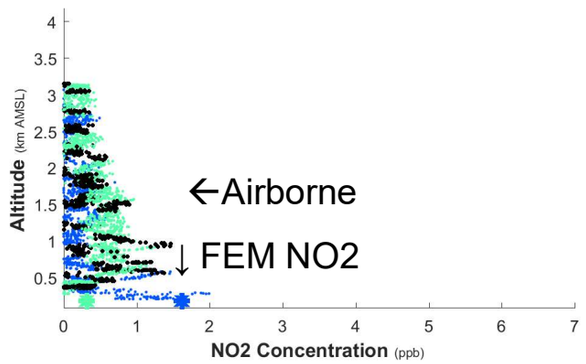
Diurnal Pandora (PGN) NO2 column and EPA FEM NO2

In situ NO2 profile snapshots

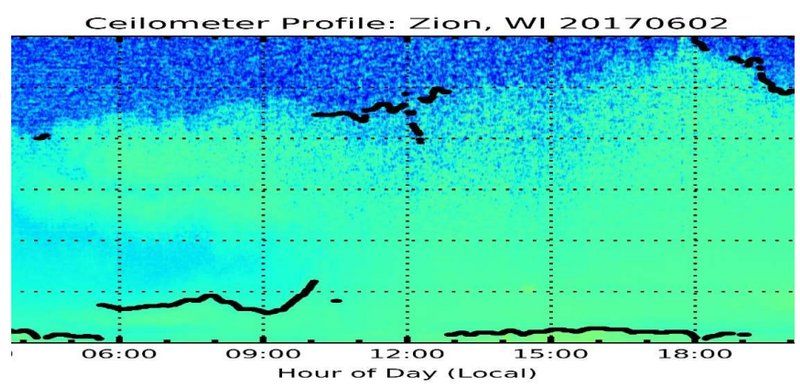
1 July 2017 Lake Michigan: **MDA8 O3 = 48 ppb**

