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

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REVISION HISTORY PAGE

Revision	Description	Release Date
Preliminary	Draft Release Prior to CDR	6/10/2015
Baseline	Establishing initial baseline document – see TEMPO-CR-7185	4/25/2023

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EXECUTIVE SUMMARY

The Tropospheric Emissions: Monitoring of Pollution (TEMPO) Instrument is a NASA Earth Venture Instrument (EV-I) project selected on November 8, 2012, in response to the second Stand Alone Mission of Opportunity Notice (SALMON-2), NNH12ZDA0060. The Smithsonian Astrophysical Observatory (SAO) under the direction of the TEMPO Principal Investigator (Pl) at SAO is the lead organization for the project, responsible for TEMPO instrument development data products and science.

TEMPO is a hosted payload designed to collect Earth radiance measurements from geostationary orbit that will enable the quantification of spatial and temporal variations of trace gases and aerosols important for understanding air quality in the troposphere. The anticipated precision, resolution, and coverage of TEMPO will enable an improved understanding of greater North American pollutant sources and sinks (fluxes) on continental, regional, and local scales and the chemical and physical processes controlling their variability over the diurnal-to-seasonal cycles.

As part of the PI-led TEMPO Science Team effort, this document outlines a best-efforts validation plan that extends beyond the Program Level Requirements Appendix (PLRAs) for the TEMPO geophysical data products of ozone, nitrogen dioxide, and formaldehyde. The best-efforts approach seeks to leverage measurement and modeling assets over the timeline of the baseline TEMPO mission, which if undertaken will result in the use of a comprehensive set of measurements (ground-based and spaceborne) for routine validation enhanced by episodic field mission efforts (airborne).

The validation plan provides a structure for the geophysical data product maturity progression. It discusses specific TEMPO validation activities, which rely on use of data from core measurement stations, networks and satellites, and airborne science field campaign over select regions with targeted measurement that can be leveraged for TEMPO validation objectives. In addition, a set of model-based efforts are discussed to aid in the TEMPO evaluation.

The success of this validation approach beyond the PLRAs depends very much on contributions from the measurement community funded outside of the TEMPO mission, including but not limited to the European Union Copernicus Programme, NASA Tropospheric Chemistry Program, U.S. Environmental Protection Agency Air, Climate and Energy Program, Environment Canada and Climate Change Research Program. The levels of enthusiasm and scientific expertise within the measurement community is high, a state suggesting a high probability of success.

Additional resources will be required to fully validate all potential TEMPO L2 data products. The TEMPO validation cadre encourages the community to consider a measurement domain that comprises rural, suburban, and urban areas; international sites in Canada, Mexico, and the Caribbean; spatial scales from synoptic to neighborhood; geophysical conditions from homogeneous to highly heterogeneous.

ACRONYMS AND ABBREVIATIONS

ABI	Advanced Baseline Imager
AC/VC	Atmospheric Composition/Virtual Constellation
AEROMMA	Atmospheric Emission and Reactions Observed from Megacities to Marine Areas
AGL	Above Ground Level
AIRS	Atmospheric Infrared Sounder
AMF	Air Mass Factor
AO	Announcement of Opportunity
ATBD	Algorithm Theoretical Basis Document
Cal/Val	Calibration and Validation
CALIOP	Cloud-Aerosol Lidar with Orthogonal Polarization
CALIPSO	Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations
CEOS	Committee on Earth Observation Satellites
CHAPS-D	Compact Hyperspectral Air Pollution Sensor-Demonstrator
CPR	Cloud Profiling Radar
CrIS	Cross-track Infrared Sounder
CTMs	Chemical Transport Models
DIAL	Differential Absorption Lidar
DISCOVER-AQ	Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality
DS	Direct Sun
DSCOVR	Deep Space Climate Observatory
DU	Dobson units
EarthCARE	Earth Cloud Aerosol and Radiation Explorer
ECC	Electrochemical Concentration Cell
EPA	Environmental Protection Agency
EOL	End of line
EPIC	Earth Polychromatic Imaging Camera
ESA	European Space Agency
EV	Earth Venture
EV-I	Earth Venture Instrument
FOR	Field Of Regard
FOV	Field Of View
FTIR	Fourier Transform Infrared Radiometer
FWHM	Full Width at Half Maximum
GCAS	GeoCAPE Airborne Simulator
GEO	Geostationary Earth Orbit
GEO-CAPE	Geostationary Coastal and Air Pollution Events
GEOS-CF	GEOS Composition Forecasting

GEOTASO	GEOstationary Trace gas and Aerosol Optimization
GOES-R	Geostationary Operational Environmental Satellite - R Series
GOME	Global Ozone Monitoring Experiment
GOME-2	Global Ozone Monitoring Experiment-2
HIRES	High Resolution
HSRL	High Spectral Resolution Lidar
IAGOS	In-Service Aircraft for a Global Observing System
IASI	Infrared Atmospheric Sounding Interferometer
IDAF	Instrument Data Analysis Facility
IOT	In-Orbit Test
L0	Level 0
L1	Level 1
L2	Level 2
L3	Level 3
LEO	Low Earth Orbit
LISTOS	Long Island Sound Tropospheric Ozone Study
MAX-DOAS	Multi Axis Differential Optical Absorption Spectroscopy
MLS	Microwave Limb Sounder
MOZAIC	Measurement of OZone and water vapour on Airbus In-service
NDACC	Network for the Detection of Atmospheric Composition Change
NIER	National Institute of Environmental Research
NRT	Near-Real-Time
NWP	Numerical Weather Prediction
OMI	Ozone Monitoring Instrument
OMPS-LP	Ozone Mapping and Profiler Suite Limb-Profile
OMPS-NM	Ozone Mapping and Profiler Suite Nadir-Mapper
OOC	On-Orbit Checkout
OWLETS-2	Ozone Water-Land Environmental Transition Study-2
PBL	Planetary Boundary Layer
PGN	Pandonia Global Network
PLAR	Post-Launch Acceptance Review
PLRA	Program Level Requirements Appendix
QA/QC	Quality Assurance/Quality Control
RAQMS	Real-time Air Quality Modeling System
RSME	Root Mean Square Error
S5P	Sentinel-5 Precursor
SAO	Smithsonian Astrophysical Observatory
SHADOZ	Southern Hemisphere ADditional OZonesondes
STAQS	Synergistic TEMPO Air Quality Science
SZA	Solar Zenith Angle

TEMPO	Tropospheric Emissions Monitoring of POllution
TOLNet	Tropospheric Ozone Lidar Network
TOMS	Total Ozone Mapping Spectrometers
TOT	Total Column
TRACER-AQ	Tracking Aerosol Convection interactions ExpeRiment-Air Quality
TROPESS	TRopospheric Ozone and its Precursors from Earth System Sounding
TROPOMI	TROPOspheric Monitoring Instrument
UV/VIS	Ultraviolet Visible
UVN	Ultraviolet/Visible/Near-Infrared
VIIRS	Visible Infrared Imaging Radiometer Suite
WMO	World Meteorological Organisation
WOUDC	World Ozone and Ultraviolet Radiation Data Centre
WRF/CMAQ	Weather Research Forecast/Community Multi-scale Air Quality

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1.0 OBJECTIVE

1.1 Specific Objectives

This document presents a validation plan for the Earth Venture Instrument-1 Tropospheric Emissions: Monitoring of Pollution (TEMPO) baseline mission Level 2 (L2) geophysical data products. The plan describes product validation maturity level, correlative data sets for product validation, and methodologies to be applied to establish the scientific validity and associated validation level of the products.

The objectives of validation are twofold; (1) assessment and communication of product quality and (2) assessment of areas for product improvement to be conducted in collaboration with the TEMPO algorithm development and science team's characterization of the performance of the L2 products. An intent of the validation plan is to present a broader scope of activities that could be conducted during the post-launch phase of TEMPO and be viewed as opportunities for broad participation or areas for enhanced validation while ensuring a minimum set of activities will be conducted to achieve a basic level of product validation.

TEMPO is a science mission under the NASA EV-I cost capped program, but it is also part of the larger Committee on Earth Observation Satellites (CEOS) Geostationary Air Quality (Geo-AQ) constellation. In addition to TEMPO, the Geo-AQ constellation includes the National Institute of Environmental Research Geostationary Environmental Monitoring Spectrometer (GEMS, NIER, Republic of Korea) and Sentinel-4 Ultra-violet/Visible/Near-Infrared (UVN) sounder (Copernicus/ESA), both of which are operational satellite missions. In an effort to be as consistent as possible with CEOS recommendations on validation needs, as described in the Geostationary Satellite Constellation for Observing Global Air Quality: Geophysical Validation Needs, Oct., 2019 (link in section 1.3), this document represents a "best efforts" approach for validation of L2 data products beyond the Program Level Requirements Appendix (PLRA), and a recognition by the science team that the EV program constraints may limit the use of TEMPO data for certain applications, which may require a greater understanding of product uncertainty and biases. This validation document is focused on bringing additional validation resources to bear on the TEMPO mission and should not be considered as being part of the PLRA.

1.2 Scope of Document

Validation is the process of assessing, by independent quantitative means, the quality of data products derived from system outputs. This document outlines a plan for validation of the TEMPO Level-2 baseline mission products discussed in section 2. It describes favorable validation approaches and identifies correlative datasets, including those from planned community field campaigns or dedicated field campaigns for TEMPO science, which will or could be used to validate the products. Activities presented under this document are meant to cover the baseline mission (launch plus 2 years) with the realization that some activities are likely to occur outside the baseline mission due to the timeframe required to achieve full product validation (Section 3).

1.3 Related Documents

[1] TEMPO Nitrogen Dioxide Retrievals Algorithm Theoretical Basis Document, v1.0, DOIs and https will be added once ATDBs once ATBDs are published, April 2023.

[2] TEMPO Ozone Profile Retrieval Algorithm Theoretical Basis Document, v1.0, DOIs and https will be added once ATBDs are published, April 2023

[3] TEMPO Formaldehyde Retrieval Algorithm Theoretical Basis Document, v1.0, DOIs and https will be added once ATBDs are published, April 2023

[4] TEMPO Cloud Parameters Retrieval Algorithm Theoretical Basis Document, v1.0, DOIs and https will be added once ATBDs are published, April 2023

[5] Geostationary Satellite Constellation for Observing Global Air Quality: Geophysical Validation Needs, CEOS AC/VC and CEOS Working Group on Calibration and Validation, v1.1, Oct. 2, 2019: (https://ceos.org/document_management/Virtual_Constellations/ACC/Documents/GEO%20AQ%20Constellation%20Geophysical%20Validation%20Needs%201.1%202Oct2019.pdf)

[6] TEMPO Green Paper: Chemistry experiments with the Tropospheric Emissions: Monitoring of Pollution instrument, March 2022, https://lweb.cfa.harvard.edu/atmosphere/publications/TEMPO-Green-Paper-March2022.pdf

2.0 INSTRUMENT & SCIENCE PRODUCT DESCRIPTION

2.1 TEMPO Instrument

TEMPO in Geostationary Earth Orbit (GEO) will measure key components of atmospheric pollution over Greater North America, from Mexico City to the Canadian tar/oil sands, and from the Atlantic to the Pacific, at high spatial and temporal resolutions. TEMPO spectroscopic measurements in the ultraviolet (UV) and visible (Vis) spans a spectral range that includes key gases of tropospheric air pollution chemistry: ozone (O_3), nitrogen dioxide (NO_2), and formaldehyde (HCHO). Thus, TEMPO will measure the major components, directly or by proxy, of the diurnal tropospheric ozone chemistry cycle. Multi-spectral observations will provide sensitivity to O_3 in the lowermost troposphere where diurnal measurements are key to understanding both air pollutant emissions and chemistry. The small spatial footprint will resolve pollution sources and distributions within cities. Together, this combination of high temporal and spatial resolution is expected to improve emission inventories, monitor population exposure, and enable effective emission-control and air quality management strategies.

TEMPO takes advantage of a commercial geostationary host spacecraft to make the first North American tropospheric trace gas measurements from GEO. The science and engineering of TEMPO builds on several decades of heritage spectrometers (GOME, SCIAMACHY, OMI, TROPOMI, GOME-2, and OMPS; Burrows et al., 1999; Bovensmann et al., 1999; Levelt et al., 2018; Munro et al., 2016; Flynn et al., 2014) operating in low-earth-orbit (LEO). These legacy instruments have demonstrated the technologies necessary to provide the measurement precision needed to retrieve the L2 geophysical products to the uncertainty thresholds required of the TEMPO mission using very similar physical retrieval algorithms. TEMPO, with its improved detector technology and pre-launch calibration results is anticipated to provide the necessary measurement quality to meet its precision thresholds despite finer spatial sampling while operating from GEO The overlap of TEMPO with legacy missions, both from a personnel and technological perspective, has increased confidence in mission success. Novel to TEMPO are hourly measurements with finer spatial sampling at the GEO geometries over an extended wavelength window. Based on our analysis, the radiometric performance under these conditions, which primarily impacts L2 product precision, is likely of less concern than the quality and spatial scale of the retrieval assumptions (e.g., trace gas a-priori vertical profile, surface reflectivity, cloud fraction), which will impact product accuracy more so than the measurement precision (e.g., Laughner et al., 2019; Judd et al., 2020; Liu et al., 2021; Tack et al., 2021). The new L2 products enabled by TEMPO will therefore need to be characterized through validation. While the characterization of product accuracy is a desired metric, especially for potential operational uses of TEMPO L2 data products, no accuracy metrics exist for these products such that assessing accuracy is beyond the current capabilities of this best effort approach.

Table 2-1 shows key characteristics of the delivered TEMPO instrument and planned measurements. More instrument details can be found in Zoogman et al. (2017), although some characteristics for the final built instrument have changed slightly. The TEMPO instrument is a UV/visible imaging grating spectrometer using two 2-D 2k x 1k charge coupled device (CCD) detectors in one focal plane covering the two bands ~293-494 nm (UV band) and ~538-741 nm (visible band), respectively. The 2k are for the spatial direction and 1k (1028) columns are for the spectral direction. The TEMPO instrument slit aligns the North/South (N/S) direction and simultaneously measures 2048 (N/S or cross-track) spatial pixels, of which 2035 pixels have good performance. Each band has 1028 spectral pixels, of which ~1016 pixels have good performance. The spectral resolution is ~0.6 nm at Full Width at Half Maximum (FWHM) and the spectral interval is ~0.2 nm.

Table 2-1 TEMPO instrument and measurements characteristics

Volume, Mass	1.4 m x 1.1 m x 1.2 m, 137kg
Average operating power	138 W
Detector size	two 2048 (spatial) x 1028 (spectral) detectors
Wavelength range	UV band: ~293 - 494 nm, Visible band: 538 - 741 nm
Spectral resolution	~0.6 nm @Full Width Half Maximum (0.54-0.63 nm)
Spectral sampling	~0.2 nm or ~3 pixels /FWHM (2.7-3.2)

Spectral co-registration[1]	< 0.1 pixel (for UV, visible, UV/visible)
Orbit	geostationary (35786 km), 91.0°W above equator
Boresight	34.45°N, 91.65°W
Instantaneous field of view	41.49 μrad (N/S) x 129.20 μrad (E/W)
Modulation Transfer Function @Nyquist	0.31-0.41 N/S x 0.38-0.49 E/W
Field of view[2]	4.92° N/S x 8.64° E/W
Spatial resolution	2.0 km (N/S) x 4.75 km (E/W) km @center of FOR
Temporal resolution[3]	~1 hour, ~2.85s snapshot / mirror step
Spectra per hour[2,3,4]	2035 N/S (cross-track) x 1226 E/W (mirror step)
Maximum Signal-to-Noise Ratio[5]	1350 @ 330 - 340 nm

[1]Smile, keystone, and UV/visible co-alignment are within 0.1 pixel.
[2]Assuming 123 μrad E/W mirror step size (6.2 μrad overlapping between 2 steps) & 1226 steps (as shown in Figure 2-1)
[3]Nominal mode. In the early morning or late afternoon, optimized mode can measure daylight portion every ~30 mins. Special mode can measure selected portions of FOR at 5-10 mins.
[4]2035 out of 2048 spatial pixels are valid pixels; 1016 out of spectral 1028 pixels are valid pixels.
[5]For the nominal radiance.

Figure 2-1 shows an optimized nominal TEMPO Field of Regard (FOR) of the Earth view over North America. In this example, TEMPO scans the FOR from east to west within one hour in 1226 mirror steps. Each mirror step is a ~2.85 s snapshot of all 2K N/S cross-track pixels. The data are split into 10 granules; each granule includes ~6 minutes of data. Due to the fixed Instantaneous Field of View (IFOV), the footprint on ground increases with the increase of viewing zenith angle or with distance from the TEMPO orbital position. It is ~2.0 x 4.75 km^2 at the center of FOR, varying from 8 km^2 in Mexico City to 21 km^2 at Canadian tar sands. Plotted on Figure 2-1 is the footprint ground sampling area for the FOR, which is in all cases <17 km^2 within the contiguous United States. In the early morning and late afternoon, TEMPO can operate in optimized scan mode, measuring the daylight portion of the FOR at 30-minute resolution. In addition, TEMPO can use up to 25% of the observation time to perform special observations in high-time scan mode, scanning the selected portion of the FOR (i.e., a N/S strip) at much higher temporal resolution (e.g., 5-10 minutes). Special observations can alternate with nominal hourly scans (e.g., 1-hour special observation followed by a 1-hour nominal scan of FOR). For Figure 2-1, an integration time of 100 ms with 26 frames is used to minimize saturation while scanning the FOR within 1 hour in 1226 mirror steps. The signal to noise ratio (SNR) of measurements depends on the measured radiance. For SNR requirement analyses since the inception of the TEMPO project, we have used the nominal radiance, which is a clear-sky average radiance over TEMPO FOR from different seasons. For the nominal radiance, the SNR at native spatial resolution maximizes at ~1350 around 330-380 nm, it is ~900 at 450 nm, and ~500-900 (~900 at 540 nm and ~500 at 740 nm) for the visible band. Below 330 nm, it quickly decreases to 750, 190, 20 at 320, 310, and 300 nm, respectively.