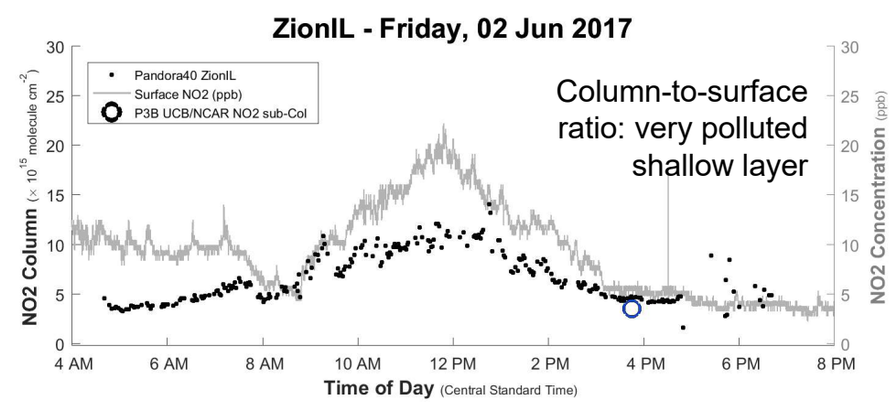


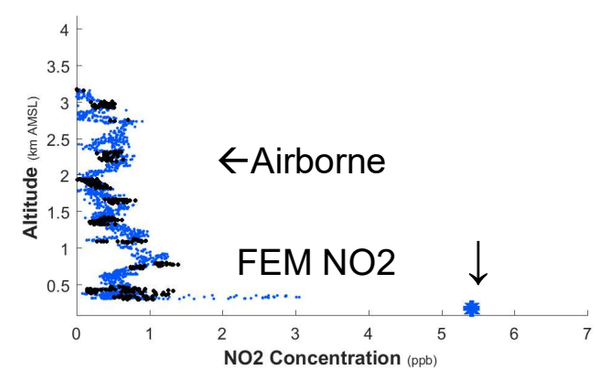




2 July 2017 Lake Michigan: **MDA8 O3 = 79 ppb**

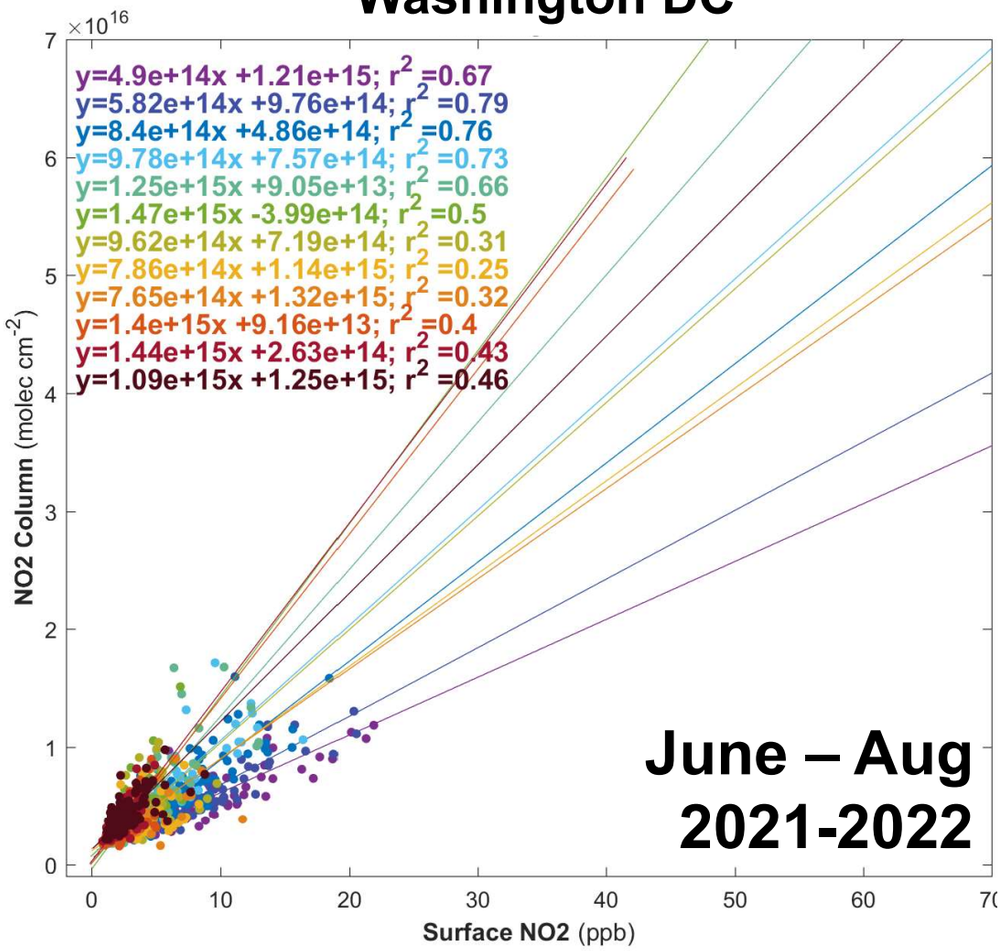




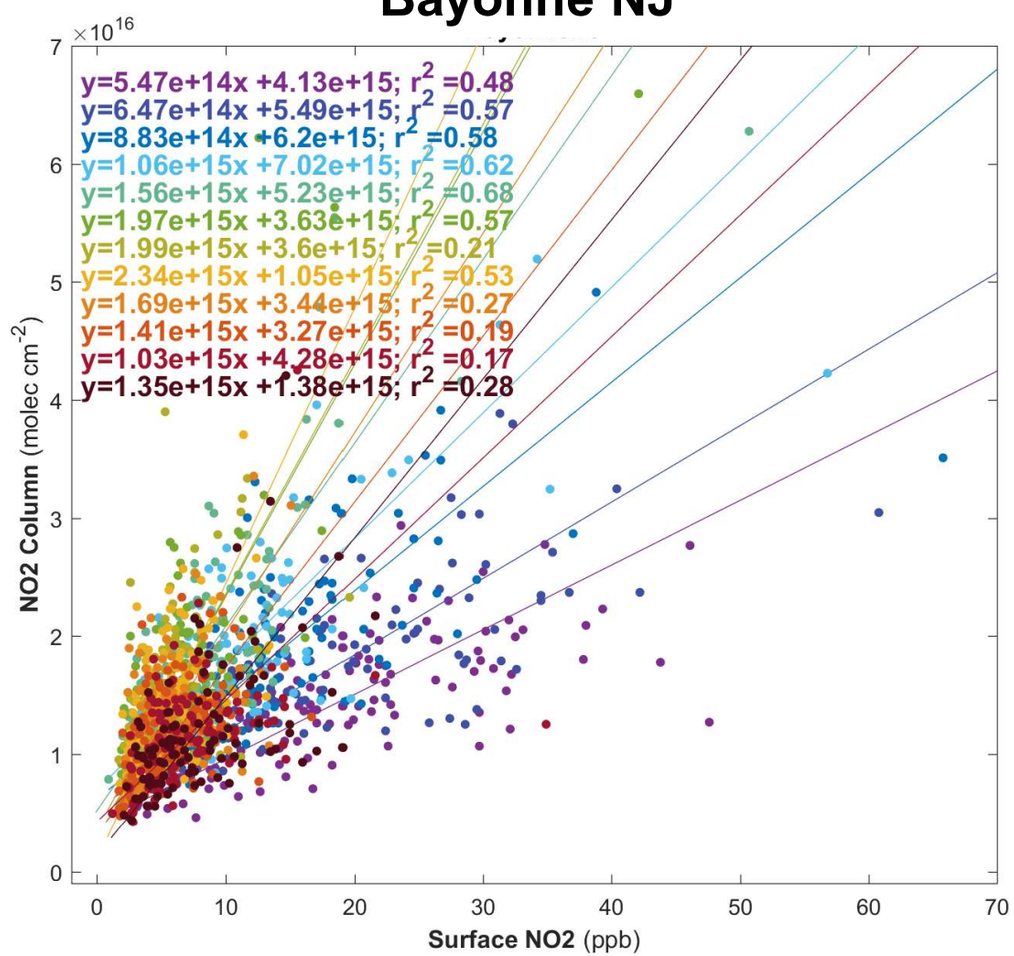


How we can use ground-based data to characterize vertical profiles overhead: NO2 column vs surface NO2 at ~20 SLAMS locations

Washington DC



Bayonne NJ

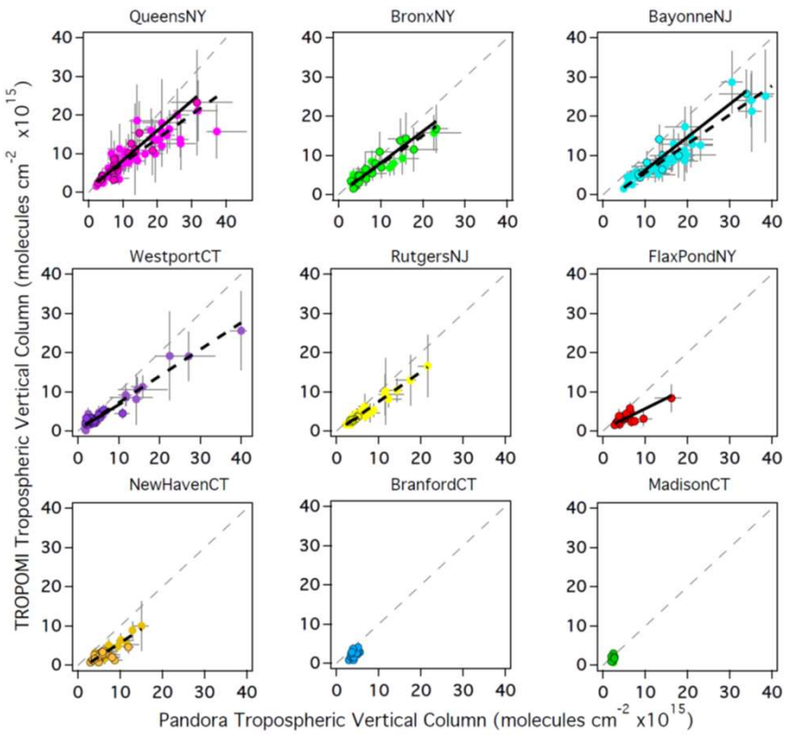


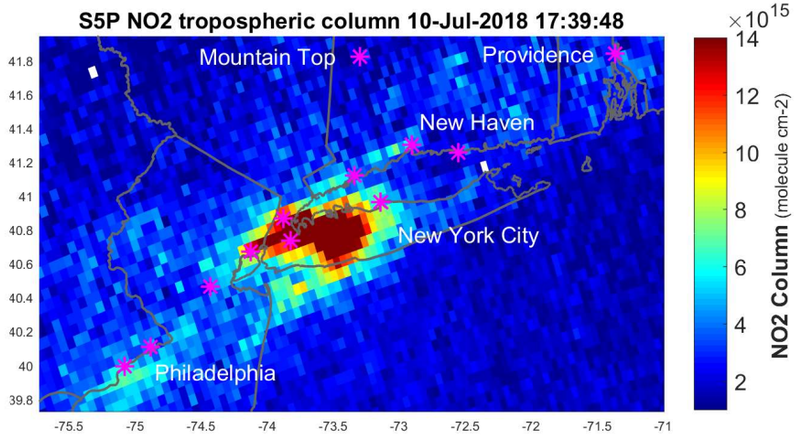
6 AM
7 AM
8 AM
9 AM
10 AM
11 AM
12 PM
1 PM
2 PM
3 PM
4 PM
5 PM

- **Midday slopes are 25% – 50% smaller at DC site than at Bayonne site.**
- **R^2 values worse at midday and afternoon than in AM.**

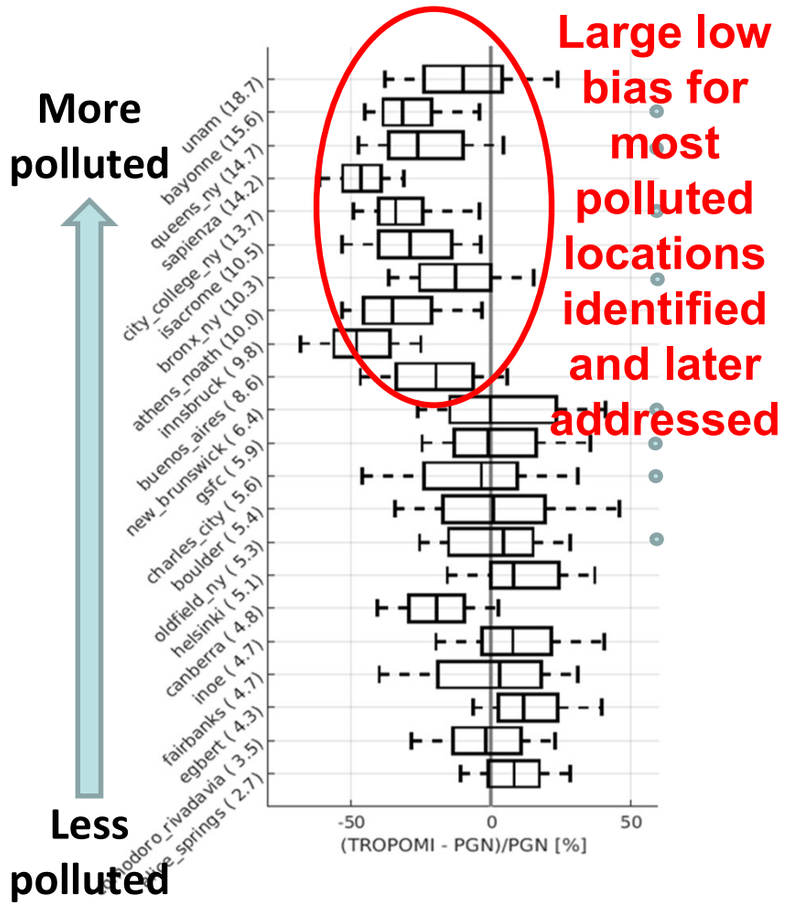
How we use Pandora directly: Routine and Systematic Evaluation of Satellite Measurements – TROPOMI NO_2 Example

Detailed validation study over New York City region during LISTOS 2018 study





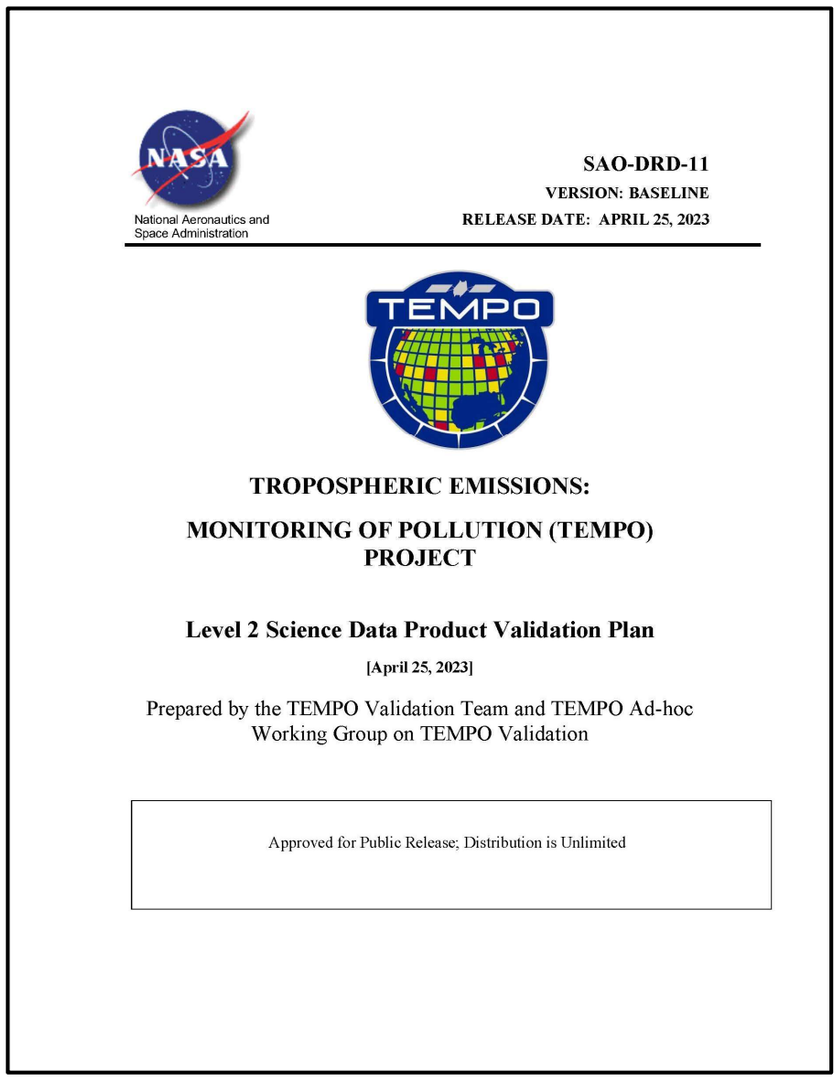
The PGN provides years-long data sets from around the world to compare with TROPOMI **(Pandoras in the OTR)**



Judd et al, Evaluating Sentinel-5P TROPOMI tropospheric NO2 column densities with airborne and Pandora spectrometers near New York City and Long Island Sound, *AMT,* 2020.

Verhoelst et al, : Ground-based validation of the Copernicus Sentinel-5p TROPOMI NO_2 measurements with the NDACC ZSL-DOAS, MAX-DOAS and Pandonia global networks, *AMT,* 2021.

TEMPO (Tropospheric Emissions: Monitoring Pollution) mission Validation Plan



National Aeronautics and Space Administration

SAO-DRD-11
VERSION: BASELINE
RELEASE DATE: APRIL 25, 2023

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

- Facilitated and led by EPA researchers in collaboration with TEMPO Science Team, NASA and NOAA.
- Outlines a best-efforts validation approach for the TEMPO for **ozone, nitrogen dioxide, and formaldehyde** data products.
- Seeks to leverage 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.

TEMPO Validation - Geophysical Data Products

Product Validation Maturity level were adopted from the NOAA GOES-R program Level 2 aerosol products:

- Beta: the product is minimally validated and may still contain significant errors; based on product quick looks using the initial calibration parameters.

- 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 operational use.

- 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 operational use.

Nitrogen Dioxide Product Validation Overview

Beta product maturity:

- NO_2-01: Distinguish high NO_2 urban areas from nearby rural areas for three select urban-rural scene combinations.
- 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.
- 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.

Provisional product maturity:

- NO_2-04: Assess performance metrics (bias/precision/uncertainty) of TropNO2 product across the CONUS for 1 month period in two season that includes a range of column densities.
- NO_2-05: Conduct deep-dive analyses for a pollution event with relatively poor performance and identify the root cause and recommend algorithm improvements.

Full product maturity:

- NO_2-06: assess accuracy, precision, and uncertainty of the TropNO_2 product across the CONUS for a wide range of representative conditions over a period of at least one year.
- NO_2-07: assess accuracy, precision, and uncertainty of the TropNO_2 product over areas of interest using data gathered during targeted field campaigns.