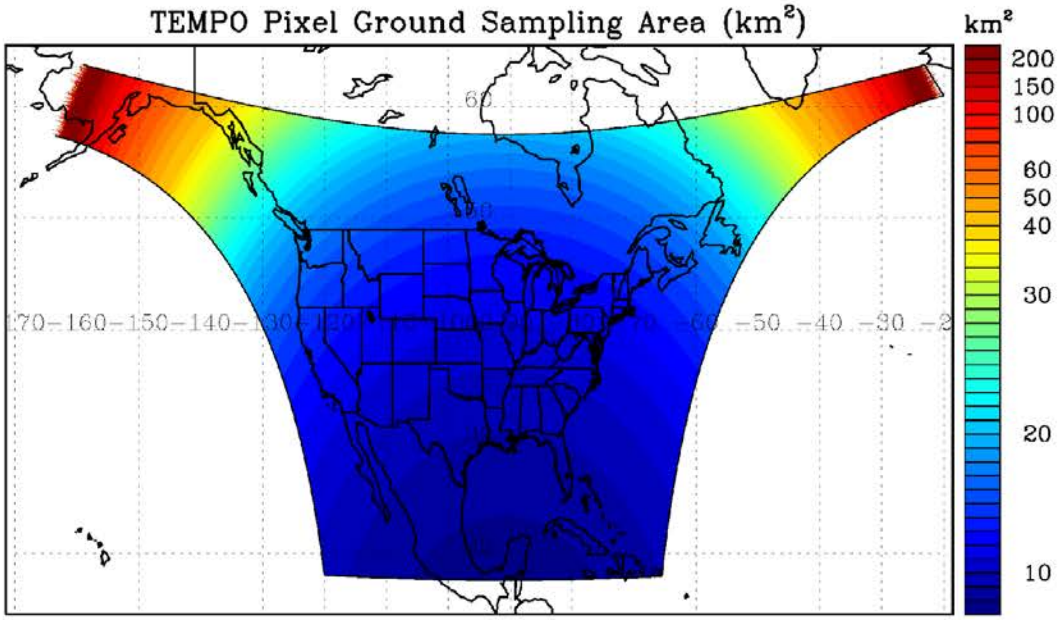

Figure 2-1 The TEMPO field of regard. TEMPO aligns its instrument slit with 2035 N/S valid pixels and scans from east to west in 1226 mirror steps within 1 hour. Shown on the FOR is the TEMPO pixel ground sampling area (km^2). The actual field of regard and number of mirror steps might slightly change due to instrument pointing and optimal scanning strategies.

2.2 Schedule

The TEMPO Mission after launch is divided into four operational phases: Launch and Orbit Transfer, Commissioning, Operations, and End of Life. The Commissioning Phase includes Spacecraft Commissioning and TEMPO Commissioning. Spacecraft Commissioning includes Bus In-Orbit Test (IOT), Payload IOT, drift to the operational orbit location, and the start of commercial services. TEMPO Commissioning includes Activation, On-Orbit Checkout (OOC), and a Post-Launch Acceptance Review (PLAR). Figure 2-2 from the TEMPO Commissioning-Plan (TEMPO-09-0024-TEMPO-Commissioning-Plan_Baseline) below shows the TEMPO Mission Operational Phases.

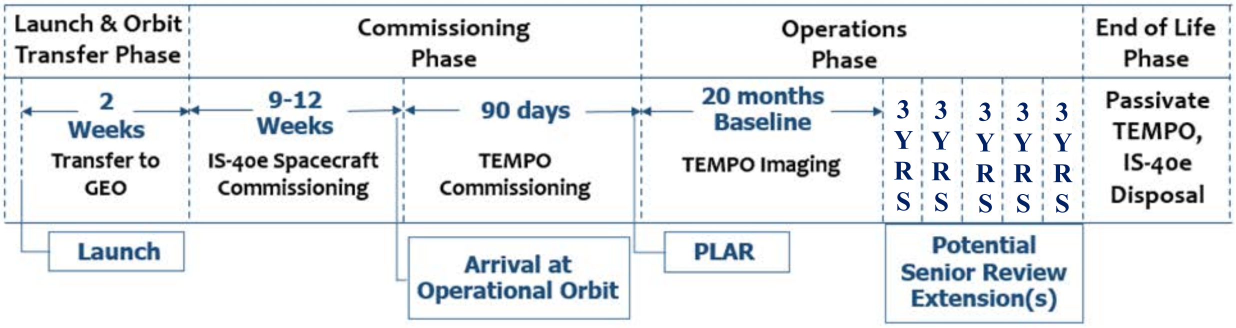

Figure 2-2 Operational Schedule for TEMPO Mission after launch.

TEMPO Commissioning, to take place after IS-40e Spacecraft Commissioning is completed, begins with Activation, which involves a series of activities to power on the TEMPO instrument, outgas the payload, and validate its functionality and performance. This activity will occur over the first 30-45 days of TEMPO Commissioning and will be better known as the spacecraft commissioning timeline evolves. The remainder of the 90-day commissioning period is allotted for OOC, which involves instrument calibration, characterizing instrument performance and refining nominal operations to be fully prepared for the Baseline mission upon successful completion of PLAR. Table 2-2 shows the tentative timeline to release the data products after PLAR and corresponding data latency based on PLRA. All data products will be archived by the NASA Langley Atmospheric Science Data Center (ASDC).

Table 2-2 Project schedule for TEMPO Data Products

Data Product	Description	Time beyond On-Orbit Checkout (OOC) to deliver initial data	Maximum data latency after first release for ≥ 80% of products
Level 0	Raw Instrument Data	2 months	Within 2 hours of receipt at SAO
Level 1	Engineering Unit (EU)-Converted Data	4 months	Within 3 hours of production of L0 and receipt of ancillary data required by the Level 0 to Level 1 algorithm at SAO
Level 2	Derived Geophysical Data	6 months	Within 24 hours of production of L1 at SAO
Level 3	Derived Gridded Geophysical Data	6 months	1 month after completion of data accumulation required for individual geophysical products

2.3 Standard Product Requirements

Table 2-3 presents the current planned L2 products for ozone, nitrogen dioxide, and formaldehyde, along with product precision and frequency requirements. The required precision in Table 2-3 is set for retrievals with four native pixels coadded at a spatial scale of ≤ 60 km^2 at the center of FOR. As the spatial resolution of 4 coadded pixels is ~40 km^2, the planned product spatial scales listed Table 2-3 meet or exceed this requirement. Note that there are no specific accuracy requirements in the PLRA and GEO-CAPE science traceability matrix but we will assess the bias of these products relative to independent measurements during the planned validation activities.

Although we have used the term "product" for each requirement, strictly speaking, these are the retrieved variables or quantities rather than stand-alone products. All the three ozone quantities can be derived from the TEMPO ozone profile algorithm, which retrieves partial columns of ozone at 24 layers including 0-2 km ozone for the first layer above the surface. Tropospheric column O_3 and total column O_3 can be integrated from the retrieved profile. Ozone profile retrievals will be performed at a coarser spatial resolution after coadding at least four pixels in the cross-track direction because it is very computationally intensive, and we do not have adequate computational resources. As 0-2 km O_3 and tropospheric column O_3 are from the ozone profile algorithm, validating these quantities often includes comparison of O_3 profiles. There is a separate TOMSV8.5 total ozone algorithm which can produce total column O_3 quickly at the native spatial resolution. Both total column NO_2 and tropospheric column NO_2 are from the TEMPO NO_2 algorithm; tropospheric column HCHO is from the TEMPO HCHO algorithm. Cloud parameters (effective or radiative cloud fraction, and cloud Optical Centroid Pressure (OCP)) are important inputs to the trace gas retrieval algorithms. Although there are no specific requirements for the cloud parameters, we have recently developed a O_2-O_2 absorption-based cloud retrieval algorithm to retrieve these two parameters. As these cloud parameters are essential to the trace gas algorithms, the cloud product also needs to be validated. Therefore, we will cover the validation of L2 ozone, NO_2, HCHO, and cloud products in this L2 science validation plan. Other products including CHOCHO, SO_2, and aerosol are baseline products in the original TEMPO proposal but were removed from the list at Key Decision Point for Phase C (KDP-C) in 2015 due to budget concerns and the fact that the TEMPO instrument is a cost-cap project. Although there is some on-going effort to produce these products along with additional operational/research products like BrO and H_2O, their algorithms have not yet been integrated to the SDPC software, and the validation of these products is not included in this L2 science validation plan.

Table 2-3 TEMPO mission Level 2 data product (variable) requirements. Note that the spatial resolution for the precision requirement is with 4 native pixels coadded, not the actual product resolution listed below.

Product Name	Product Horizontal Resolution N/S x E/W @ center of FOR[1]	Product Precision	Frequency[2]
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	1.0×10^{15} molecules cm^{-2}	1 hour
Tropospheric Column NO_2	2.0 x 4.75 km^2	1.0×10^{15} molecules cm^{-2}	1 hour

Tropospheric column HCHO	2.0 x 4.75 km^2	1.0 × 10^{16} molecules cm^{-2}	3 hours

[1]Measurement requirements are met up to 70° SZA for O_3, NO_2, and HCHO products.

[2]The temporal revisit does not indicate sampling rate as the nominal spatiotemporal sampling is fixed (~1226 E/W mirror steps per hour, with a total of 1226E/W x 2035 N/S pixels ~2.5M pixels per hour, so that each measurement is a snapshot of ~2.85 seconds) and the nominal product will always be produced hourly. "Frequency" here means the number of measurements (typically hourly) that can be averaged to see if the product meets the precision requirements.

3.0 VALIDATION APPROACH

The TEMPO PLRA related to validation states, "Compare space-based and ground-based retrievals of products using correlative data collected from daytime (solar zenith angles $\leq$ 70° for all products) observations at least one month each season from at least three (3) ground validation sites in the US to identify and correct regional-scale and diurnal systematic biases in the space-based products and to demonstrate required precisions in polluted clear-sky scenes to the levels listed in Table 2-2. At the validation sites, Pandora solar spectral-radiometer measurements will be the primary source of correlative data for trace gas column densities. Ozonesondes will contribute to the validation of the O_3 mixing ratio on a best effort basis."

The PLRA requirement of three ground sites for validation of TEMPO products will be met. There are more than 60 Pandora instruments within the TEMPO FOR that will serve as the primary ground-based network for validating NO2, HCHO, and total column ozone. With the development of TOLNet after the finalization of TEMPO PLRA, there are eight operating Lidar stations that will serve as the primary ground-based network for validating TEMPO tropospheric and 0-2 km ozone. At the discretion of the TEMPO science team, the remainder of the "best efforts" validation approach presented in this document may be used to aid in validation results for the PLRA.

The evolving validation maturity of TEMPO Level 2 products beyond the PLRA is described by three levels: Beta, Provisional, and Full validation. Once SAO has approved the Level 1b (L1b) products for Level 2+ data processing, validation analysis of the L2+ data product will begin towards Beta maturity. Further levels of maturity (Provisional and Full validation) require a longer-term data record. A general description of the three maturity levels follows:

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.

Adopted from the GOES-R ABI Product Validation Plan (PVP) for Suspended Matter/Optical Depth and Aerosol Size Parameters, Figure 3-1 contains a more descriptive set of activities associated with the three product maturity levels, along with quantitative statements as to how validation activities might relate to the current state of data products.

Beta Validation

Preparation Activities
- Initial calibration applied (L1b).
- Rapid changes in product input tables, and possibly product algorithms, can be expected.
- Product quick looks and initial comparisons with ground truth data (if any) are not adequate to determine product quality.
- Anomalies may be found in the product and the resolution strategy may not exist.

End state
- Products are made available to users to gain familiarity with data formats and parameters.
- Product has been minimally validated and may still contain significant errors.
- Product is not optimized for operational use.

Provisional Validation

Preparation Activities
- Validation and quality assurance (QA) activities are ongoing, and the general research community is now encouraged to participate.
- Severe algorithm anomalies are identified and under analysis. Solutions to anomalies are in development and testing.
- Incremental product improvements may still be occurring.
- Users are engaged in the Customer Forums (L2+ products only), and user feedback is assessed.

End state
- Product performance (L1b or L2+) has been demonstrated through analysis of a small number of independent measurements obtained from selected locations, periods, and associated ground-truth/field program efforts.
- Product analysis are sufficient to communicate product performance to users relative to expectations.
- Documentation of product performance exists that includes recommended remediation strategies for all anomalies and weaknesses. Any algorithm changes associated with severe anomalies have been documented, implemented, tested, and shared with the user community.
- Testing has been fully documented.
- Product ready for operational use and for use in comprehensive calibration/validation activities and product optimization.

Full Validation

Preparation Activities
- Validation, QA, and anomaly resolution activities are ongoing.
- Incremental product improvements may still be occurring.
- Users are engaged and user feedback is assessed.

End state
- Product performance for all products is defined and documented over a wide range of representative conditions via ongoing ground-truth and validation efforts.
- Products are operationally optimized, as necessary, considering mission parameters of cost, schedule, and technical competence as compared to user expectations.
- All known product anomalies are documented and shared with the user community.
- Product is operational.

Figure 3-1 TEMPO Level 2 & 3 product maturity levels qualitative descriptors

By applying the qualitative descriptors to all validation stages of the TEMPO L2 data products the following product-specific performance indicators (PSPIs) are thresholds for each maturity level.

Nitrogen Dioxide Product Validation Overview:

Three PSPIs have been defined to attain Beta maturity for TEMPO NO_2.

- 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.

Two additional PSPIs have been defined to attain Provisional maturity. These tests will quantify bias, precision, and uncertainty for an extended period that includes some but not all seasonal variability. This extended period must be sufficient for the user to evaluate whether the product is ready for operational testing. The PSPIs that support Provisional maturity are listed below.

- NO_2-04: Assess performance metrics (bias/precision/uncertainty) of the tropospheric NO2 product across the CONUS for 1 month period in two seasons, preferably summer and winter, that includes a range of column densities.
- NO_2-05: Conduct deep-dive analyses for an episode with relatively poor product performance, identify the root cause and recommend algorithm improvements.

Finally, two PSPIs have been defined to attain Full maturity by further extending the conditions under which NO_2 bias, precision, and uncertainty performance is quantified to include a seasonally representative number of independent measurements. The PSPIs that support Full maturity are listed below.

- 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.
- NO_2-07: Assess bias, precision, and uncertainty of the tropospheric NO2 product over areas of interest using data gathered during targeted field campaigns.

Ozone Products Validation Overview:

Three PSPIs have been defined to attain Beta maturity for TEMPO O_3 products.

- O_3-01: Distinguish high tropospheric O3 areas resulting from stratospheric intrusion or pollution transport or pollution from nearby normal or low O3 areas for three select high-low O3 scene combinations.
- 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.
- 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.

Two additional PSPIs have been defined to attain Provisional maturity. These tests will quantify bias, precision, and uncertainty for an extended period that includes some but not all seasonal variability. This extended period must be sufficient for the user to evaluate whether the product is ready for operational testing. The PSPIs that support Provisional maturity are listed below.

- 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.
- 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.

Finally, two PSPIs have been defined to attain Full maturity by further extending the conditions under which tropospheric O_3 bias, precision, and uncertainty performance is quantified to include a seasonally representative number of independent measurements. The PSPIs that support Full maturity are listed below.

- 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.
- O_3-07: Assess bias, precision, and uncertainty of the tropospheric product over areas of interest using data gathered during targeted field campaigns.

Formaldehyde (HCHO) Product Validation Overview

Three PSPIs have been defined to attain Beta maturity for TEMPO HCHO .

- HCHO-01: Distinguish high HCHO concentrations from background concentrations. Given HCHO retrieval noise levels, these qualitative evaluations may use spatial or temporal averaging.
- HCHO-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.
- HCHO -03: Identify two radiatively homogenous, cloud-clear, low HCHO 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.

Two additional PSPIs have been defined to attain Provisional maturity. These tests will quantify bias, precision, and uncertainty for an extended period that includes some but not all seasonal variability. This extended period must be sufficient for the user to evaluate whether the product is ready for operational testing. The PSPIs that support Provisional maturity are listed below.

- HCHO-04: Assess performance metrics (bias/precision/uncertainty) of HCHO 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 HCHO.
- HCHO-05: Conduct deep-dive analyses for an episode with relatively poor product performance, identify the root cause of the discrepancy and recommend algorithm improvements.

Finally, two PSPIs have been defined to attain Full maturity by further extending the conditions under which HCHO bias, precision, and uncertainty performance is quantified to include a seasonally representative number of independent measurements. The PSPIs that support Full maturity are listed below.

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

4.0 Post-Launch Validation Activities

4.1 Early Orbit (Pre-Beta) Assessment by TEMPO Algorithm Team

During the Commissioning Phase and the period immediately following On-Orbit Checkout an initial assessment of the TEMPO L1B and 2 products will be carried out by the algorithm teams. This assessment is to ensure the product generation is performing as expected and to identify potential areas of focus before the data products proceed to the Beta Validation phase. This effort will involve cursory-level comparisons of key geophysical parameters with independent measurements correlated in time and space.

4.2 Science Product Validation and Evaluation

Science product validation and evaluation efforts to the degree feasible will begin during the Commissioning Phase with main validation occurring over the Operational Phase of the TEMPO mission. Validation will include systematic long-term validation of the geophysical data products over a dynamic range of the products and of their observation conditions, which include solar zenith angles, cloud properties, surface albedo, and abundance of pollutant. This will be accomplished primarily through the use of LEO satellites and ground-based correlative measurements, synergetic science field campaigns along with indirect assessment and evaluation with chemical transport models and other correlative measurements such as surface concentration air quality network data and small-sensor networks of quality.