Primary correlative measurement systems for validation of TEMPO Measurements and Baseline Products:

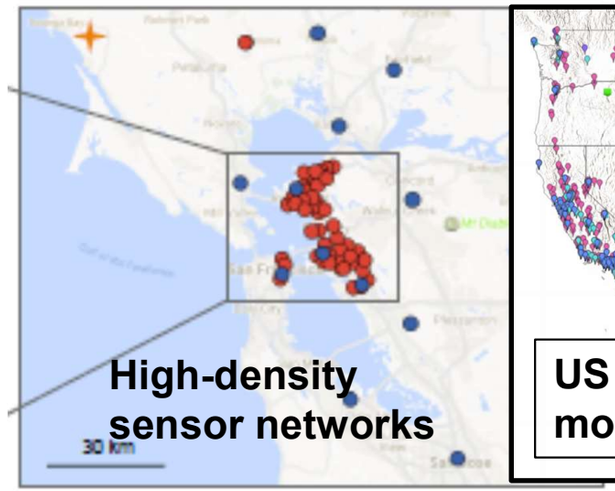
Product Name	Product Horizontal Resolution N/S x E/W @ center of FOR[1]	Product Precision	Air Quality relevant (All in surface- 1 km) Product Precision	Frequency[2]	Ground-based data sources	Satellite data sources
Total Column O_3	2.0 x 4.75 km^2	3%		1 hour	Brewer, Dobson, PGN (pandora)	TROPOMI, OMI, OMPS
Tropospheric Column O_3	8.0 x 4.75 km^2 (4 N/S across-track pixels coadded)	10 ppbv	10 ppb	1 hour	Ozonesonde, TOLNET	TROPOMI, OMI, OMPS
0-2 km O_3 selected scenes	8.0 x 4.75 km^2 (4 N/S across-track pixels coadded)	10 ppbv	10 ppb	2 hours	Ozonesonde, TOLNET	
Total Column NO_2	2.0 x 4.75 km^2	1.0 × 10^{15} molecules cm^{-2}	0.4 ppb	1 hour	PGN (pandora) Direct Sun	TROPOMI, OMI, OMPS
Tropospheric Column NO_2	2.0 x 4.75 km^2	1.0 × 10^{15} molecules cm^{-2}	0.4 ppb	1 hour	PGN (pandora) Direct Sun and MAX-DOAS	TROPOMI, OMI, OMPS
Tropospheric column HCHO	2.0 x 4.75 km^2	1.0 × 10^{16} molecules cm^{-2}	4.0 ppb	3 hours	PGN (pandora) Direct Sun and MAX-DOAS, FTIR MAX-DAOS	TROPOMI, OMI, OMPS

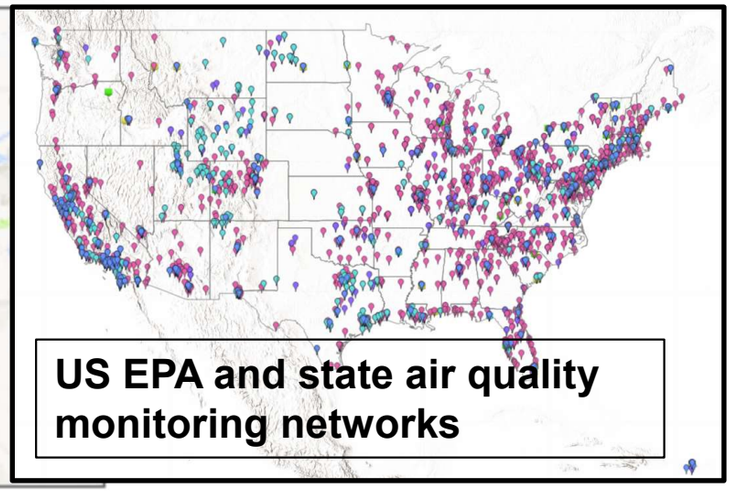
Measurement research under the ACE Research Program over the past decade provided a foundation for EPA involvement in TEMPO Validation.

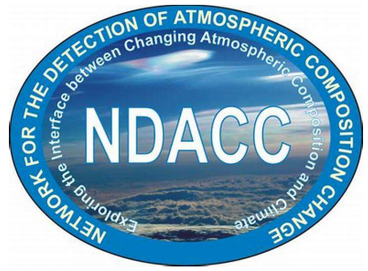
The integration of key (chemical and meteorological) measurements within the existing air quality networks will contribute to an improved assessment of TEMPO product precision plus an improved assessment of biases, and possibility allow an assessment of product accuracy.

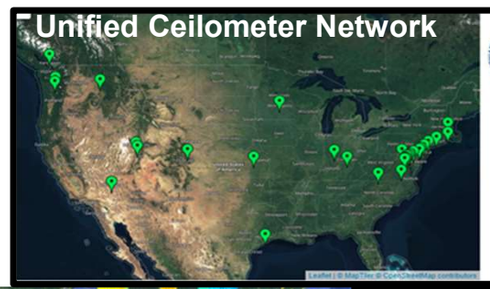
Wrap-Up

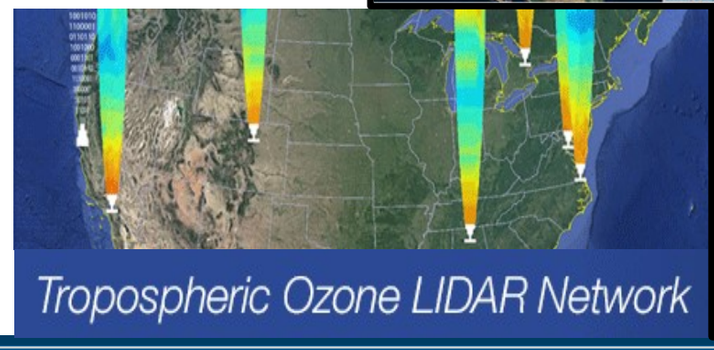
- A concerted effort is developing for validation of TEMPO data products which is based on leveraging both operational and research air quality observing systems.
- TEMPO validation efforts will provide routine and systematic (on-going) validation through the PGN, NDACC, and satellites along with more complex (episodic) validation via planned science campaigns with focus on satellite data and local air quality.
- For the first time, validation measurements for a satellite mission are being integrated within the existing air quality network
- The validation plan provides a framework for facilitating greater use of satellite data products, the emerging TEMPO validation paradigm is focused on providing information on the reliability and accepted uses of data products.