The TEMPO ATBDs contain the detail on processes and inputs to retrieve trace gas abundances from the solar backscatter radiance measurements, including the inputs for converting the slant column to a vertical column density via the air mass factor (AMFs). Uncertainties in AMF calculations can be a large source of uncertainty for NO_2 and HCHO L2 data products, particularly over pollutants areas (Boersma et al., 2007; Martin et al., 2002). Primary factors which drive this uncertainty is the AMF sensitivity to surface reflectance, clouds, aerosols, and a priori profile information (Lorente et al., 2017). Within the baseline mission of 20 months the initial validation is focused on assessing the quality of the L2 data products with correlative measurements, as an in-depth evaluation of major factors impacting product uncertainty is beyond the current scope. Retrieval sensitivity (e.g., scattering weights, averaging kernels) and a-priori profiles will also be taken into account, if possible and appropriate, to evaluate and improve uncertainties resulting from a priori errors.

For each region of interest, the main comparison metrics will be the spatial and temporal correlations and gradients, mean bias, standard deviation, root mean square of the differences, and linear regression slope. Given the novelty of fine-spatial scale measurements, best efforts special emphasis will be placed on pairwise validation efforts at spatial scales of one TEMPO pixel. The spatial, diurnal, daily, monthly, seasonal variation, and trend of the mean biases and other metrics can be assessed to check the spatiotemporal consistency of TEMPO products.

4.2.1 Validation with satellite measurements

Intercomparisons with correlative measurements from satellites form a key part of TEMPO product assessment and are complementary to validation using ground-based and airborne measurements. Satellite-based measurements provide ample cross-validation opportunities with large spatial coverage and similar spatial resolution, but only at one time per day from LEO or hourly from the Lagrange-1 point L_1 for EPIC measurements of total and tropospheric ozone columns. Obtaining satellite coincidences minimizes errors due to spatiotemporal collocation and sampling and make it easier to conduct comparisons as a function of various geophysical parameters such as cloud fraction and cloud-height, surface albedo, and viewing geometry. In particular, satellite-based instruments will provide the TEMPO algorithm team a tool to perform immediate validation during pre-beta assessments leveraging the rich legacy of any relevant prior or ongoing validation efforts. Table 4-1 lists satellite instruments that will have products available for TEMPO intercomparisons.

Table 4-1 Satellite instrument[1] datasets for intercomparison with TEMPO baseline products

Instrument[1] (agency)	Product providers	Species of interest	Satellite(s)	Equator Crossing Local Time	Spatial resolution (km^2)

TROPOMI (ESA,EUMETSAT)	EUMETSAT	NO_2, HCHO, O_3 (total and profile)	Sentinel-5P	13:30	3.5 x 5.5 (nadir)
OMI (NASA/ESA/NIVR)	NASA, ESA	NO_2, HCHO, O_3 (total and profile)	Aura	13:45	13 x 24 (nadir)
GOME-2(B/C) (ESA,EUMETSAT)	EUMETSAT	NO_2, HCHO, O_3 (total and profile)	Metop-B Metop-C	9:30	40 x 80
OMPS-NM (NASA/NOAA)	NASA, NOAA	HCHO, O_3 (total and tropospheric O_3)	Suomi NPP JPSS-1, JPSS-2	13:35	50 x 50 (nadir) 12 x 17 (nadir)
OMPS-LP (NASA/NOAA)	NASA	O_3 (stratospheric profile & column)	Suomi NPP JPSS-2	13:35	~125 along track, 3 samples across track
MLS (NASA)	NASA	O_3 (stratospheric profile & column)	Aura	13:45	6 (across) x 200 (along)
IASI (ESA,EUMETSAT)	EUMETSAT	O_3 (total and profile)	Metop-B Metop-C	9:30	4 x 12 (center of cell)
AIRS (NASA)	NASA	O_3 (TROPESS)	Aqua	13:30	13 x 24 (if combined with OMI) or 45 x 45
CrIS (NASA/NOAA)	NASA	O_3 (TROPESS)	SNPP JPSS1, JPSS2…	13:30	14 X 14
Sentinel-5 (ESA,EUMETSAT)	EUMETSAT	NO_2, HCHO, O_3 (total and profile)	Metop-SG-A1 Metop-SG-A2 (launch≥2024)	9:30	7.5 x 7.5
EPIC (NASA)	NASA	O_3 (total/tropospheric),cloud height, cloud fraction, aerosols	DSCOVR	N/A (Lagrange-1 orbit)	~20 x 20

[1]OMI, MLS, AIRS, MODIS, CPR and CALIOP data availability is contingent on continuing operations of EOS Aura, Terra, Aqua, CloudSAT and CALIPSO satellites.

Upon generation of initial TEMPO data products and prior to release for science team involvement and validation, the SAO Team will conduct an assessment of each data product. This will involve limited comparisons by qualitatively checking the spatiotemporal distribution of TEMPO products against those correlative satellite products to make sure the retrievals look reasonable without showing very large retrieval biases or spatiotemporal dependent anomalies. For higher-level validation, careful quantitative intercomparison and analysis will be conducted. The intercomparisons will focus on geographic regions of interest representative of different scenarios within TEMPO's domain. The goal is to explore retrieval performance as a function of geophysical parameters and observation geometries.

4.2.1.1 LEO instruments

The instruments listed in Table 4-1 are all anticipated to be in orbit at the time of TEMPO launch with the exception of the Sentinel-5 instruments (scheduled launch in 2024). Other than

EPIC/DSCOVR and ABI/GOES-R series, these instruments collect measurements from LEO, in a sun-synchronous orbit that passes over the equator at the same local solar time each day and measuring a given location once per day. Standalone TEMPO-LEO comparisons will help assess TEMPO Level 2 products and provide a unique intersection with the Geo-AQ constellation members, GEMS and Sentinel-4 . For total column ozone and broader band spectral L1B validation, DSCOVR/EPIC provides hourly sunlit disc measurements from the Lagrange-1 orbit at 20km x 20km spatial resolution and can further link GEO missions for commonly measured variables.

Many of these LEO instruments are nadir-viewing UV/visible instruments similar to TEMPO and provide similar measurements of NO_2 and HCHO with high sensitivity to the lower atmosphere, total O_3 and O_3 profiles. OMPS-NM operates only in the UV and as a result measures NO_2 from weaker spectral absorption features. CrIS, AIRS, and IASI are all infrared sounders with variable vertical sensitivity to O_3 primarily limited to the upper and middle atmosphere. In addition to providing the TEMPO baseline products NO_2, HCHO, total O_3 and O_3 profile, some of these missions also provide products for SO_2, water vapor, BrO, CHOCHO, and aerosol-layer heights presenting opportunities for validation of non-baseline TEMPO Level 2 products that are not included in this validation plan.

O_3 profile algorithms from both LEO instruments and EPIC use an UV-only approach (even for the GOME-2 instruments that have visible channels), and thus have less sensitivity to lower tropospheric O_3 in comparison to retrievals derived from TEMPO UV combined with visible wavelengths (Zoogman et al., 2017). The infrared (IR) instruments, IASI, AIRS and CrIS, and the microwave sounder, MLS, are included in Table 4-1 as they have been used in combination with OMI/GOME-2/OMPS/TROPOMI to perform joint UV/IR or microwave retrievals to enhance sensitivity to lower tropospheric O_3. This has been done as part of the TRopospheric Ozone and its Precursors from Earth System Sounding (TROPESS) Project (Fu et al., 2013, 2018, https://tes.jpl.nasa.gov/tropess/), in Europe (Cuesta et al., 2015) and with AURA science team (Ziemke et al., 2006). Limb viewing O_3 profiles by MLS and OMPS-LP have been used for validating stratospheric O_3 profiles and columns, such as in previous OMI validation with MLS data (Liu et al., 2021; Huang et al., 2018).

4.2.1.2 NO_2 and HCHO intercomparisons

NO_2 and HCHO total column products can be or are provided by all UV/visible LEO instruments listed in Table 4-1. Of the instruments currently on orbit, the Sentinel-5P/TROPOMI instrument provides observations with the finest spatial resolution while maintaining a similar precision to coarser missions. As a result, TROPOMI will be the priority LEO instrument for initial TEMPO comparisons. TROPOMI NO_2 and HCHO products are routinely assessed using measurements from the NDACC zenith sky DOAS network, Pandora network and MAX-DOAS instruments (NO_2) and the NDACC FTIR network and MAX-DOAS instruments (HCHO) (De Smedt et al., 2021; Verhoelst et al., 2021; Vigouroux et al., 2020), with results available through the Validation Data Analysis

Facility. TEMPO-LEO comparisons will span two times of the day, at ~9:30 AM (GOME-2) and at ~ 1PM LST (OMI, OMPS, TROPOMI) providing opportunity to assess different assumptions about the a priori vertical profiles and other input parameters incorporated in the various products and their diurnal variability. When comparing L2 products, we will adjust for product profile differences using scattering weights to both evaluate errors due to a-priori profiles and to narrow down to other sources of error. The OMI and OMPS operational HCHO products (González Abad et al., 2015, 2016) were developed and are maintained by the SAO TEMPO algorithm team and share a spectral fitting and retrieval framework with TEMPO. As a result, these products will be useful for comparisons with TEMPO for algorithm verification.

4.2.1.3 O_3 intercomparisons

TEMPO's total O_3 from both TOMS V8.5-based total O_3 and the O_3 profile algorithms can be validated using multiple satellite datasets. TROPOMI provides measurements collected at 13:30 local time with a pixel spatial resolution close to that of TEMPO. Comparison of the TEMPO TOMS V8.5-based total ozone product with OMPS/OMI/EPIC total O_3 provides algorithmic consistency to aid identification of differences due to differing detector characteristics and observation geometries. Combining the intercomparison with GOME-2 total O_3 at its 9:30 overpass with the afternoon comparison assesses the diurnal variation of total O_3 performance to some extent. Intercomparison with EPIC total O_3 and tropospheric O_3 as a function of hour during the day can be used to assess the diurnal variation of the quality of retrieved total and tropospheric O_3.

The O_3 profile in the stratosphere and corresponding stratospheric ozone column will be evaluated with spatial-temporally collocated high vertical resolution limb observations from MLS and OMPS-LP with and without applying TEMPO retrieval averaging kernels following Liu et al. (2010) and Huang et al. (2018). The entire O_3 profile will first be compared to latest V2 OMI retrievals which is based on the SAO UV-only O_3 profile algorithm to minimize algorithm differences and will also be compared with TROPOMI and GOME-2 operational retrievals from other groups to assess the retrieval performance during both morning and early afternoon. Due to similar vertical resolution, retrieval averaging kernels do not need to be similarly applied as does those with MLS or OMPS-LP observations. However, differences due to a-priori assumptions can still be accounted for using averaging kernels and a-priori profiles from both retrievals. TEMPO tropospheric O_3 columns can be compared to those from OMI, TROPOMI, GOME-2, OMPS, and EPIC products either from O_3 profile retrievals or from residual-based techniques. Intercomparison with morning overpass LEO (GOME-2) and afternoon overpass LEO (e.g., TROPOMI, OMI, OMPS), and with EPIC as a function of local time can assess the diurnal variation of the retrieval performance of TEMPO tropospheric ozone. O_3 profiles, especially tropospheric O_3 and 0-2 km ozone, will also be compared with spatiotemporally collocated TROPESS joint UV/IR products to assess the capability and performance of TEMPO UV/Visible retrievals to capture O_3 enhancement in 0-2 km above the surface and in the troposphere.

DSCOVR (Deep Space Climate Observatory) is a satellite mission in operation since June 2015 observing the entire sunlit Earth from an orbit near a gravitational balance Lagrange-1 (L_1) point

1.5 million km from Earth. The instrument onboard DSCOVR relevant to TEMPO is EPIC (Earth Polychromatic Imaging Camera). EPIC is a ten-channel narrow band CCD camera ranging from 317 nm to 780 nm. Science products are obtained once per hour during the Northern Hemisphere (NH) summer season and once per 90 minutes during NH winter. Its continuous synoptic (sunrise to sunset) view of the sunlit side of Earth from L_1 provides quasi-geostationary observations for comparison with TEMPO, overlapping view geometries at noon local solar time over the TEMPO orbital slot longitude (91.0° W). DSCOVR-EPIC's spatial resolution for scientific products is about 20 km x 20 km near the center of each Earth image.

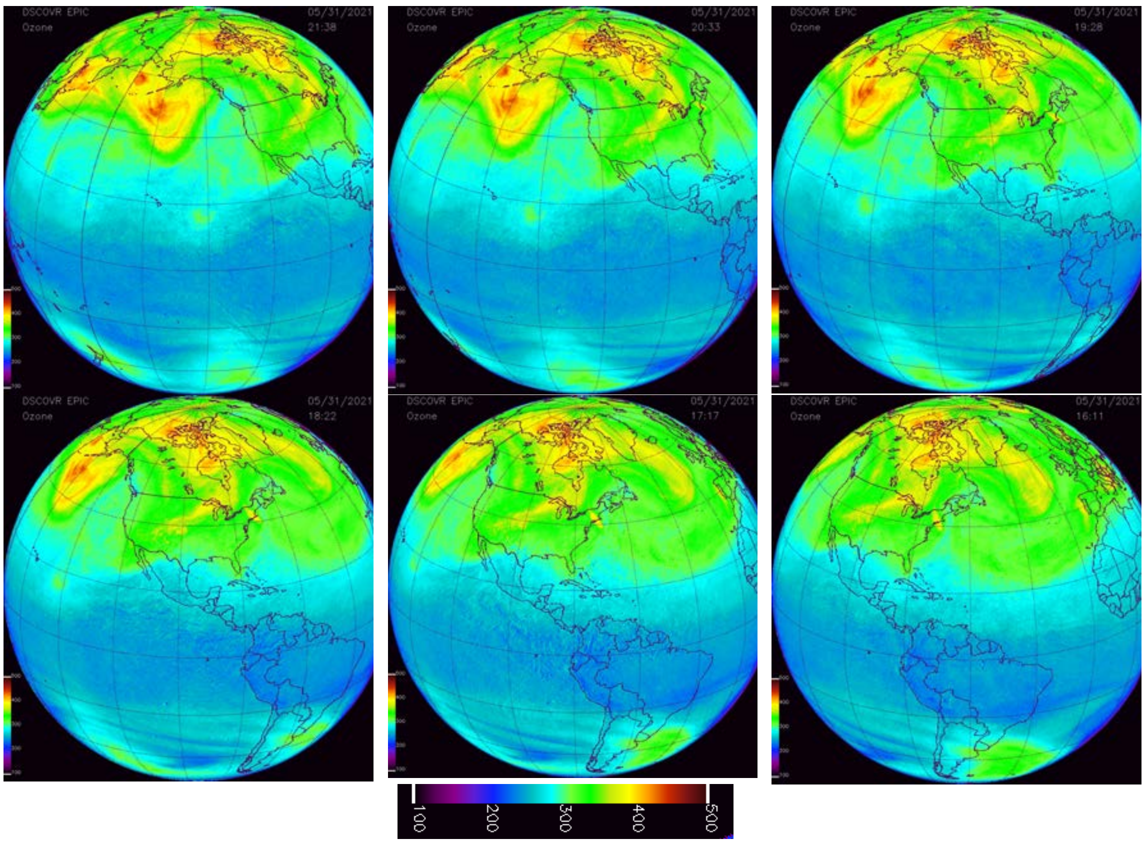

Figure 4-1 Examples of a sequence of EPIC ozone data from 31 May 2021 at 21:38, 20:33, 19:28, 18:22, 17:17, and 16:11 GMT in the TEMPO FOV. Note that the variability of ozone is compressed because of the wide color scale.

EPIC has two total ozone products from two different groups (Kramarova et al., 2021; Huang et al., 2022), covering the regions of interest to TEMPO as shown in Figure 4-1 for ozone. Both products are similar to the TEMPO total ozone algorithm with tropospheric ozone columns derived by subtracting model stratospheric ozone columns from total O_3. Therefore, these products can be used for intercomparisons with TEMPO total ozone using both the total ozone and O_3 profile algorithms and tropospheric ozone column. EPIC data can also be used to validate cloud fraction, cloud height, aerosol amounts, and plume height. Additionally, its radiance products are of interest for backscattered radiance validation of TEMPO calibration. This effort will build off the EPIC project that has significant experience in developing scene matching with other near-Earth satellites.

4.2.1.4 Cloud intercomparisons

The purpose of the TEMPO O2-O2 clouds is to support the TEMPO trace gas retrievals. The product includes Effective Cloud Fraction (ECF) and cloud Optical Centroid Pressure (OCP) which are required for TEMPO trace gas retrievals. The algorithm is adapted from NASA's OMI O2-O2 cloud algorithm (Vasilkov et al., 2018), with the use of the SAO trace gas spectral fitting algorithm.
While numerous instruments provide cloud information, different products make different assumptions and approximations, and have different purposes and limitations. As a result, the retrieved cloud products are usually not directly comparable (Compernolle et al., 2021). Consequently, differences among cloud products are expected. Nonetheless, inter-comparisons can still be useful for understanding the characteristics of different cloud products, checking the overall reasonableness, and inferring the cloud influences on trace gas retrievals. The satellite cloud products below are among the datasets to be considered for this purpose.