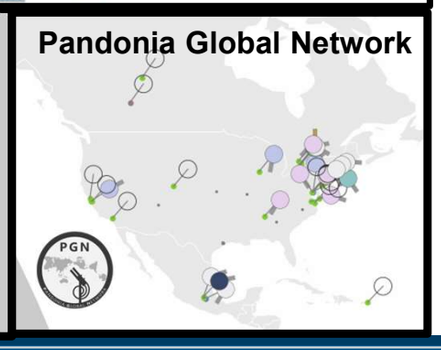






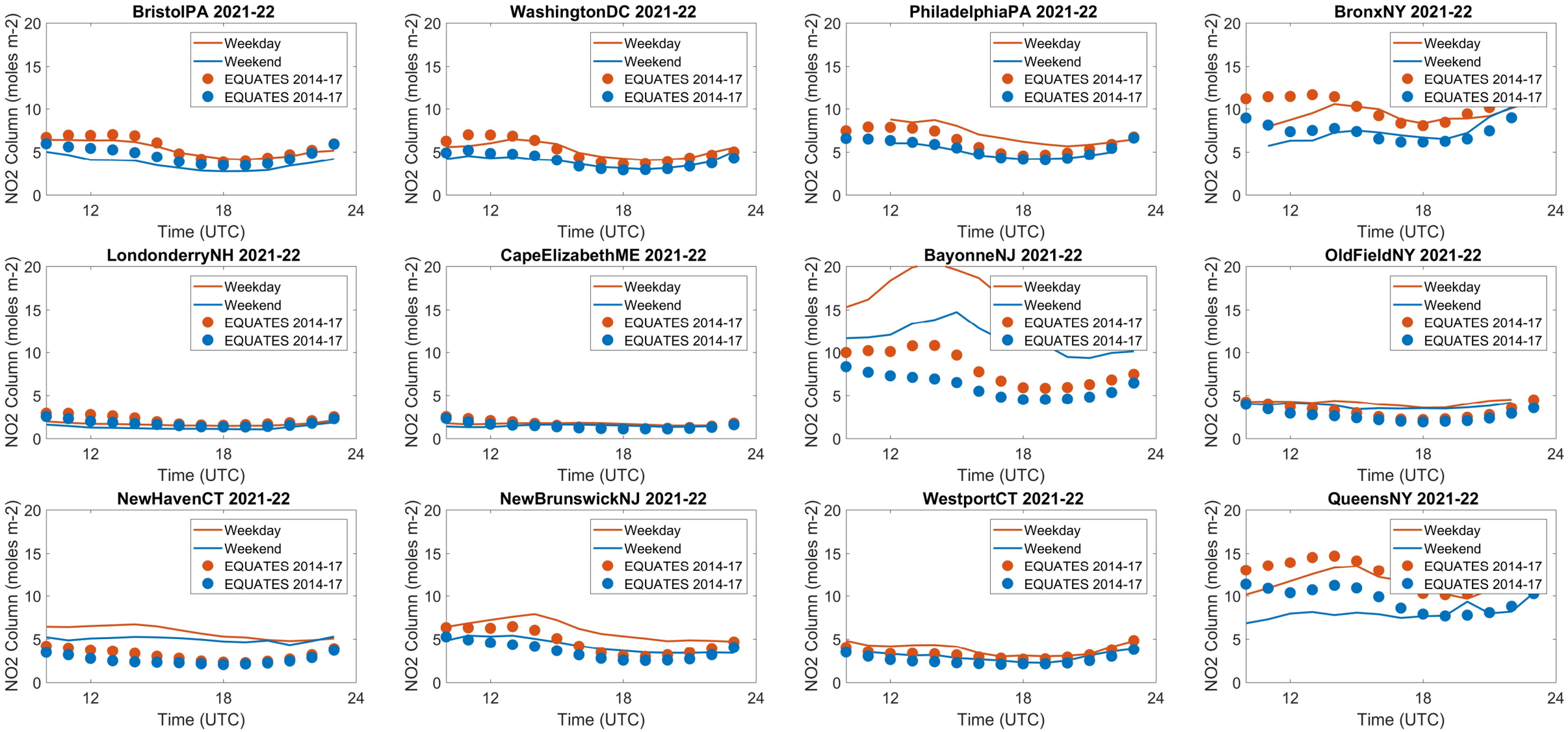






Extras

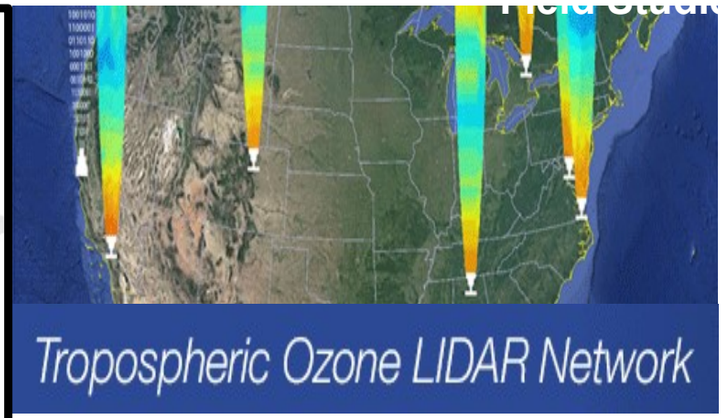
More than a validation source: PGN vs EQUATES (offset in time by ~6 years)

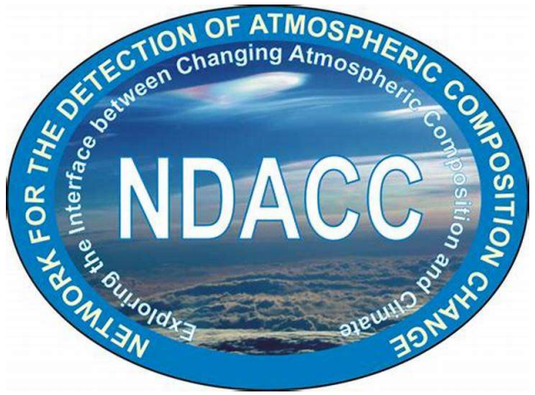


Summary

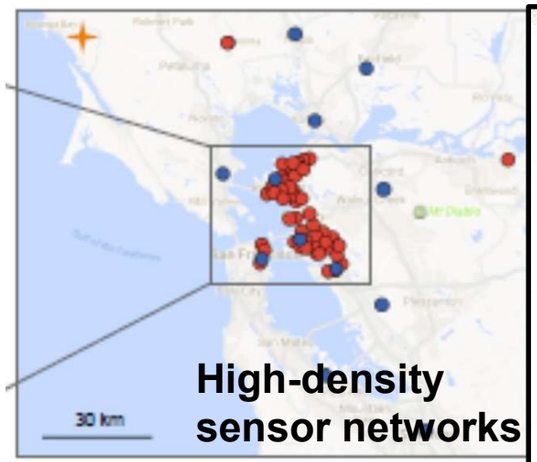
- EPA/ORD was key partner in TEMPO, especially relating to data product validation planning and implementation, and data accessibility
- EPA/ORD has worked with state agencies and federal partners to develop PGN as a TEMPO validation resource directly co-located at a subset of science-focused air monitoring networks like PAMS and NCORE.
- Routine and systematic data collection is an important validation asset to enhance the applicability of satellite-based data products for EPA applications, and also directly provides an evaluation resource for EPA tools like EQUATES/CMAQ

Correlative measurements for routine and systematic validation of TEMPO data products – ground networks