The Visible Infrared Imaging Radiometer Suite (VIIRS) on board Suomi NPP and NASA-NOAA JPSS satellites provide Level 2 cloud products at a spatial resolution of 750 m. These products include cloud mask, cloud type and cloud phase, cloud top information (i.e., pressure, height, temperature and layer), cloud base height, cloud optical and microphysical properties (e.g., optical depth, effective radius, liquid water path, ice water path). Cloud fraction is not directly available from VIIRS, but cloud mask can be used to compute cloud fractions for larger areas and subsequently used for comparisons with TEMPO. The TROPOMI NPP cloud fraction employs this approach. The VIIRS cloud top pressure is derived from the cloud top temperature product using the Numerical Weather Prediction (NWP) profiles, where the cloud top temperature is retrieved from IR observations. The VIIRS cloud top heights can be averaged onto the TEMPO pixels to compare with the TEMPO cloud pressure. Suomi NPP VIIRS clouds have been used to validate TROPOMI clouds (Compernolle et al., 2021). TROPOMI clouds can also be compared with TEMPO clouds, though it is noted that TROPOMI clouds are based on different assumptions which will naturally lead to differences with respect to TEMPO (Compernolle et al., 2021).
The GOES-R Advanced Baseline Imager (ABI) cloud is an attractive option for comparison with TEMPO cloud because both are observing North America from a GEO orbit. In addition, the ABI has high spatial (2 km) and temporal (10 min or better) resolutions. As a result, the ABI product can be exploited to better co-locate with TEMPO as well as to provide information on sub-pixel and sub-hourly variability.

The standard EPIC Level 2 cloud product include cloud mask, cloud effective pressure/ height, and cloud optical thickness (Yang et al., 2018). The cloud effective pressure is the most relevant to TEMPO clouds and is derived from the O2 A-band and B-band pairs under the assumption of mixed Lambertian-Equivalent Reflectivity where the surface and clouds are approximated with Lambertian reflectors. Clouds are assumed to have an albedo of 0.8. The effective cloud fraction is derived during the retrieval of cloud effective pressure. These assumptions are similar to those used for TEMPO. Furthermore, EPIC resolves daytime cloud variations, providing an opportunity to compare with TEMPO's hourly observations.

The CloudSat Cloud Profiling Radar (CPR) and the CALIPSO Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) provide vertical profiles of clouds. These are nearing end of life but will be used to examine TEMPO clouds in case of overlapping observations. The Earth Clouds, Aerosols and Radiation Explorer (EarthCARE) satellite to be launched in 2024 will provide 3D cloud structure measurements using its lidar, radar and imager with a ground pixel size of ~500 m.

4.2.1.5 GEO constellation algorithm intercomparisons

With algorithm and/or input reader modifications, GEMS and Sentinel-4 retrieval teams may be able to produce independent NO2, HCHO and O3 (total and UV-only profile) products for comparison with the operational TEMPO Level 2 products. Similar limited studies have been performed recently by the TEMPO and Sentinel-4 algorithm teams as part of GEMS validation, using GEMS Level 1C data in TEMPO/Sentinel-4 algorithms to produce complementary independent Level 2 GEMS products. These types of efforts can provide valuable input to the TEMPO algorithm team and help to isolate the impacts of various parameters in spectral fitting and air mass factor calculations. Importantly, they also provide context for TEMPO, GEMS and Sentinel-4 measurements within the global air quality constellation.

4.2.2 Validation with ground-based correlative measurements

The Brewer-Dobson-Networks have served as the primary ground-based remote sensing measurements for O_3, providing long, uninterrupted, well-maintained, homogeneously calibrated time-series for satellite validation. Over the past decade the Pandonia Global Network (PGN) and Tropospheric Ozone Lidar Network (TOLNet) have emerged as complementary networks with a primary focus on O_3, NO_2, and HCHO, with each TOLNet location containing both an ozone lidar and pandora spectrometer. The combination of these three networks provides a set of routine and systematic correlative observations which can be used for TEMPO validation.

4.2.2.1 Pandonia Global Network: Pandora (Direct Sun + MAX-DOAS)

4.2.2.1.1 Instrument and method summary

During the baseline mission, a primary means of validation of the TEMPO L2 NO_2 and HCHO data products is to compare them with equivalent ground-based measurements from the Pandonia Global Network (PGN- https://www.pandonia-global-network.org/). In early 2022 the PGN contains approximately 60 Pandora instruments distributed across the TEMPO FOR. Figure 4-2 shows the distribution of the Pandoras across the TEMPO FOR plotted with TROPOMI Tropospheric Vertical Column NO_2 averages for 2018 (May-December). The distribution of the Pandoras is heavily weighted to polluted urban areas. Rural or remote sites are few but include sites in coastal Puerto Rico outside Fajardo, in Konza Prairie outside Manhattan, KS, in Altzomoni outside Mexico City, in the Berkshire Mountains outside Cornwall, CT, in Egbert outside Toronto and on Table Mountain NW of Los Angeles, CA.

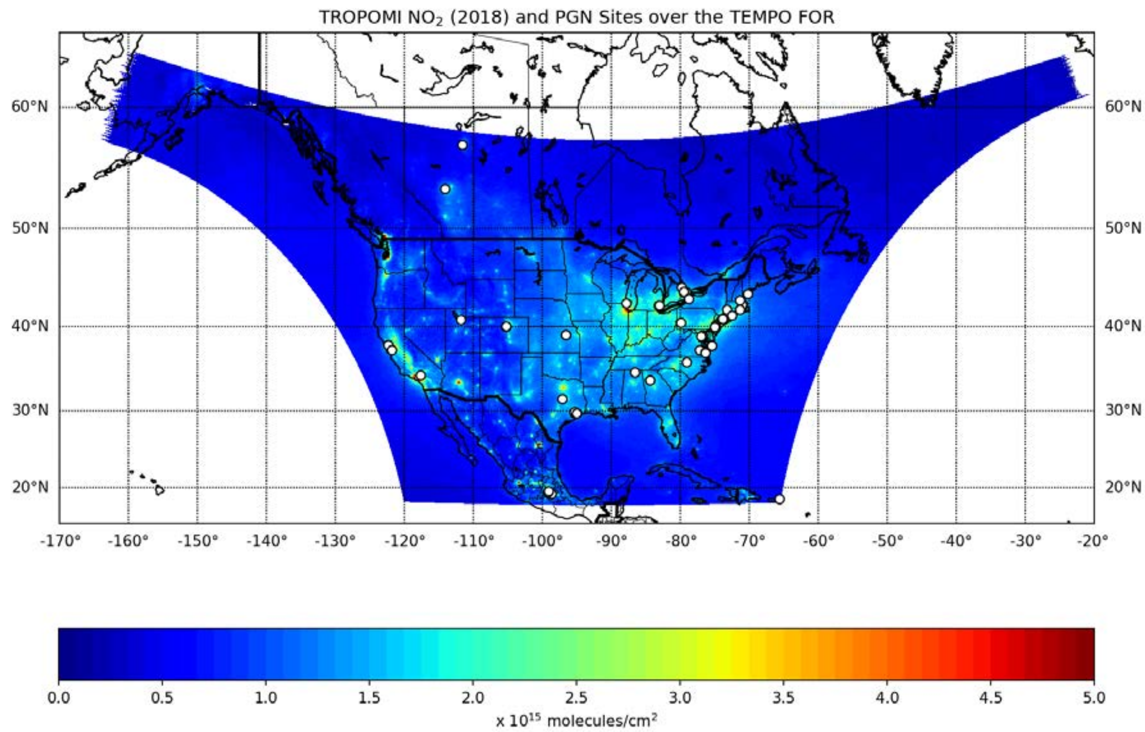

Figure 4-2 Pandora spectrometer locations (white circles) within the TEMPO FOR with TROPOMI Tropospheric Vertical Column NO_2 (May-Dec 2018).

Pandora L2 data products are available with open access in near-real time from the PGN website. Standard Level 2 NO_2, HCHO, and O_3 data products for Pandora from the latest Blick processing software, version 1.8 (v1.8), includes the generation of the following L2 data products: total column NO_2, HCHO and O_3; NO_2 and HCHO tropospheric column; NO_2 and HCHO surface concentration; and tropospheric profile of HCHO and NO2.

PGN is a collection of consistently designed and calibrated instruments capable of collecting high-quality direct-sun, direct-moon and sky-scan MAX-DOAS) spectrally resolved UV/Visible radiances. The PGN adheres to spectrometric quality standards by providing robust laboratory and field calibration, analysis protocols and pre-defined QA/QC determinations. The spatial sampling and spectral quality depend on the sampling mode. The direct-sun mode measurement has a 2.4 degree field of view (FOV) FWHM due to the addition of a diffuser in the view path, which captures the solar disc (~0.53 degrees) and negligible diffuse scatter. For a solar zenith angle of 0 degrees, the 0.53 degree solar disc implies the diameter of conical sampling of approximately 10 meters at 1 km altitude AGL. At a solar zenith angle of 70 degrees, the diameter of conical sampling is 24 m and the path reaches 1 km altitude AGL at a distance of 2.75 km from the instrument location along the solar azimuth. The inference of trace gas abundance in direct-sun mode requires quantification of the pollutant in a carefully selected reference spectra via extrapolation. One of two extrapolation methods are operationally used to infer the abundance within the reference spectra with bias improving as a longer time series of measurements are incorporated into the analysis (Luftblick, 2022). One month of accumulated clear-sky data is usually sufficient. The bias of this extrapolation is the largest driver of PGN DS total column product bias for NO_2, and likely on par with the spectral fitting uncertainty and potential artifacts for the less robust HCHO product. Any error associated with the extrapolation will be maximum for midday observations and minimum at large solar zenith angles.

The sky scan mode has a 1.5 degree FOV and samples sky-scattered photons. When accounting only for single scattering, the instrument observes the atmospheric absorption of NO_2 and HCHO along the view path. Vertical profile information can be obtained when spectra recorded at view zenith angles ranging from near-horizon (89 degrees) to zenith (0 degrees) are referenced to one another. In a multiple scattering atmosphere and with a bright surface reflectance, effective pathlengths increase. The effects of scattering can be accounted for by applying radiative transfer models, lookup tables, or by correcting products through use of information retrieved from simultaneous spectral fitting of gases with well-known abundances (e.g., O_2-O_2 dimer).

Due to the lack of an absolute calibration the bias and precision for Pandora L2 NO_2 and HCHO data product can vary by instrument. The operational total NO_2 (DS) is high quality, with an overall precision of about 0.5 % and estimated bias of 0.1 DU. The PGN L2 suite of data products will serve as a primary ground-based measurement for all validation maturity levels, beta, provision, full.

4.2.2.1.2 Pandora Advantages and Challenges for validation

Known sources of inconsistency between TEMPO L2 NO_2 and PGN data products are use of different spectroscopic assumptions and the different volumetric spatial overlap, as noted in TROPOMI validation efforts (Verhoelst et al., 2021).

While Verhoelst et al. (2021) noted differences with the NO_2 cross sections used in TROPOMI and Pandora algorithms as a source of inconsistency between the measurements, recent updates to v1.8 algorithm improve upon the treatment of the tropospheric and stratospheric cross section which had previously resulted in known biases. As per the Pandora Blick1.8 manual 1.8.4: Section 6.8.2, the PGN v1.8 product is attempting to resolve or diminish this reported source of inconsistency.

While both PGN and TEMPO provide retrievals of column integrated NO_2 and HCHO, spatial incongruities between Pandora and TEMPO measurements can periodically cause large differences between the two instrument platforms, especially where trace gas sources or sinks are spatially variable. These effects are likely to be most notable for NO_2 based on the steeper gradients observed in the past, from both remote sensing platforms and in situ (e.g., Judd et al., 2019). In analyses spanning long time periods, the impacts of spatial mismatches on NO_2 column comparisons between TEMPO and PGN will diminish unless the differences are driven by persistent sources of NO_2 gradients.

Several approaches will be useful for characterizing near-field, persistent NO_2 gradients and thus their potential impacts on TEMPO validation. Figure 4-3 illustrates the combined viewing geometries of Direct Sun (DS) and Multi-Axis sky scans (MAX-DOAS) for Pandora which are expected to aid in assessing viewing geometry issues for TEMPO validation. The standard PGN operational measurement routines now include MAX-DOAS in addition to DS measurements. The combination of DS and MAX-DOAS retrievals can provide an independent measurement of spatial variability surrounding the ground site. When combined with sites with a surface based NO_2 or HCHO measurement the retrievals can provide an independent evaluation of the profile shape factor. At low sun elevations, Pandora DS measurements sample a larger volume of the atmosphere (i.e., proportional to the secant of the solar zenith angle) and are thus expected to be more spatially comparable. In fast DS mode, PGN NO_2 products can provide data on a timescale of seconds. Highly variable native time sample data would indicate the extent that the atmospheric column over a site is influenced by near-field sources of NO_2 variability. Finally, simulated or measured vertical wind information can be combined with Pandora DS measurements on multiple days to generate an estimate of near-field sources of variability.

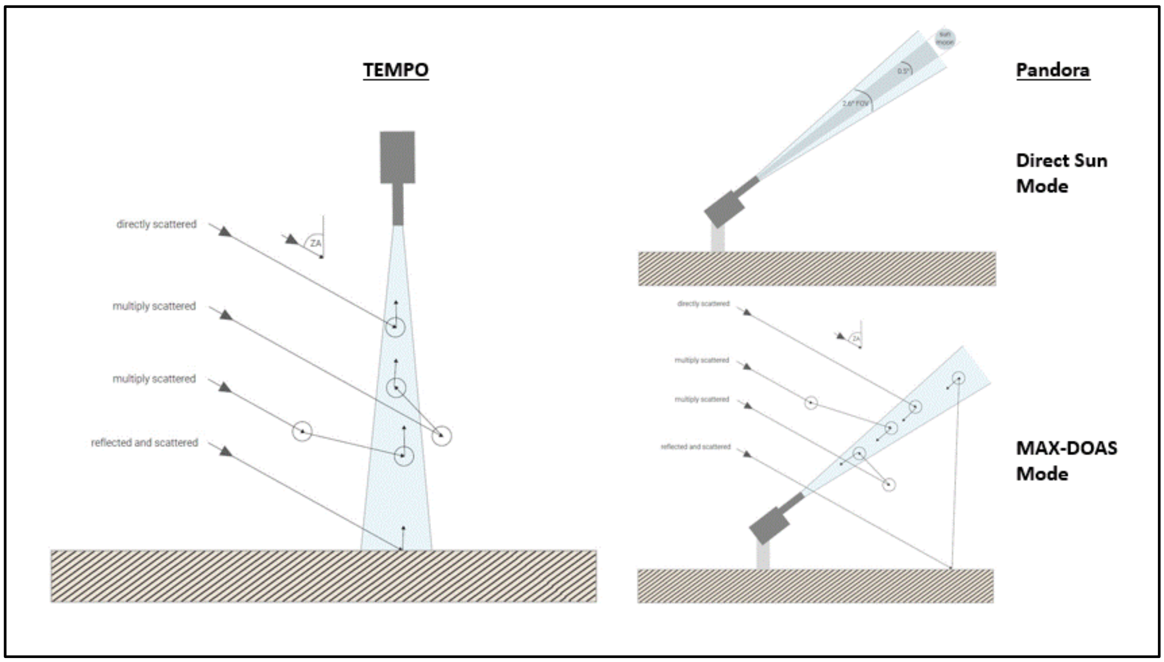

Figure 4-3 Scattering impacts on viewing geometry for TEMPO and Pandora DS and MAX-DOAS modes (adopted from PGN).

4.2.2.1.3 PGN/TEMPO L2 HCHO/NO_2 Validation Maturity Thresholds

The overarching validation maturity level guidelines are described in Section 3. PGN measurements will support specific validation analyses undertaken by individual scientists in collaboration with SAO of all TEMPO L2 Total Column NO_2 and HCHO Tropospheric Column NO_2 through all product maturity levels. Total Column comparisons will be compared to Pandora Direct Sun (DS), Multi-Axis sky scans (MAX-DOAS), and a combination of both measurements. Regression analysis will be conducted with standard statistical metrics reported, mean difference, RSME, correlation coefficient. Given the level of interests from other groups conducting validation activities, we encourage any outside groups to conduct analysis to contribute to a larger body of results for use by the TEMPO science team and the community.

In support of TEMPO beta validation analysis combined PGN/TEMPO data analysis will include a Beta maturity preliminary validation report. For Beta maturity, it is envisioned that PGN data will be most useful for providing an initial assessment of high solar and view zenith angle geometry retrievals (early morning, late afternoon, far north, west, and east). These locations and times of day present the most novel and challenging observation geometry and are not covered by heritage LEO observations. To that end, existing PGN sites near the tar Sands of Canada (polluted NW), Houston, TX (polluted south central), Manhattan KS (unpolluted central), Table Mountain, CA (mixed SW), Port Elizabeth, ME (mixed NE) and Queens, NY (polluted, NE), currently span a range of low and high TEMPO view angles and varying NO_2 column abundances indicating the network is well situated to provide early assessment of data quality at the edges of the TEMPO field of view, in addition to providing full diurnal coverage.

In support of Provisional Maturity Level, PGN/TEMPO validation reports are likely to contribute by assessing quantitative accuracy and precision thresholds at polluted and non-polluted locations to identify any systematic biases.

In support of Full Maturity Level, PGN/TEMPO validation analyses are likely to contribute by providing detailed metrics on impacts of individual sources of bias and uncertainty in the TEMPO L2_NO2_TOT and L2_HCHO_TOT retrieval algorithms (e.g., influence of clouds, diurnal cycle, seasonal cycles, city-scale profile shape factor variability).

4.2.2.2 Specific TEMPO Validation Activities

TEMPO L2 NO_2 summed column data (troposphere + stratosphere) will be compared to measurements from all Pandoras within the FOR with available total column data. Linear regression comparisons of coincident total column NO_2 will be generated as the first available TEMPO L2 NO_2 data become available. Initial coincidence criteria for TROPOMI validation were defined in Judd at et. (2020) and Verhoelst et al. (2021). However, we expect temporal averaging times between Pandora and TEMPO may differ based on a variety of factors to be explored, particularly for the unique demands of TEMPO viewing at large solar and view zenith angle factors as TEMPO products progress through validation maturity levels. Plots, correlation coefficients and mean bias will be reported as part of routine reports and made available through SAO or at the official TEMPO data archive located at NASA Langley Atmospheric Science Data Center.

TEMPO L2 column data will be compared to measurements from a subset of Pandoras within the FOR with available total column HCHO data. For HCHO comparisons a subset of Pandora instruments will be selected based on an assessment of data quality using data from the prior years (2019 or later) as a result of instrument upgrades implemented to address a formaldehyde interference in the pandora measurement (Spinei et al., 2021). Linear regression comparisons of coincident total column HCHO will be generated as the first available TEMPO L2_ HCHO data become available. Initial coincidence criteria between Pandora and TEMPO will be defined based on the temporal and spatial averaging time for TEMPO L2 data products. Plots, correlation coefficients and mean bias will be reported as part of routine reports and made available through SAO or at the official TEMPO data archive located at NASA Langley Atmospheric Science Data Center.

TEMPO L2 NO2 and HCHO data products will be made available to research groups conducting Fourier-Transform InfaRed (FTIR) spectroscopy and Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements within the TEMPO FOR, including but not limited to Environment and Climate Change Canada, National Center for Atmospheric Research, and Universidad Nacional Autónoma de México (UNAM) to contribute validation analysis on a best effort basis.

4.2.2.3 Tropospheric Ozone Lidar Network (TOLNet)

4.2.2.3.1 Instrument and method summary

A primary means of validation of the TEMPO L2 O_3 profile and tropospheric and 0-2 km O_3 partial column data products is to compare them with equivalent ground measurements from the Tropospheric Ozone Lidar Network, TOLnet.
(https://www-air.larc.nasa.gov/missions/TOLNet).

Prior to the launch of TEMPO, TOLNet will have eight instruments distributed across the TEMPO FOR. Figure 4-4 shows the distribution of the TOLNet sites within the U.S. and southern Canada. The distribution of the TOLNet instruments is organized through a combination of federal labs (NASA/NOAA/ECCC) and universities (UAH, CCNY, Hampton U). Table 4-2 lists the TOLNet sites, with a proposed weekly observing schedule during periods of selected scenes with cloud fractions less than 0.2.

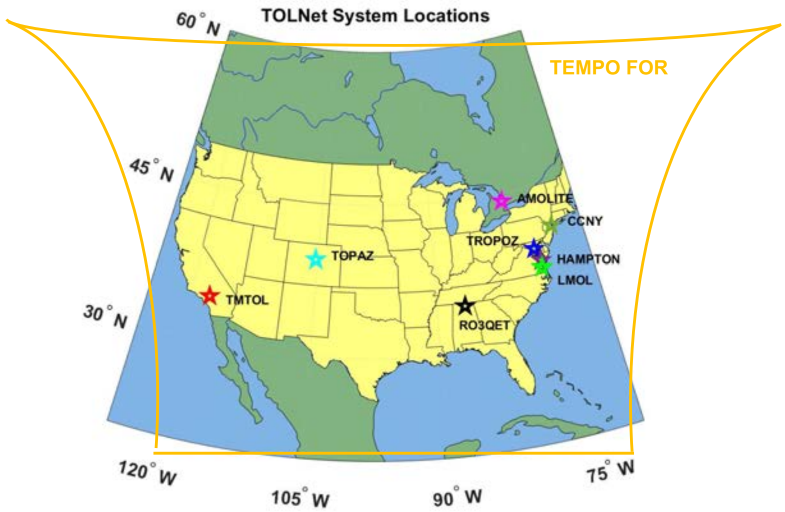

Figure 4-4 TOLNet Locations Across the TEMPO Field of Regard.

The proposed effort maximizes TOLNet station manual and semi-autonomous/remote operations given available resources. Most TOLNet sites with appropriate averaging can provide information about the 0-2km and Tropospheric O_3 partial columns. To maximize value at each TOLNet site, we propose Table 4-2 to highlight the observational capabilities. If a site is not able to retrieve daytime ozone profiles to the tropopause (or requirements based on Table 2-2), then nighttime profiles and averaging may be used in select scenes to retrieve the ozone at altitude where daytime limitations exist. This results in a hybrid product of daytime profiles (where ozone structure/gradients change diurnally in the PBL and lower FT) and nighttime or pre-dawn upper free tropospheric profiles (where ozone is less variable).

Table 4-2 List of TOLNet sites and measurements/instruments at these sites.

Site	Daytime + Nighttime Hybrid		Dedicated Pandora (Y/N)	Surface	Ceilometer
Product	0-2km	Full Trop.			
NASA GSFC	X	X	Y	O_3, NO_2	Y
NASA LaRC	X	X	Y		Y
JPL/TMF	X	X	Y	O_3	Y
UAH	X	X	Y		
NOAA CSL	X	X	N		
ECCC	X	X	Y		
Hampton U		X	Y		Y
CCNY	X	X	Y		Y

TOLNet has recently been adopted by the LaRC ASDC and profiles of ozone, uncertainty, and retrieval meta-data is available at: https://asdc.larc.nasa.gov/project/TOLNet. The file contents, structure, and naming conventions comport with the GEOMS format. This standard high resolution (HIRES) TOLNet product will be emphasized for process science studies, similar to the most current archived data with short time slicing (<20 min), moderate to high effective vertical resolution, and not standardized (but ideally in-house processing is performed).

For TEMPO evaluation, especially for the 0-2km product, a HIRES (TEMPO) product will be provided using a consistent temporal and vertical resolution scheme across the entire network. The TEMPO a-priori and averaging kernels will be applied to this data to allow for consistent end-products for TEMPO and associated model validation/evaluation. Figure 4-5 shows an example of how TOLNet is being used to validate TROPOMI O_3 profiles in the troposphere. TOLNet is currently processed on a centralized computer to provide these common products to the end-user and validation community.

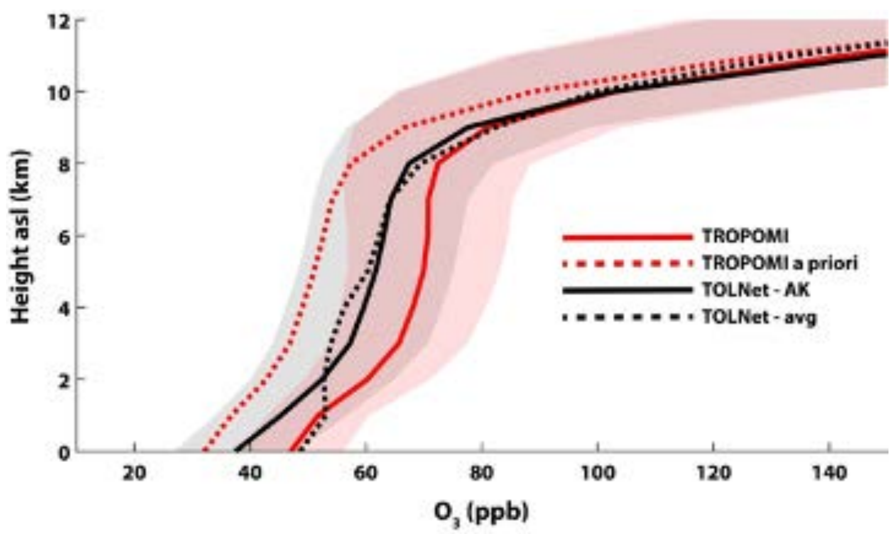

Figure 4-5 Comparison of TOLNet (Table Mountain Facility) and TROPOMI O_3 profiles

4.2.2.3.2 TOLNet Operating Schedule – Routine (at Home Institution) Mode

To rigorously understand the representativeness of TEMPO profile retrievals, especially in the vertical, a dedicated and consistent data set from existing ground-based O_3 lidars and co-located ancillary measurements in needed (e.g., ceilometer, Pandora spectrometer – Section 4.2.2.1, ozonesondes – Section 4.2.2.3). These proposed sites could be the 7-8 “home” institutions operating on a fixed schedule within the bounds of level of effort and appropriate atmospheric conditions *(e.g.,* cloud fraction <0.2). This can be accomplished with the standard TEMPO hourly scans or more intensive repeated sampling.

In early 2020, NASA TOLNet created an internal forecasting alert system utilizing chemical transport models run through NASA, NOAA, and NCAR that can generally forecast relevant events of interest 1-5 days prior to reaching each TOLNet site. During TEMPO operations, this forecast system can be used to identify opportunities for higher frequency TEMPO scans in coordination with TOLNet observations to characterize ozone pfiles pre- and post-events related to aged or fresh stratosphere-troposphere transport, wildfire/biomass/agricultural burning, and regional photochemical ozone episodes. Using this alert framework in conjunction with the special-operations scan patterns available by TEMPO, TOLNet is able to better coordinate network wide observations during events that are generally challenging to characterize with field campaign airborne methods, such as those that traverse multiple states or geographic land use regions. An example of this is below in Figure 4-6.

By increasing the dwell time for a day before and after each forecasted episode, TOLNet sites will also be able to provide the necessary statistics to complete a tertiary goal of exploring the temporal and diurnal representativeness of the standard TEMPO retrieval in a variety of mixed atmospheric scenes. This will add critical context to the standard TEMPO retrieval and improve our fundamental understanding of transport events within the scientific community. Furthermore, given TOLNet’s greater sensitivity and measuring depth at nighttime, overnight measurements can provide statistics for indirectly understanding daytime ozone at higher altitudes at regional scales as opposed to daytime only TOLNet measurements.

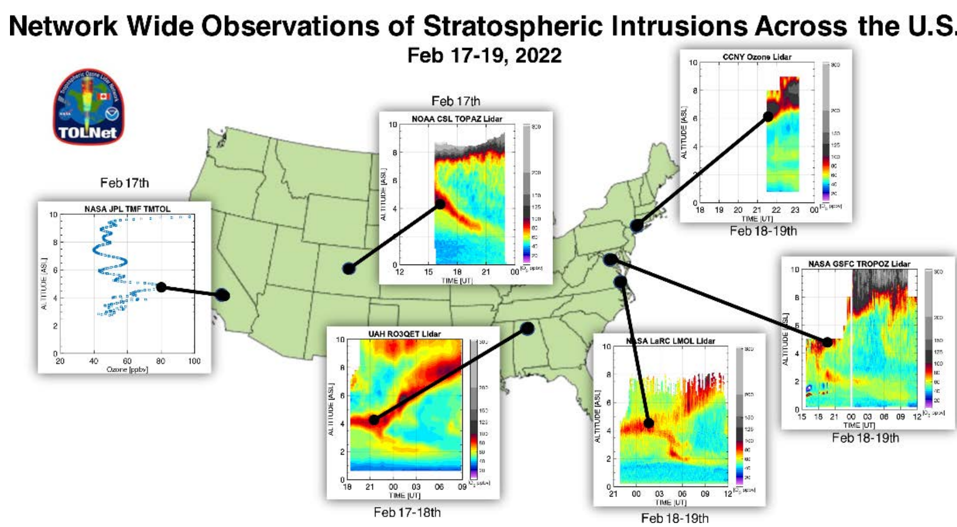

Figure 4-6 Network-wide Observations from TOLNet characterizing a continental-wide stratospheric intrusion episode from Feb 17-19, 2022

The emphasis on network wide observational efforts will be to increase sampling frequency at TOLNet sites as resources allow to more fully explore the representativeness of the TEMPO O_3 0-2km products. For instance, how do TEMPO retrievals perform in scenes that are:

a. clean vs polluted (w.r.t ozone and particulate matter)
b. complex scenes such as coastlines or mountainous terrain
c. high sun angles vs. low angles and different times of the day
d. cloud-free vs. cloudy
e. surface albedo/land type impact on the TEMPO retrievals

The overall goal of this activity is to demonstrate through measurement analysis that the baseline precision for TEMPO O_3 measurements has been met at target sites across application areas and retrieval conditions. Techniques that have been developed for previous ground-based intercomparison campaigns, including validation of satellite data products, will be applied for TEMPO validation. TEMPO O_3 retrievals will also be compared with modeled fields in order to rationalize the differences in measurement area to the TEMPO ground footprints. Error budgets, including biases, will be developed relying on techniques developed for O_3 which will be much improved before TEMPO launch. An essential difference with respect to previous spaceborne measurements of tropospheric ozone is the hourly (or more frequent) diurnal-sampling capability of TEMPO.

4.2.2.3.3 Specific TEMPO Validation Activities

TOLNet will participate in several collaborative activities in the validation period. The collaborative activities include STAQS, AEROMMA, GOTHAAM, and CUPiDS which will provide airborne payloads with in situ and remote sensing measurements relevant to TEMPO air quality science on board the NASA JSC G-V, NASA DC-8, NOAA Twin Otter, NSF C-130 aircraft, and a SeaRey amphibious aircraft.

Continuous tropospheric ozone profiles add a critical component needed to understand processes relevant to air quality and pollution transport with TEMPO. TOLNet will contribute most heavily in the New York City area in summer 2023 (with at least 3 systems operated by NASA, NOAA, and CCNY) with additional support in the Chicago area by the UAH RO3QET, Los Angeles by the JPL TOLNet lidars, and Toronto areas by the ECCC AMOLITE lidar.

The framework for TOLNet participation in these field campaigns stems from measurements strategies and collaborations developed during airborne air-quality studies over the previous decade. Additional long-term fixed-location sites will continue to operate at their home institution location within the TEMPO FOR to continue to accrue ozone profiles for validation activities. Outside of campaign deployments in 2023, all TOLNet sites are expected to operate and maintain observations presented in Table 4-2.

4.2.2.4 Ozonesonde stations

4.2.2.4.1 Instrument and method summary

Balloon-borne electrochemical concentration cell (ECC) ozonesondes measure the vertical ozone profile from the surface to over 30 km altitude at 100-150 m vertical resolution, with uncertainties and accuracies close to 5%. They are launched at multiple locations in North America, rendering ozonesondes an ideal candidate for validating the TEMPO instrument’s 0-2 km, tropospheric column, and total column ozone products.

The measurement principle of the ECC is based on the reaction of ozone in a neutral-buffered potassium iodide (KI) solution, such that approximately two electrons flow in the ECC's external circuit for each ozone molecule absorbed into the solution (Smit, Thompson, and ASOPOS 2.0, 2021; Tarasick et al., 2021). The raw ECC current is converted into an ozone partial pressure and transmitted to a ground station for data collection. Ozonesondes are always coupled with a meteorological radiosonde, so pressure, temperature, humidity, and GPS data are also collected in conjunction with the ozone measurements. Ozone data are typically reported as partial pressures (mPa) and can be converted to various other quantities (e.g., Dobson Units, volume mixing ratio, number density, if not provided) using the coincident radiosonde meteorological measurements.

4.2.2.4.2 Station locations and TEMPO validation activities

A network of past and currently operational long-term ozonesonde stations within the planned TEMPO FOR and supported by ECCC, NOAA, NASA, and other agencies in North America are listed in Table 4-3. Most of these stations launch ozonesondes once per week. The stations each follow the recommendations of the Assessment of Standard Operating Procedures for OzoneSondes (ASOPOS) 2.0 expert panel (Smit, Thompson, and ASOPOS 2.0, 2021) to ensure the highest quality data are collected. The ozone measurements also include a full accounting of their uncertainties for every partial pressure value. All of the stations in North America operate using one of two ECC ozonesonde manufacturers: Environmental Science (En-Sci; Westminster, CO, USA) or Science Pump Corporation (SPC; Camden, NJ, USA). The data are publicly archived at the World Ozone and Ultraviolet Data Centre (WOUDC; https://woudc.org/data/explore.php?lang=en), NOAA GML (https://gml.noaa.gov/aftp/data/ozwv/Ozonesonde/), and the Network for the Detection of Atmospheric Composition Change (NDACC; https://www-air.larc.nasa.gov/missions/ndacc/data.html) repositories.

Table 4-3 Long-term ozonesonde stations within the planned TEMPO field of regard.

Station Name		**Lat (°)**	**Lon (°)**	**Notes**
Edmonton		53.54	-114.1	Weekly launches
Goose Bay		53.31	-60.36	Weekly launches
Port Hardy		50.68	-127.38	Weekly launches
Yarmouth		43.87	-66.11	Weekly launches
Trinidad Head		40.8	-124.16	Weekly launches
Boulder		40	-105.25	Weekly or more frequent launches
Beltsville		39.05	-76.88	Once monthly, more frequent during pollution episodes
Wallops Island		37.93	-75.48	Weekly launches
Huntsville		34.72	-86.64	*Inactive as of 2020*
Idabel		33.9	-94.75	*Inactive as of 2016*
Houston		29.72	-95.34	Occasional measurements also collected at El Paso and San Antonio, TX, generally in spring/summer

In addition to the long-term stations noted above, ozonesondes are launched on a more frequent basis, up to once per day or more, as part of intensive air-quality campaigns to monitor day-to-day evolution of the ozone profile. In the recent past, frequent ozonesonde profiling occurred during DISCOVER-AQ, OWLETS-1&2, LISTOS, TRACER-AQ, etc. This strategy will also be implemented during planned STAQS/AEROMMA/GOTHAAM campaigns in 2023. A combination of the operational measurements at existing stations, and more frequent campaign-based profiling will enable TEMPO ozone validation studies for both episodic pollution events and long-term measurement stability.

4.2.2.5 Dobson/Brewer

The Brewer and Dobson instruments have served as the primary ground-based remote sensing measurements for total ozone column providing long, uninterrupted, well-maintained, homogeneously calibrated time-series for satellite validation especially prior to the emergence of the PGN of Pandora instruments in the last decade. For example, they have been used in validating GOME and OMI total ozone from TEMPO's heritage ozone profile algorithm (Liu et al., 2005; Bak et al., 2015) and in validating ESA's Climate Change Initiative GOME-type Total Ozone Essential ClimateVariable (GTO-ECV) (Koukouli et al., 2015; Garane et al., 2018) and TROPOMI total ozone (Garane et al., 2019).