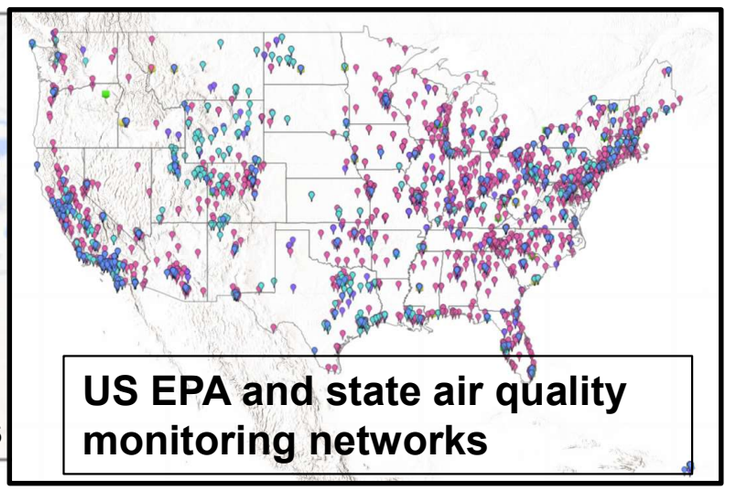




Unified Ceilometer Network



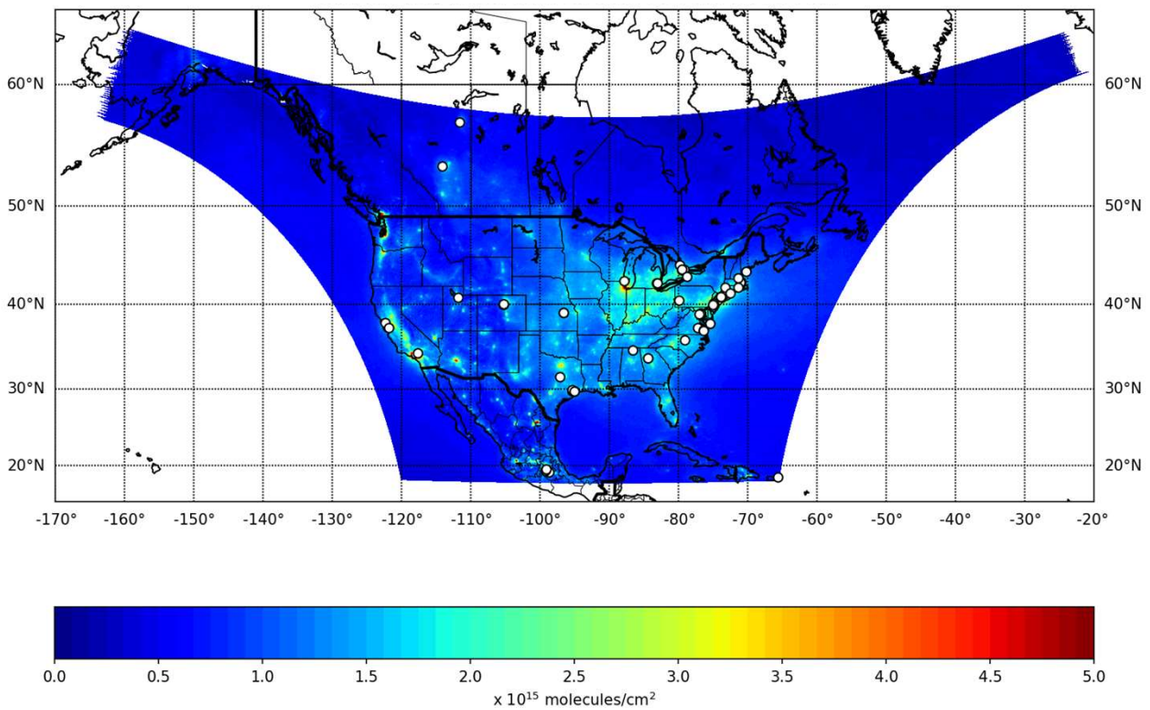
High-density sensor networks



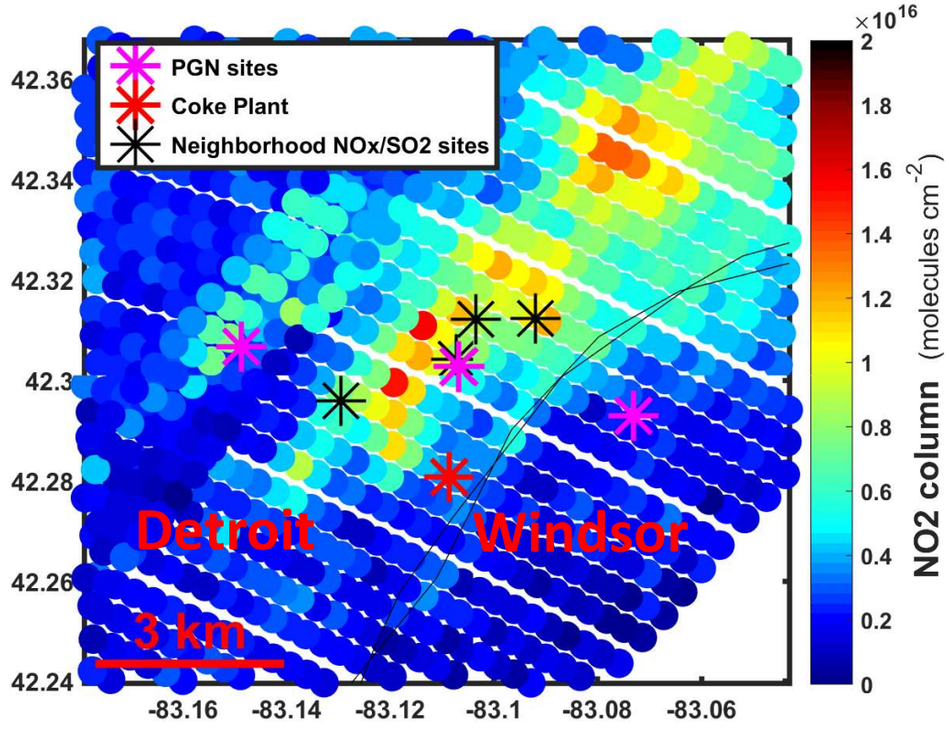
US EPA and state air quality monitoring networks

Photochemical Assessment Monitoring Stations (PAMS) Enhanced Monitoring has allowed EPA ORD to collaborate with SLT Agencies to build out the Pandonia Global Network in conjunction with NASA and the European Space Agency across the U.S. for use in validating the TEMPO satellite mission

Pandonia Global Network Locations
in TEMPO Field of Regard



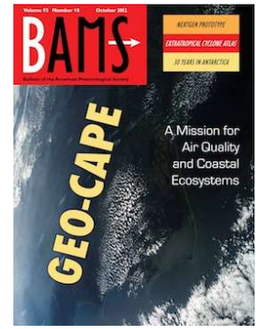
NASA GCAS NO2 column – MOOSE 2021



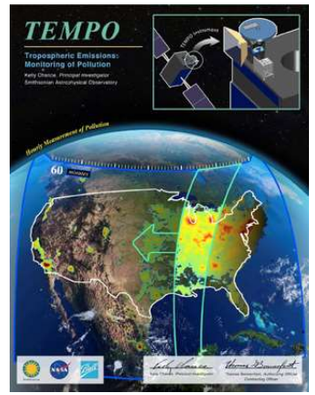
In addition to partnering on the larger TEMPO validation effort across North America, EPA and ECCC have contributed long-term total column NO2, O3, formaldehyde and SO2 measurements to Dearborn, Detroit and Windsor. One of several locations across the FOR to assess TEMPO sub-pixel variability for NO_2, HCHO, and SO_2 and improve our understanding of satellite/surface air quality inferences at neighborhood scales