Dobson instruments are spectrophotometers that measures 3 pairs (so-called A, C, and D pairs, one ozone absorbing wavelength and one non-absorbing wavelength) of solar spectrum falling onto separate slits. The difference in the sunlight attenuation between the pair is used to discern the amount of the total column ozone in the atmosphere; the double pair method is used to minimize the impacts of atmospheric aerosol interference on the spectral observations (Komhyr et al. 1993, Komhyr et al., 1989). It measures the total ozone column, typically three times per day (10 am, noon, and 2 pm standard local time). It can operate in both direct sun and zenith sky modes. Direct sun observations are made under clear sky conditions and through an optically thin cloud. Under cloudy conditions, the zenith sky observations are used to determine the ozone column. Further information about Dobson instrument operations can be found in the WMO GAW Report (https://gml.noaa.gov/ozwv/dobson/GAW183-Dobson-WEB.pdf). NOAA Global Monitoring Laboratory (GML) is the custodian of the Dobson World standard instrument D083, which is calibrated at the NOAA's Mauna Loa observatory every two years using the Langley Technique. Dobson regional standards are calibrated to D083 approximately every four years.

The Brewer spectrophotometer (Kerr et al., 1985) went into commercial production in the early 1980s. The Brewer instrument measures spectral irradiance at six wavelengths ranging from 303.2 to 320.1 nm. The measurement at 303.2 nm is only used to check the spectral wavelengths. The channel at 305.3 nm is used to retrieve the sulfur dioxide (SO_2) column and the ozone column is retrieved from a combination of five longer wavelengths (306.3, 310.1, 313.5, 315.8, and 320.1 nm) (Kerr, 2002). There are two types of Brewers in use today: single and double Brewers. The latter is known to better reduce the impact of straylight on the measurement than the single brewer does (Gröbner et al., 1998). The basic measurement principle for the Brewer instrument is the same as the Dobson. However, The Brewer grating spectrometer has an improved optical design over the Dobson spectrometer, as it measures the intensity of five operational wavelengths quasi-simultaneously, and it is fully automated to take measurements continuously every ~10 mins during the sunlit part of the day. The Environment and Climate Change Canada (ECCC) Brewer network calibrates its standard instruments (the Brewer triad) at Mauna Loa using the Langley plot method (Fioletov et al., 2005) and all other station instruments in the ECCC network are calibrated against the triad using traveling standards (Zhao et al., 2021).

The principle behind the measurements of the Dobson and Brewer instruments is generally the same. Both Dobson and Brewer total ozone retrieval algorithms use the effective ozone absorption coefficients derived from Bass and Paur (1985) at fixed effective ozone temperatures. Due to different wavelengths and thus different temperature dependence between these two measurements, there are seasonal and systematic differences in the retrieved total ozone (Vanicek, 2006). The difference can also depend on the choice of ozone cross sections. Redondas et al. (2014) evaluated the effects of cross sections and temperature dependence on the Dobson and Brewer retrievals. The seasonal dependence of the differences between the results from the various instruments is greatly reduced with the application of temperature-dependent absorption coefficients, with the greatest reduction obtained using the University of Bremen (IUP) ozone cross sections (Serdyuchenko et al., 2013; Gorshelev et al., 2013). NOAA GML has several of Dobson's total column records processed using the IUP ozone absorption cross sections. The temperature dependence in Dobson is corrected using the ECMWF (European Centre for Medium-Range Weather Forecasts) effective temperatures. The IO3C and WMO GAW ozone/UV SAG initiated reprocessing of all Dobson and Brewer records collected at the WOUDC. This work is expected to be completed by the end of 2023.

For the ground-based validation of the TEMPO total ozone column, 7 Dobson stations (mostly in USA with one in Mexico) and 5 Brewer stations in Canada from the WMO GAW network measure total ozone in the TEMPO field of regard. These stations have been identified (see Table 4-4) that archived their data in 2022 (with the exception of Dobson observations at Caribou, which stopped in 2018 and will be restarted in early 2023). The Dobson and Brewer data are submitted to the WMO Ozone and UV Data Center (WOUDC, www.woudc.org) regularly. The once-a-day representative (selected as the most accurate type among multiple observations) Dobson total column data are archived at the WOUDC twice per year after the thorough quality control and verification of instrument calibrations. Both daily mean and individual Brewer measurements are submitted to WOUDC three times a year. More frequent (monthly) and individual (not daily mean) updates for NOAA GML Dobson data (not final records, but quality assured) are available from GML aftp website (https://gml.noaa.gov/aftp/data/ozwv/Dobson/). Brewer data can also be found from the Canadian Brewer Network (http://exp-studies.tor.ec.gc.ca/).

We will use Dobson and Brewer total ozone to validate the total ozone from both TEMPO total ozone and ozone profile algorithms. Individual total ozone measurements (rather daily mean) will be used to validate the diurnal variation of total ozone. Both Dobson/Brewer operate in direct-sun and zenith-sky modes. Direct-sun measurements will be mainly used due to higher quality (Garane et al., 2018).

Table 4-4 List of Dobson/Brewer stations within the TEMPO field of regard.

Inst (Br/DB)	WOUDC Station ID	GAW ID	Station Name	Station Country	Latitude	Longitude	Elevation masl m	Contributor Name
DB	192	MXC	Mexico City	Mexico	19.33	99.18	2268	Mexico IG[1]
DB	106	BNA	Nashville	USA	36.25	-86.57	182	NOAA GML[2]
DB	341	HNX	Hanford	USA	36.32	-119.63	73	NOAA GML
DB	107	WAI	Wallops Island	USA	37.87	-75.52	4	NOAA GML
DB	67	BLD	Boulder	USA	40.02	-105.25	1634	NOAA GML
BR	65	TOT	Toronto	Canada	43.78	-79.47	198	ECCC[3]
DB	19	BMK	Bismarck	USA	46.77	-100.75	511	NOAA GML
DB	20	CBM	Caribou	USA	46.87	-68.02	192	NOAA GML
BR	290	SAT	Saturna Island	Canada	48.78	-123.13	0	ECCC
BR	76	GOB	Goose Bay	Canada	53.32	-60.38	66	ECCC
BR	21	EDT	Edmonton	Canada	53.57	-113.52	668	ECCC
BR	77	CHL	Churchill	Canada	58.75	-94.07	35	ECCC

[1]Mexico of Institute of Geophysics, [2]NOAA Global Monitoring Laboratory, [3]Environment and Climate Change Canada

4.2.3 Validation with Correlative Airborne Measurements

Correlative airborne measurements for TEMPO NO_2 and HCHO column products and the ozone profile product can be split into three categories: UV-VIS airborne spectrometers, ozone airborne Differential Absorption Lidar (DIAL), and in situ profile collection. These measurements are largely confined to opportunities linked with field studies focused on air quality, rather than systematic collections in time. However, these datasets can provide detailed observations of the horizontal and vertical spatial distribution of these trace gases to help assess root causes of biases and uncertainty in TEMPO L2 products. The sections below focus on specific strategies that can be applied in terms of the approach to data collection and follow-on processing strategies that can contribute to TEMPO L2 trace gas column or profile (ozone) product validation during known future opportunities in 2023 and beyond.

4.2.3.1 UV-VIS Airborne Spectrometers

Airborne spectrometers, similar to TEMPO, collect scattered light in the UV-VIS spectrum that has traveled through Earth's atmosphere to each respective instrument. The high spectral resolution data are used to retrieve NO_2 and HCHO column densities by quantifying the absorption fingerprints in the absorption windows of each trace gas. NASA has multiple of these airborne instruments, both matured as well as under development:

- The GeoCAPE Airborne Simulator (GCAS) was developed in support of NASA's 2007 Decadal Survey GEO-CAPE geostationary satellite mission (Kowalewski and Janz, 2014).

This instrument has a 45-degree field of view, providing a swath width of ~ 7 km at a flight altitude of 28,000 feet with a spatial resolution demonstrated as 250 x 560 m on the NASA G-V aircraft.

- The GEOstationary Trace gas and Aerosol Optimalization (GEOTASO) instrument was also supported by NASA as a risk-reduction for geostationary observations from TEMPO and GEMS (Leitch et al., 2014). The instrument also has a 45-degree field of view, though has a large physical footprint inside airborne platforms and, therefore, is less compatible with other complementary airborne instruments (e.g., the High Spectral Resolution Lidar-2 as discussed in Sect. 4.2.3.2; Hair et al., 2008) unless flown on larger aircraft.
- Still under development: The Compact Hyperspectral Air Pollution Sensor–Demonstrator (CHAPS-D) could push the envelope in terms of spatial resolution by observing at 40 m resolution at a flight altitude at 28,000 feet though at the expense of swath width (FOV of 15 degrees) (Swartz et al., 2021).

The details in the rest of this section will focus on GCAS as the most likely contributor to TEMPO validation with identified future opportunities, however these ideas can also be applied to other airborne spectrometers.

UV-VIS airborne spectrometer measurements will support specific validation analyses undertaken through field campaigns and in collaboration with SAO for TEMPO L2_NO2 TotCols and TropCol and HCHO TotCols. These measurements are expected to support validation at the provisional and full product maturity levels, primarily due to timing of forthcoming field campaigns.

4.2.3.1.1 UV/VIS Airborne Spectrometer Advantages and Challenges for validation

Uncertainty in the NO_2 and HCHO retrievals from airborne spectrometers and from TEMPO are similar and originate from the slant column spectral fit, reference spectrum uncertainty, and uncertainty in air mass factor (AMF) calculations which are reliant on assumptions about surface reflectivity, clouds, and assumptions about the vertical distribution of each trace gas. As demonstrated in multiple field campaigns, airborne spectrometers:

- retrieve tropospheric columns at sub-kilometer and approximately kilometer resolution for NO_2 and HCHO, respectively. This retrieval results in dozens of pixels mapped to each coincident TEMPO pixel to improve uncertainty related to slant column spectral fit.
- are not as heavily influenced by spatial heterogeneity in comparison to TEMPO or other satellite measurements comparisons vs. Pandora and can be used to estimate the representativeness error that might be expected between datasets (Tang et al., 2021).
- provide an additional dataset to assess the sensitivity of the retrieval to a priori assumptions used within AMF calculations. This sensitivity includes assumed vertical profiles, surface reflectivity input, and cloud fraction assumptions.

4.2.3.1.2 Proposed methodology for airborne spectrometer correlative

comparisons

Figure 4-7 shows an example of how airborne spectrometer data was used to validate the TROPOMI NO2 product. Based on use of UV-VIS airborne spectrometers for validation of TROPOMI (Judd et al., 2020), initial proposed methodology for validation is as follows:

1. Evaluation of any systematic biases in airborne spectrometers; data using data collected over multiple networks of Pandora spectrometers. GCAS retrievals have been demonstrated to no systematic biases with an uncertainty of ±25% in comparison to Pandora
2. Coincidence criteria between the airborne and TEMPO measurements should, at a minimum, consider the time difference between measurements (no greater than 30 minutes), fractional coverage of the TEMPO pixel by airborne spectrometer data, and cloud conditions. Sensitivity studies could consider a shortened temporal window than 30 minutes, especially if TEMPO is operating in a special scan mode with finer temporal resolution, but TROPOMI NO2 evaluations showed large temporal impacts beyond 30 minutes.
3. Calculate a TEMPO scale column density by doing a spatial average of airborne data within a TEMPO pixel along with statistics relating to the sub-pixel variation using standard deviation or percentiles.
4. Apply appropriate linear regressions and calculate difference and percent difference statistics. These statistics could be applied to data subsets based on sub-pixel variability and pollution level.

The above criteria were built for NO2 datasets but will be adapted for HCHO validation efforts as well. TEMPO product validation with airborne spectrometers should emphasize evaluating based on time of day (i.e., repeated systematic flight sampling several times in the same day to capture diurnal variability) as a unique aspect of geostationary observations but should also extend toward cloud coverage and different surface scenes.

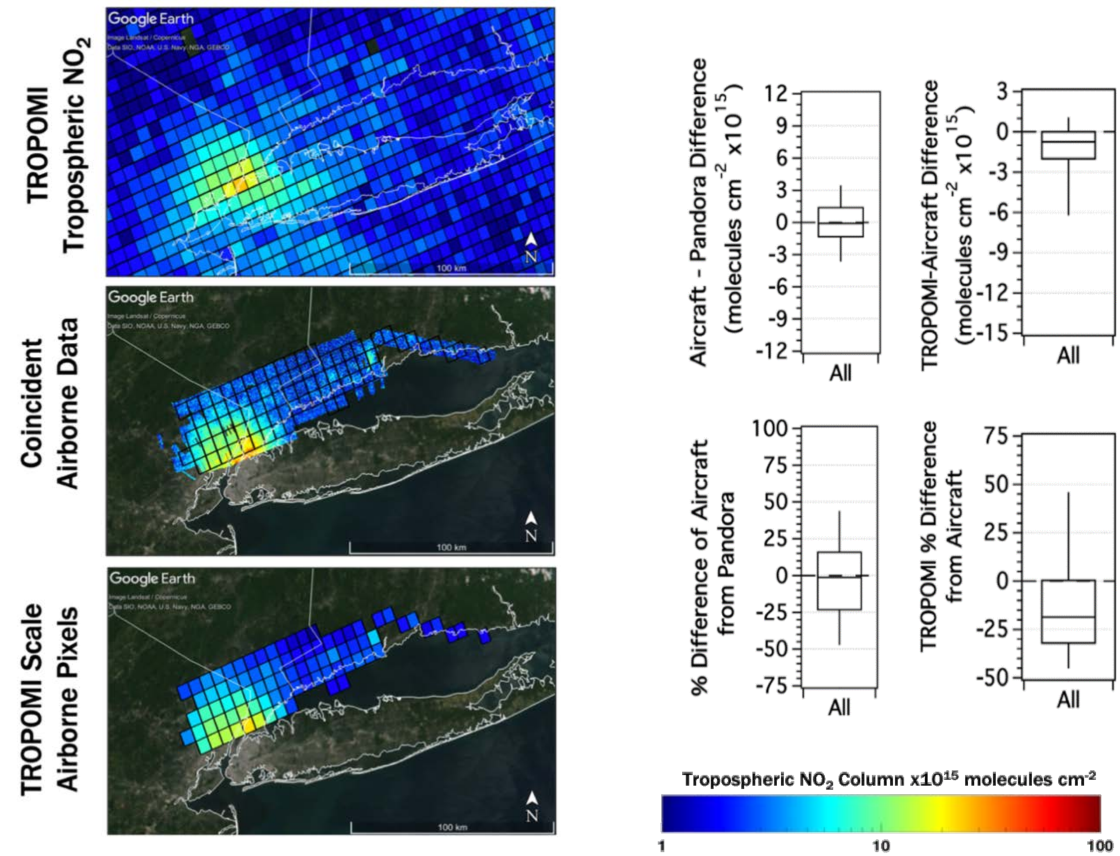

Figure 4-7 The maps on the left show how the airborne data compares to TROPOMI tropospheric NO_2 on June 30^{th} (top) in comparison to airborne spectrometer data at its native sub kilometer resolution within +/- 30 minutes from the TROPOMI Overpass(middle) and aggregated to the TROPOMI pixel scale (bottom; showing pixels with > 75% spatial coverage). The box plots show the difference and percent difference between Pandora and airborne spectrometers and TROPOMI and airborne spectrometers showing about a 20% low bias in TROPOMI during the Long Island Sound Tropospheric Ozone Study in 2018 (12 days of data). Figure adapted from Judd et al., 2020.

4.2.3.2 Ozone Differential Absorption Lidar

Using active remote sensing, ozone profiles can be measured by airborne lidars via the Differential Absorption Lidar (DIAL) technique. Scientists at NASA Langley Research Center operate two systems capable of these observations on NASA airborne platforms:

- DIAL/High Spectral Resolution Lidar (HSRL) can be deployed on larger aircraft (e.g., NASA DC8) observing ozone both nadir and zenith of the aircraft (Richter et al., 1997; Browell et al., 1998)

- HSRL2/DIAL is a more compact version of the lidar capable of flying on smaller remote sensing platforms (e.g., NASA G-V or B200) observing ozone profiles nadir of the aircraft (Hair et al., 2008; Hair et al., 2018)

This section will focus on the latter instrument (HSRL2/DIAL) as the most likely contributor to TEMPO ozone profile validation through opportunities related to planned field studies with the airborne spectrometers on the NASA G-V.

HSRL2/DIAL measurements will support specific validation analyses undertaken through field campaigns and in collaboration with SAO for TEMPO L2 0-2km and (in specific cases) free tropospheric ozone partial columns in the ozone profile product. They are expected to support validation at the provisional and full product maturity levels, primarily due to timing of forthcoming field campaigns.

4.2.3.2.1 HSRL2/DIAL Advantages and Challenges for Validation

The main differences between HSRL2/DIAL and TEMPO ozone profiling observations are their spatial resolution and the independent nature of their different remote sensing techniques (active vs. passive) to distinguish the ozone characteristics vertically through the atmosphere. Below are highlights of the airborne HSRL2/DIAL instrument that would provide value in comparing to collocated TEMPO measurements:

- The DIAL method of retrieving average ozone in vertical layers is different compared to the TEMPO retrieval. Ozone number densities are calculated (similar to TOLNet – see Sec. 4.2.2.2) using a known differential absorption cross section between the DIAL wavelengths and does not require additional model inputs, such as an a priori profile. Conversion to mixing ratios (ppbv) requires air density from reanalysis data.
- HSRL2/DIAL retrieves nadir profiles along the aircraft flight track, which nominally flies at 8-9 km in altitude during air quality science flights. The instrument could be flown at a higher altitude (aircraft dependent) to profile the entire troposphere for free tropospheric validation. This higher altitude flight would be at the expense of less signal-to-noise or averaging resolution for TEMPO evaluation of the 0-2 km product.
    - Nominal resolutions of the retrieved ozone concentration profile product are sampled at 300 m in altitude over a minute of integration (~13 km spatial coverage on the NASA G-V). However, integrated values at a coarser vertical resolution (1 or 2 km) can be achieved at a 10 second averages (~2 km) amounting to a spatial resolution finer than a TEMPO pixel in nominal flying conditions at 8-9 km altitude. The ability to sub-sample HSRL2 at different vertical resolutions along with surface monitoring data will also be able to contribute a better understanding how/where/when 0-2km ozone relates to surface air quality.

The systematic errors in DIAL ozone are dominated by the impact of aerosol scattering between the offline and online wavelengths in the presence of strong vertical gradients in the backscatter profile. Unique to this instrument, the HSRL capability allows for identification and correction of this aerosol impact using the calculated wavelength dependence of the backscatter and extinction at the 355 nm and 532 nm wavelengths. As of now, this random uncertainty for the ozone profile is estimated to be 10% or 5 ppbv when averaged at the nominal resolution (1min, 300m). These HSRL aerosol measurements can also be valuable for evaluating any eventual TEMPO aerosol product.

HSRL2/DIAL observations have been demonstrated showing a mean bias of -1.2% and standard deviation within 6% in comparison to ozonesonde measurements on average from near-surface to 7-8km altitude (Hair et al., 2018). Additional comparisons to ozonesondes are also being conducted from the recent TRACER-AQ campaign.

4.2.3.2.2 Proposed methodology for HSRL2/DIAL correlative comparisons

The airborne HSRL2/DIAL's strength will be in the evaluation of pixel-to-pixel variance for individual samples from the TEMPO instrument across the sampling domain and to assess the lower pieces of information in the ozone vertical profile at high resolutions. The baseline precision requirement for TEMPO's 0-2 km product is reported at 10 ppbv for a nominal mixing ratio of 40 ppbv (Zoogman et al., 2017). The airborne campaigns planned should allow for the assessment of how well TEMPO captures horizontal gradients. For example, this dynamic range (> 10 ppbv within the boundary layer) was captured by HSRL2/DIAL during the TRACER-AQ mission in Houston, Texas on high ozone days (e.g., Figure 4-8) and are well within the expected uncertainty of the HSRL2/DIAL. The comparison between a TEMPO like product and HSRL2/DIAL has not yet been demonstrated but below are some comparison criteria to consider.

1. All comparisons will have to take into consideration different temporal and spatial sampling between TEMPO and HSRL2/DIAL. Multiple samples from the airborne lidar will likely be collected within a TEMPO pixel, therefore the statistics (mean, median, standard deviation, percentiles) can be calculated and compared to the nearest in time TEMPO pixel. Temporal criteria should be assessed between observations (< 30 minutes based on nominal repeat scan times).
2. Sampling under different conditions should be evaluated. For example, retrievals over land and open water in addition to conditions with enhanced ozone in the FT above lower values in the PBL and vice versa and under different aerosol loading, if possible.
3. With the flight lines, techniques to be explored between HSRL2/DIAL curtains could be the ability to interpolate for the creation of a gapless map in which to compare to TEMPO, however the best option for interpolation techniques (e.g., kriging, nearest neighbor) would still need to be explored.

4. Validating the free tropospheric partial profile with HSRL2/DIAL will need to take into consideration of the aircraft altitude, tropopause height, and physical ozone features present within the free troposphere (e.g., boundary layer venting, stratospheric/tropospheric exchange, long range transport). Validation of the free troposphere should only be considered during

instances where the aircraft is above the tropopause.

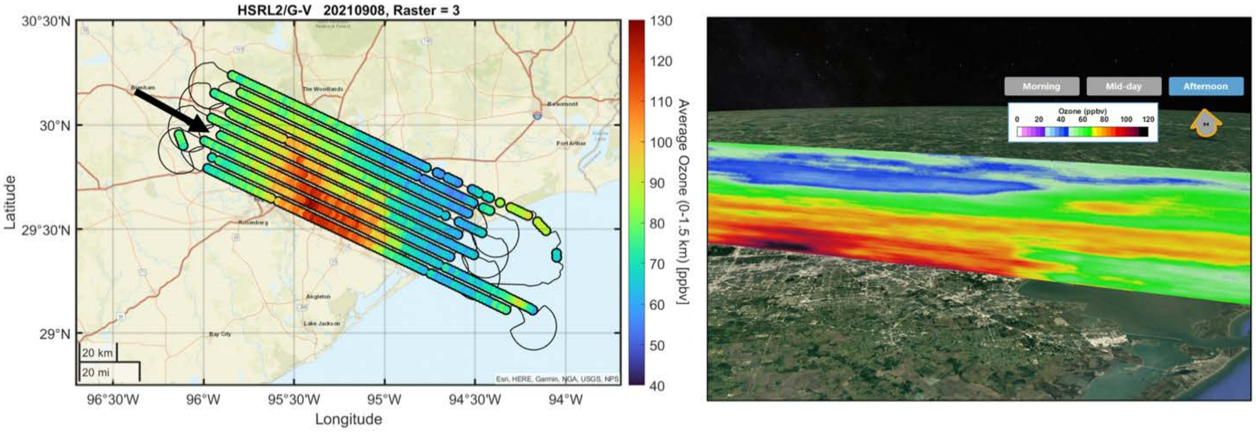

Figure 4-8 Example of partial column mixing ratios from 0-1.5 km (left) as well as the vertical profile from surface to approximately 7 km (right) from HSRL2/DIAL during the TRACER-AQ mission during the final raster of a high ozone day on September 8th, 2021 demonstrating the ability of the instrument to resolve ozone partial columns with a dynamic range wider than the precision expected from TEMPO 0-2km partial column and the ability to discern vertical features in ozone through the boundary layer and free troposphere. The black arrow aligns with the ozone curtain that is visible on the right.

4.2.3.3 Aircraft in situ profiles

Airborne platforms carrying in situ instrumentation are diverse in terms of maneuverability, endurance, speed, and payload size. Due to the diversity of in situ instruments available for NO_2, HCHO, and ozone, this section will not identify specific instrument. Instead, this section will focus more on the quality of trace gas in situ data required as well as sampling strategies that would be most beneficial for validation of TEMPO L2 trace gas products. More specifically, when/where available, in situ measurements will support specific validation analyses undertaken through field campaigns and in collaboration with SAO for TEMPO L2_NO2 TotCols and TropCol, HCHO_TotCols, and O_3 profile product for the troposphere, free troposphere, and the 0-2 km product. In situ measurements are expected to support validation at the provisional and full product maturity levels, due to timing of forthcoming field campaigns.

4.2.3.3.1 In situ Derived Column Advantages and Challenges for Validation

In situ aircraft measurements of trace gas concentrations are fundamentally not the same measurement as the vertically and spatially integrated column densities TEMPO retrieves from backscattered sunlight. The best way to match TEMPO column data with airborne in situ measurements is through the derivation of column densities through the integration of airborne in situ profile data. Challenges associated with validation with in situ aircraft data result from the limitations in horizontal and vertical spatial coverage of the in situ derived profiles, temporal representativity, and how these spatiotemporal variations conflict with a priori assumptions in the retrieval.

To limit assumptions made, the best way to create derived in situ column observations is through the execution of vertical profiling with the airborne platform with high frequency and high-quality instrumentation. The optimal vertical profile would be at the horizontal scale of a TEMPO pixel (i.e., 2.5 x 5 km) or finer to be able to evaluate TEMPO products at a pixel-by-pixel scale. However, in situ profiles typically (but not always) cover areas spanning multiple pixels and therefore that representativity should be accounted for.

Derived in situ profiles can also miss key details vertically through the column where the airborne platform is unable to sample. Examples of missed features could be near-surface pollution where larger aircraft are unable to sample due to operational restrictions or, for smaller aircraft, free tropospheric features if the profiles are limited in altitude. Most signal with respect to NO_2 and HCHO is confined to the boundary layer, therefore profiles as low as possible and over areas where in situ ground measurements exist should be given high priority for TEMPO validation.

TEMPO observations represent what could be considered an instantaneous measurement, however vertical profiles can take tens of minutes and, therefore, the comparison could be impacted by temporal variance. Uncertainties accounting for temporal variance will need to be considered in data comparisons. The length of time it takes to collect a profile will also limit the number of coincidences that can be compared to TEMPO.

4.2.3.3.2 Methodology considerations for TEMPO and airborne in situ correlative comparisons

Methodology for in situ sampling for TEMPO validation need to consider the data quality of the in situ instrumentation sampling on board these in situ platforms as well as the sampling paths flown in order to derive an in situ based column density measurement for comparison.

1. **Data quality:** To achieve validation of TEMPO L2 trace gas column products, the precision and accuracy of in situ measurements are crucial to consider especially on an airborne platform that requires faster response than fixed ground-based monitors due to their movement through the atmosphere.

   The baseline required precision for NO_2 and HCHO column densities is $1x10^{15}$ molecules cm^{-2} and $1x10^{16}$ molecules cm^{-2}, respectively. Previous in situ airborne collected profiles in urban areas have shown that NO_2 and HCHO column densities are confined to the atmospheric boundary layer or mixed layer (or the lowest 1-2 km of the atmosphere, e.g., Choi et al., 2020). A column of 0.5 ppb of NO_2 at STP integrated over 1 km of atmosphere results in a column density of approximately $1.25x10^{15}$ molecules cm^{-2}. This demonstrates the importance of high quality NO_2 measurements with uncertainty requirements of better than 0.5 ppbv for validation. Research grade measurements during previous NASA studies have demonstrated exceeding this threshold with uncertainties an order of magnitude smaller (e.g., from DISCOVER-AQ and KORUS-AQ; Choi et al., 2020). Instruments with uncertainties too high to be used assessing precision, may still be able to contribute assessing systematic biases in polluted environments. Given the larger precision requirement for HCHO columns from TEMPO, in situ HCHO measurements would have less stringent requirements for accuracy and precision for validation. However, there are many demonstrated capabilities with detection limits achieving sub-ppb levels, but with variable levels of accuracy resulting in biases between co-measured HCHO values (Zhu et al., 2020).

In situ airborne ozone measurements are not appropriate for validating the TEMPO total ozone column product due to the majority of the column being above the ceiling of airborne platforms. However, airborne in situ data could contribute toward the validation of the lower portion of the ozone profile product (namely the 0-2 km and free tropospheric components to this profile). Each of these partial columns have a precision requirement of 10 ppbv, which is achievable by research grade ozone airborne measurements.

2. **In situ profile collection methods:** Common flight strategies for collecting and deriving in situ column densities include aircraft spirals, low-altitude approaches over airports, or sets of vertically stacked flight lines (examples in Figure 4-10). Each method has unique benefits and tradeoffs.
    a. In situ spirals are the simplest to match spatially and temporally with TEMPO. For example, during DISCOVER-AQ (Figure 4-9), a typical 5 km spiral spanned several TEMPO pixels though would be vertically stacked over those same pixels. Smaller aircraft can achieve even smaller spiral footprints (perhaps down to 1 km).
    b. Low-passes over airport runways in busy airspaces where spirals are not often performed allow measurements as close to the surface as possible to provide a critical connection to surface-based measurements.
    c. Vertically stacked flight segments allow for systematic profiling across multiple TEMPO pixels with equal vertical sampling within the profile. However, this strategy can still miss features between flight altitudes and takes the most amount of time, creating another source of uncertainty reflecting temporal variance between in situ samples and TEMPO observations. Vertically stacked in situ profiles could be performed in conjunction with the airborne or ground-based DIAL measurements to capture features between the DIAL curtains.

There should be a balance between the temporal frequency of airborne profiling during flights vs. the vertical extent of the profile. The most beneficial profile collection should focus on the extent of the boundary layer into the lower free troposphere (i.e., ~3 km in many areas) where most of the variance in the troposphere is occurring for NO_2 and HCHO (Flynn et al., 2016; Choi et al., 2020; Schroeder et al., 2016). However, periodic full tropospheric profiling would be beneficial (at least 1x per flight if the platform is capable) to capture the regional slower varying free tropospheric details about relevant trace gas species as well as provide a datapoint for validating the free tropospheric ozone product.

Airborne in situ measurement availability for TEMPO trace gas column validation will be limited in time and space (confined to research air quality studies). Therefore, when considering vertical profile sampling for TEMPO validation, the focus should be dedicated in regions where there are known or suspected challenges in evaluating TEMPO products as identified by Pandora or other reference methods for validation. Some effects that must be considered include intra-pixel heterogeneity, varying surface albedo, SZA, vertical profile shape factor, cloud and aerosol interference, and temporal evolution during the in situ observation period.

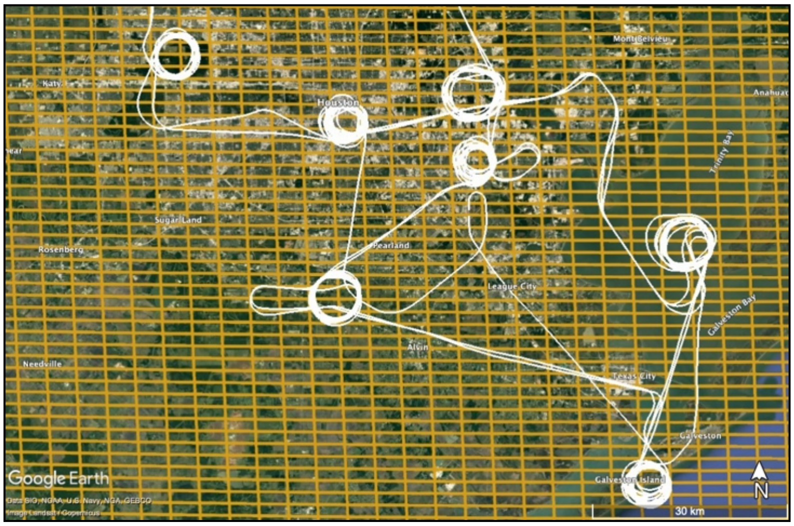

Figure 4-9 Example flight lines for collecting and deriving in situ column densities include aircraft spirals, low-altitude approaches over airports, or sets of vertically stacked flight lines.

4.2.3.3.3 Potential airborne activities during TEMPO's baseline mission

Federally supported 2023 air quality field studies: STAQS/AEROMMA-CUPIDS/GOTHAAM

In the summer of 2023, at least three federally funded research campaigns will be operating aircraft within the TEMPO field of regard: (1) NASA Synergistic TEMPO Air Quality Science (STAQS), (2) NOAA Atmospheric Emissions and Reactions Observed from Megacities to Marine Areas (AEROMMA), and (3) NSF Greater New York Oxidant Trace gas Halogen and Aerosol Airborne Mission (GOTHAAM). Below are brief descriptions with a listing of measurements that could contribute to TEMPO validation.

- ➔ The NASA Synergistic TEMPO Air Quality Science (STAQS) mission in scheduled for the summer 2023 (https://www-air.larc.nasa.gov/missions/staqs/index.html). GCAS and HSRL2/DIAL will be integrated onto the NASA G-V aircraft and provide high resolution NO_2 and HCHO column and ozone profiling measurements for the purposes of accelerating TEMPO related science early in its satellite mission. Known cities that will be sampled are Los Angeles, New York City, and Chicago amounting to over 100 flight hours. Flight strategies will include data collected systematically over the same area (nominally 50 x 135 km box) each day up to three times per day which will include overflights of ground based PGN sites and additional datasets from the NASA DC-8 supporting NOAA AEROMMA. Observational data from STAQS will be publicly available within six months after completion of the campaign in August 2023.
- ➔ NOAA plans to contribute airborne observations from the Atmospheric Emissions and Reactions Observed from Megacities to Marine Areas (AEROMMA) for validation of TEMPO during the summer of 2023 (https://csl.noaa.gov/projects/aeromma/). The

payload includes in situ instrumentation of trace gases, aerosols, and aerosol optical properties. The NASA DC-8 will aim for 4-5 flights each over Los Angeles, New York City, and Chicago, including vertical profiling. The DC-8 aircraft will also coordinate with airborne remote sensing platforms, including the NASA G-V equipped with GCAS and HSRL2/DIAL. In the New York City domain, NOAA Twin Otter will be deployed as part of the Coastal Urban Plume Dynamics Study (CUPIDS) equipped with a MAX-DOAS instrument capable of profiling HCHO and NO2 and Doppler Wind Lidar. These observations can be used to evaluate TEMPO L2 products of NO_2, O_3, and HCHO. Observational data from the AEROMMA field campaign are expected to be finalized by September 2024 and will be archived on the NOAA CSL website (https://csl.noaa.gov/projects/aeromma/data.html).

- ➔ Funded by NSF and led by academic researchers, the Greater New York Oxidant Trace gas Halogen and Aerosol Airborne Mission (GOTHAAM) aims to better understand the atmospheric chemistry in relation to secondary aerosol formation in the region of New York City with the combination of biogenic, anthropogenic, and marine precursors (https://gothaam.science/). While this study is not focused on TEMPO validation, its airborne payload on the NSF C130 will include boundary layer observations of NO_2, O_3, and HCHO.