GEO-CAPE → TEMPO

- GEO-CAPE (GEOstationary Coastal and Air Pollution Events)
  - **A NASA Earth Systematic Mission recommended by the 2007 National Research Council Decadal Survey**
  - Provide first-ever high spatial & spectral resolution observations of North America multiple times per day
    - Atmosphere: ozone, aerosol, and related observations key to co-management of air quality and short-lived climate forcers
    - Ocean: key water quality, ocean chemistry, and ecological science in coastal waters including response to environmental change
  - North American contribution to integrated global observing systems for air quality and coastal biogeochemistry
  - **First GEO-CAPE science definition workshop held in Chapel Hill, NC (2008) and Final Community Workshop hosted at EPA in Research Triangle Park, NC (2015).**
  - Planned to be implemented as 1 or more hosted payloads on commercial satellites (Fishman et al., BAMS, Oct 2012)

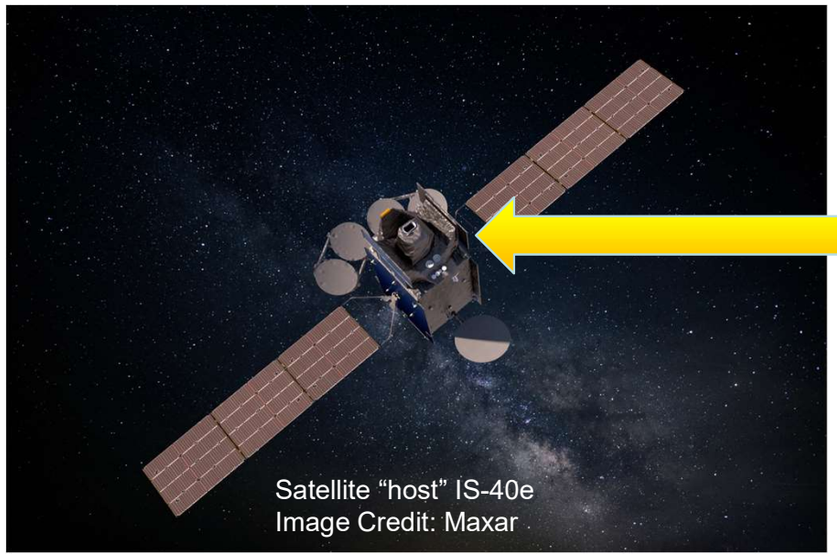


- TEMPO (Tropospheric Emissions: Monitoring of Pollution)
  - A NASA Earth System Science Pathfinder mission selected Nov 2012 via Earth Venture-Instrument
  - Measures air pollution over North America hourly and at high spatial resolution
    - UV-Vis ozone (O_3), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), formaldehyde (H_2CO), glyoxal ($C_2H_2O_2$), aerosol
    - Multi-spectral observations provide first-ever satellite measurement of O_3 in the lowermost troposphere
  - Planned launch as a geostationary commercially-hosted payload before 2020 allows TEMPO to be a component of the first global constellation for pollution monitoring, along with the European and Korean geostationary missions now in development and the NOAA GOES-R series

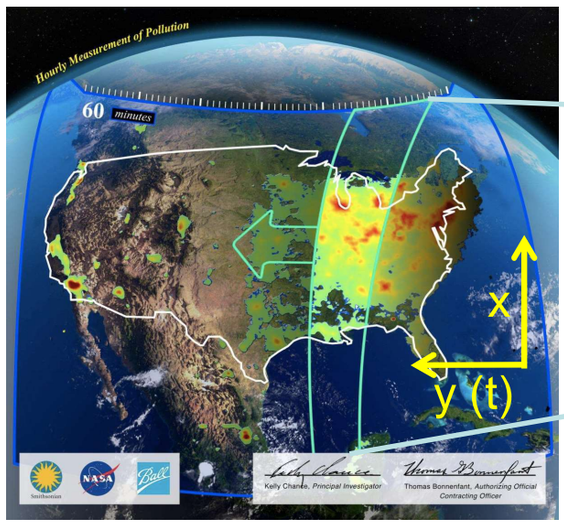


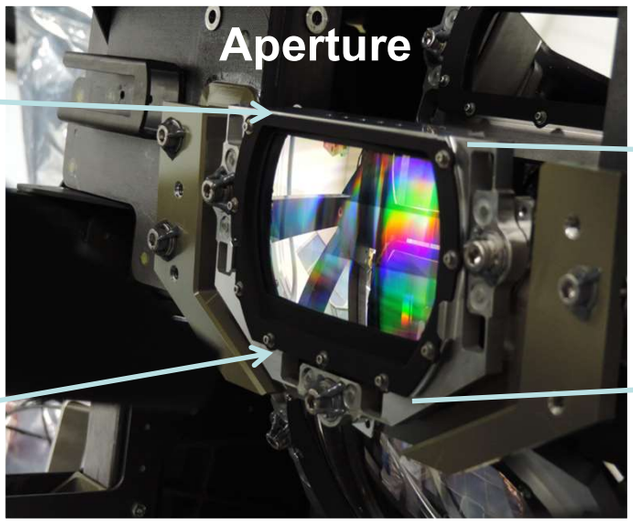
- **Geostationary Carbon Cycle Observatory (EVM-2) (GeoCarb) and Geosynchronous Littoral Imaging and Monitoring Radiometer (EVI-5) (GLIMR) are other parts of the larger GEO-CAPE mission – CEMM involvement in GLIMR**

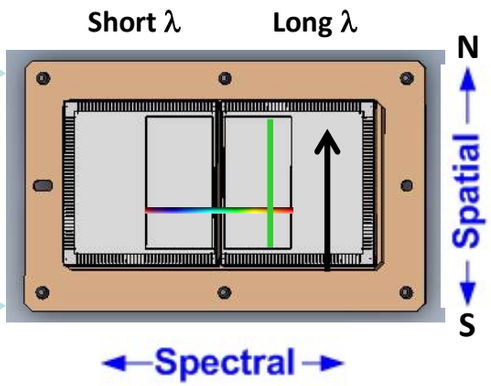
Instrument Overview



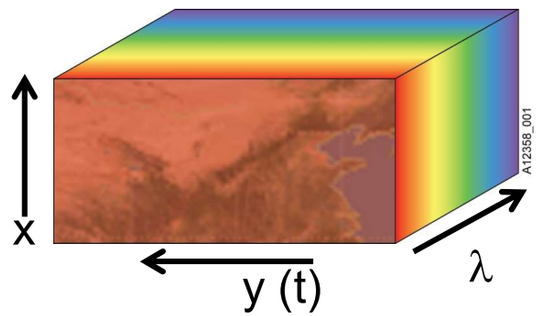
- Wavelength range = UV~293 – 494 nm and VIS 538 – 741 nm
- Spectral resolution = ~0.6 nm @Full Width Half Maximum (0.54-0.63 nm)
- Two 2048 (spatial) x 1024 (spectral) pixel CCD detectors
- Step/stare 2-axis scan mechanism
- *Each mirror step is a ~2.85 s snapshot of all 2K N/S cross-track pixels.*
- *60 minute E→W scan of FOR in 1226 mirror steps*
- *Orbit = geostationary (35786 km), 91.0° W above equator*
- *Spatial resolution 2.0 km (N/S) 4.75 (E/W) @ center of FOR*
- Instrument Control Electronics (ICE) mounted below spacecraft deck
- Images co-added on board before data downlink
- **Mass**: 137 Kg **Power**: 138W **Volume:** 1.4m x 1.1m x 1.2 m





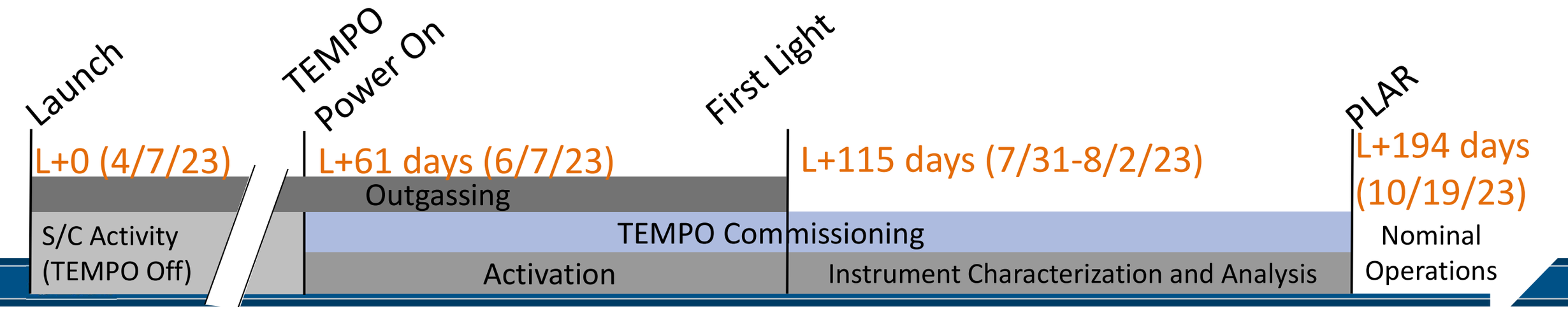


Downlink, spatial bin, image reconstruction



TEMPO Commissioning

- **TEMPO commissioning (6/7-10/18/2023):**
  - ✓ **TEMPO power on 6/7**
  - ✓ **Dry out and cool down (6/9-7/13):**
  - ✓ **Additional activation: scan mirror tuning, command load testing, etc.**
  - ✓ **First light (7/31-8/2): solar measurements & Earth imaging**
  - ✓ **23 Instrument Characterization and Analysis (ICA) activities**
  - ✓ **Post Launch Acceptance Review (PLAR) on October 18-19, 2023**
  - ✓ **Release the data products to the public in April 2024**



TEMPO offers key measurements directly aligned with EPA research as directed under Clean Air Act as Amended

Clean Air Act, codified as 42 U.S.C. 7403 - Research, investigation, training, and other activities

(a)RESEARCH AND DEVELOPMENT PROGRAM FOR PREVENTION AND CONTROL OF AIR POLLUTION The Administrator shall establish a national research and development program for the prevention and control of air pollution and as part of such program shall—

(1)conduct, and promote the coordination and acceleration of, research, investigations, experiments, demonstrations, surveys, and studies relating to the causes, effects (including health and welfare effects), extent, prevention, and control of air pollution;

(b)AUTHORIZED ACTIVITIES OF ADMINISTRATOR IN ESTABLISHING RESEARCH AND DEVELOPMENT PROGRAM In carrying out the provisions of the preceding subsection the Administrator is authorized to—

(2) cooperate with other Federal departments and agencies, with air pollution control agencies, with other public and private agencies, institutions, and organizations, and with any industries involved, in the preparation and conduct of such research and other activities;

(c)AIR POLLUTANT MONITORING, ANALYSIS, MODELING, AND INVENTORY RESEARCH In carrying out subsection (a), the Administrator shall conduct a program of research, testing, and development of methods for sampling, measurement, monitoring, analysis, and modeling of air pollutants. Such program shall include the following elements:

(3)Development of improved methods and technologies for sampling, measurement, monitoring, analysis, and modeling to increase understanding of the sources of ozone precursors, ozone formation, ozone transport, regional influences on urban ozone, regional ozone trends, and interactions of ozone with other pollutants. Emphasis shall be placed on those techniques which—

(A)improve the ability to inventory emissions of volatile organic compounds and nitrogen oxides that contribute to urban air pollution, including anthropogenic and natural sources;

(C)improve the ability to identify and evaluate region-specific prevention and control options for ozone pollution.

GAO Report (2020) Modernize the National Air Quality Monitoring System: Excerpts relevant to TEMPO Satellite Data

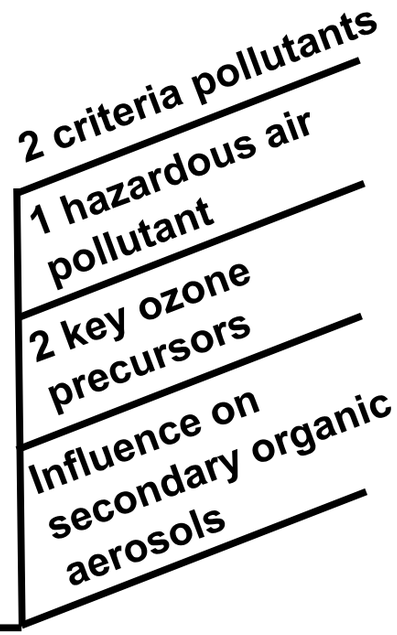
- The information needs are (1) local-scale, real-time air quality; (2) air toxics; (3)persistent and complex pollution; and (4) using low-cost sensors and satellites.

- Air quality managers, researchers…are increasingly using emerging technologies to obtain information on air quality, but many…(of) these users need more information on the reliability and accepted uses of these technologies. These technologies include remote sensors on satellites operated by NOAA and NASA.

- Satellites can provide information on air pollutants over large areas, including areas that are difficult or impossible to monitor with traditional monitoring methods.

- Satellite-based sensor data can be difficult to interpret, especially for pollution at ground level. In addition, deployed satellite-based sensor technologies currently only measure a few pollutants, including particulate matter, **ozone**, sulfur dioxide, **nitrogen dioxide**, **formaldehyde**, and carbon monoxide.

- State and local agencies use information from satellites to supplement air quality monitoring for limited purposes but said that they would likely increase their use of satellite data if they had more information on appropriate applications.



Report can be found at: https://www.gao.gov/products/gao-21-38