Progressive Aerodyne SeaRey-University of Alabama at Huntsville

Operated by the University of Alabama at Huntsville, an amphibious Progressive Aerodyne SeaRey aircraft currently configured with an in situ ozone and particulate matter measurements has the potential for adding other instruments. This aircraft is capable of making in situ measurements at various altitudes in the PBL (0-4 km) using stacked flight lines designed to sample TEMPO pixels (example in Figure 4-10). These measurements can provide correlative values to assess the precision and accuracy of the TEMPO 0-2km ozone. If available, instruments to measure NO_2 and HCHO PBL vertical distributions could be added to the payload. SeaRey in situ measurements can also provide a testbed for initial assessment of TEMPO retrieval potential. These flights are occurring now (four flights as of 7.21.2022) before TEMPO's launch and can allow the analysis teams to develop detailed assessment tools that would apply directly to the TEMPO assessments. These tools would include exploring the trade space of flight patterns, altitudes, environmental conditions, and retrieval parameters. Following TEMPO's launch, aircraft measurements using the techniques developed during the pre-launch phase can provide early assessment and guidance on the accuracy and precision of the TEMPO retrievals. Flying in conjunction with ground-based observations (e.g., by TOLNet lidars and Pandora instruments) the SeaRey aircraft can contribute significant information about the horizontal and vertical distributions of TEMPO gases and aerosols.

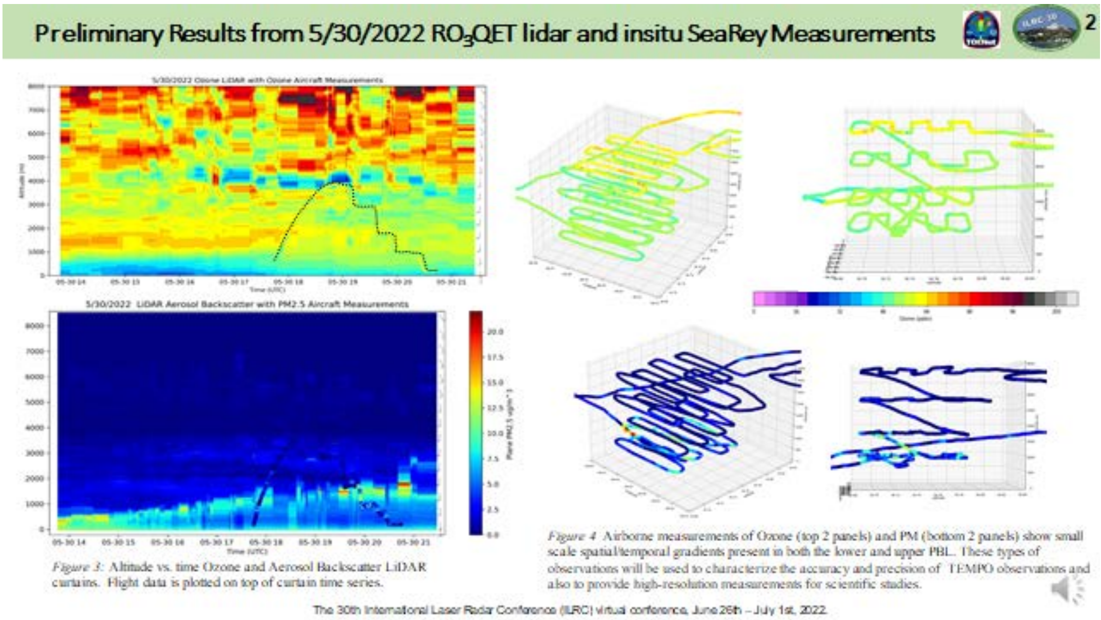

Figure 4-10 SeaRey measurements at four PBL altitudes along rectangles of TEMPO pixel size (~2x5km) of ozone mixing ratios and particulate matter amounts (right panels) with TOLNet/RO3QET time/height measurements of ozone and aerosol backscatter (left panels) over Huntsville AL on 5.30.2022.

In-service Aircraft for a Global Observing System (IAGOS)
Supported by leading research organizations, universities and weather services from Germany, France and the U.K, IAGOS provides atmospheric composition measurements on commercial aircraft (https://www.iagos.org/) around the globe. This data becomes available to researchers at a much lower latency (typically 1-2 years) than the opportunities listed above; however, this data would provide perspective on tropospheric and near-surface ozone in regions of the TEMPO field of regard unsampled by other aircraft. Relevant to TEMPO products, the most likely candidate for use in validation is their ozone profiling capabilities. For example, in 2021, ozone profiles were collected at flights into and out of 52 airports in the TEMPO field of regard. However, the horizontal extend of these profiles will be much larger than what is optimal (unlike a spiral profile) given standard extent of commercial aircraft approaches and therefore is critical for this to be accounted for in validation exercises.

4.2.4 Evaluation with Chemical Transport Models

Chemical transport models (CTMs) can play an important role in TEMPO validation activities by providing a means of including non-coincident measurements in the validation process. This is referred to as "indirect validation" (Loew et al, 2017) and is accomplished by comparison between the CTM and non-coincident validation measurements to determine the biases and RMSE and then comparison between the CTM and TEMPO L2 retrievals to determine the biases between the CTM and TEMPO L2 retrievals. Comparison of these two sets of CTM biases and RMSE can be used to indirectly assess the biases between TEMPO and the non-coincident validation measurements. This indirect validation approach has been used to evaluate OMI HCHO retrievals using GEOS-Chem and on-coincident in-situ airbonne measurements from 12 different field campaigns (Zhu at al., 2020). For this purpose, we will apply simulations of WRF/CMAQ, WRF/Chem, RAQMS, and GEOS-CF during the summer of 2023 TEMPO validation field campaigns (e.g., Synergistic TEMPO Air Quality Science (STAQS)) and other coincident and collaboration field campaigns (e.g., (AEROMMA, CUPiDS, GOTHAAM).

An example of the first part of this process is illustrated using high-resolution (1.3 km) WRF/CMAQ simulations and GEOTASO NO2 columns during the 2017 Lake Michigan Ozone Study (LMOS). The overall duration of a typical GEOTASO flight during LMOS was slightly over 3 hours with each leg of the raster taking ~20 minutes, consequently, only a limited number of the flight legs would be coincident with the nominal TEMPO 1-hour sampling. By mapping the WRF/CMAQ model predictions to the raster flight we are able to compare WRF/CMAQ predictions to all of the GEOTASO raster legs to characterize the model bias and RMSE and then compare the WRF/CMAQ predictions to the hourly TEMPO measurements. Figure 4-11 shows statistical comparisons between the WRF/CMAQ and GEOTASO for all 17 flights during June 2017. Overall, the WRF/CMAQ model NO_2 columns have a fairly high (r=0.79) correlation (accounting for 62% of the GEOTASO variance) and a small bias (0.15 mol/cm^{2}x10^{15}) that is most evident for observed NO_2 columns that are around 1 mol/cm^{2}x10^{15}. This bias is within the overall uncertainty of the GeoTASO NO_2 retrieval which can range from 45-100% for clean (NO_2 columns <3mol/cm$_2$x10^{15}) regions (Nowlan et al, 2016).

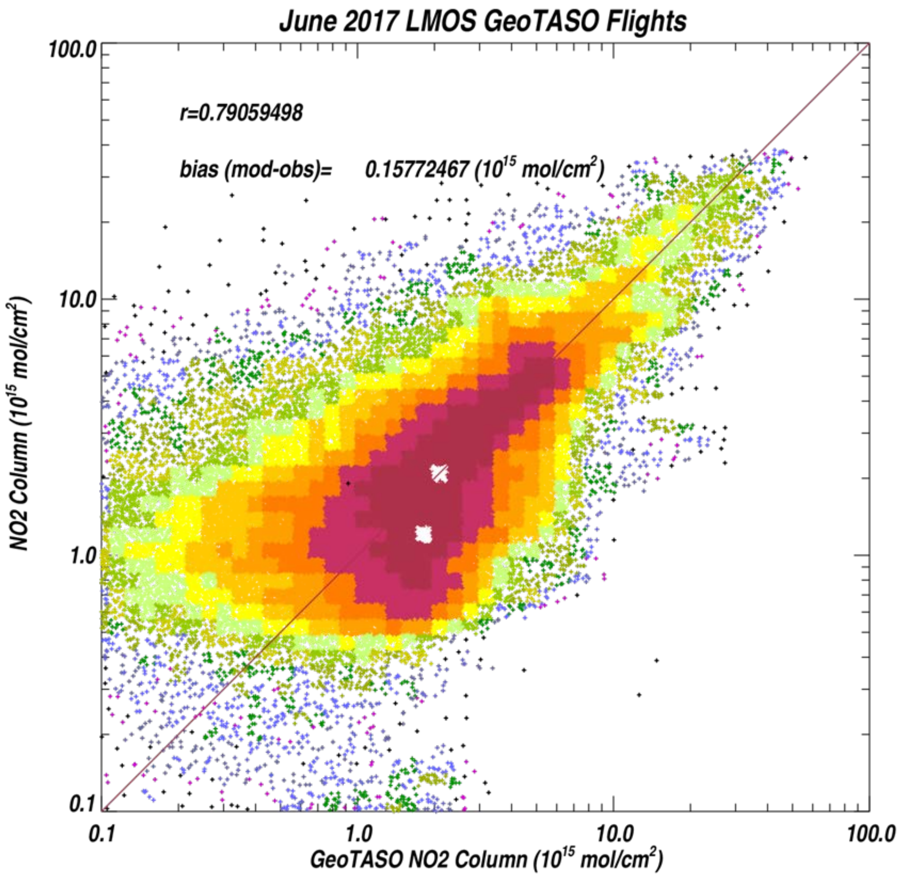

Figure 4-11 Scatter plot of WRF/CMAQ versus GeoTASO NO_2 column (mol/cm^2x10^{15}) for all 17 June 2017 GeoTASO flights during LMOS

An important fact in the accuracy of vertical column densities (VCDs) of trace gas retrievals in the troposphere are the model-predicted Air Mass Factor (AMF) values used in the retrieval. Uncertainties that arise from errors/biases in the GEOS Composition Forecast (GEOS-CF) NO_2 profile shape, which will be used as the a priori vertical profile source in the operational TEMPO retrievals, can introduce large errors in the TEMPO L2 retrievals. AMF uncertainties associated with the model vertical profile can be assessed by using multiple CTMs with different physical and chemical parameterizations and different horizontal spatial resolutions in the TEMPO AMF calculation (Judd et al, 2020). Figure 4-12 shows comparisons between TROPOMI and Pandora NO_2 columns using the standard 1x1 degree TM5 NO_2 profile and NO_2 vertical profiles from a higher resolution (12 km) NAM/CMAQ simulation during the 2018 Long Island Sound Tropospheric Ozone Experiment (LISTOS). Overall median percent differences (low biases) are reduced from -33% to -19% when higher resolution NO_2 vertical profiles are used in the AMF. To assess the uncertainty in the AMF calculations due to modeled shape profiles, and the impact they have on the TEMPO L2 data, we will statistically evaluate multiple CTMs (e.g., WRF/CMAQ, WRF/Chem, GEOS-CF) with non-coincident validation measurements to quantify model biases and RMSE and then apply those CTM vertical profiles as the a priori information in the TEMPO retrieval algorithm.

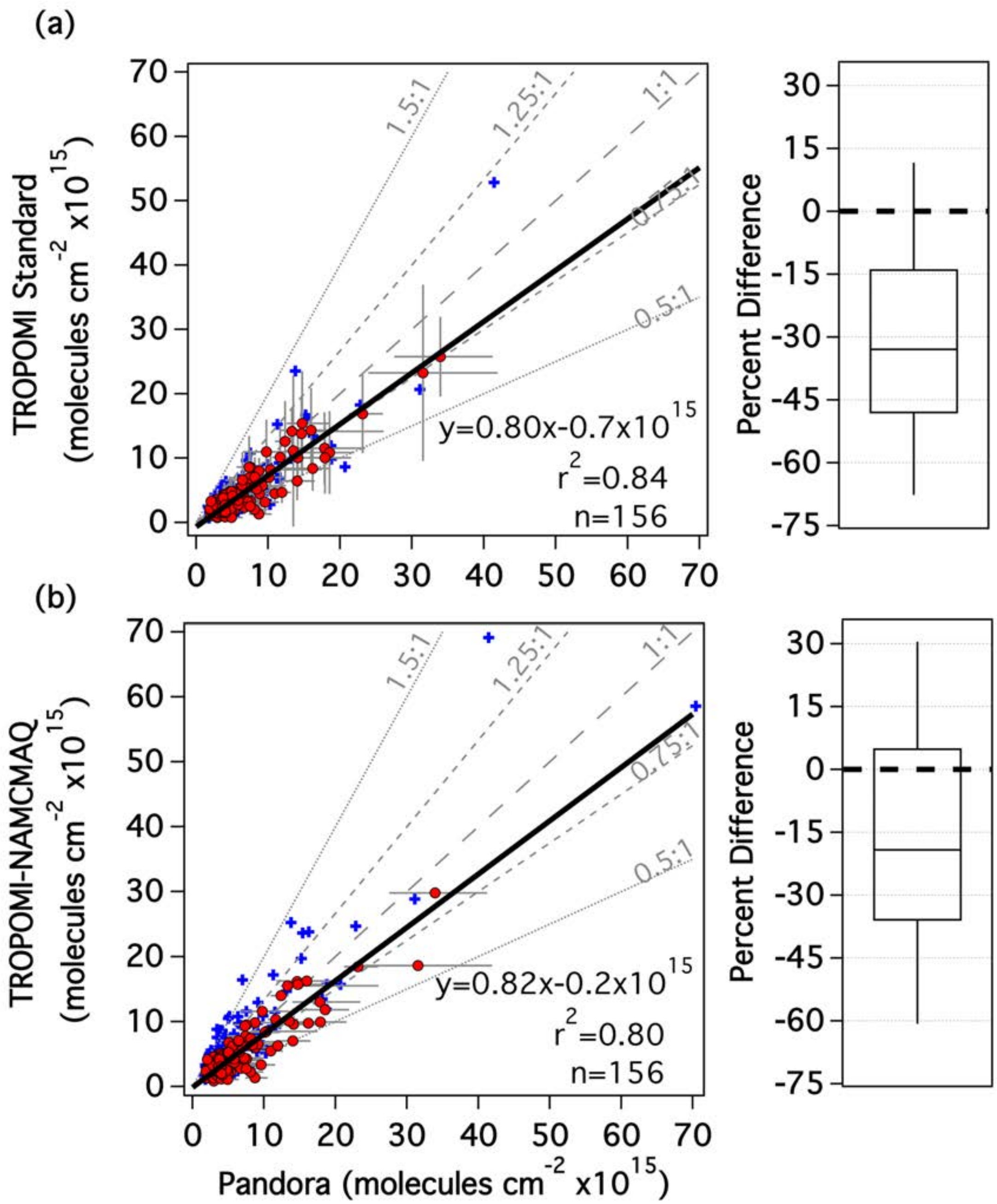

Figure 4-12 Scatter plots of TROPOMI versus Pandora NO_2 columns (mol/cm^2x10^{15}) using the standard TM-5 (upper panel) and higher resolution NAM/CMAQ (lower panel) NO_2 profiles for the AMF (reproduced from Judd et al, 2020)

High resolution CTMs can also be used to understand how spatial heterogeneities can influence Pandora Direct Sun NO_2 column and MAX-DOAS NO_2 profile retrievals, which have different viewing geometries and are therefore sampling different atmospheric slant columns.

4.2.5 Comparison of TEMPO with the MERRA-2 assimilation model

The Modern-Era Retrospective Analysis for Research and Applications Model (MERRA) is very well suited for validation studies of TEMPO. MERRA combines data assimilation from LEO satellites with 3D chemical and dynamics modeling. The result is a conversion of near noon polar orbit satellite data into synoptic data for the entire Earth. This means that ingested data from OMI, OMPS and other polar orbiting satellites incorporated into MERRA can be matched at a wide range of local times (Sunrise to Sunset). The applicability of the MERRA model has been demonstrated by comparison with synoptic time dependent measurements from DSCOVR/EPIC (Herman et al., 2018). For TEMPO, the use of MERRA-2 will provide a unique validation tool.

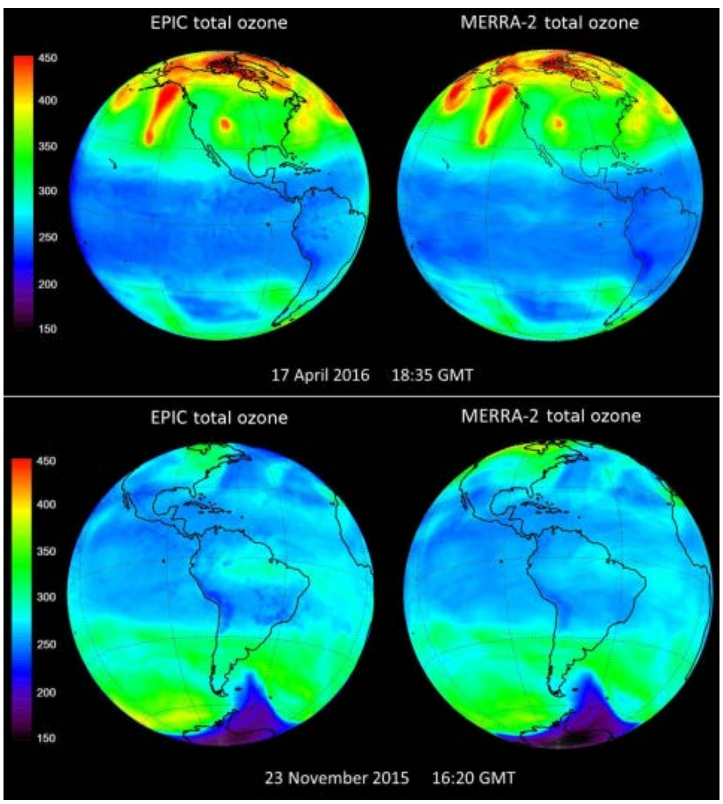

Figure 4-13 Comparison of EPIC total column ozone with the MERRA-2 assimilation model ozone.

MERRA-2 is produced with the latest version of the GEOS atmospheric data assimilation system. The assimilated data includes atmospheric motion vectors from AVHRR; surface wind speeds from SSMIS; surface wind vectors from the *Meteorological Operational Satellite-A* (*MetOp-A*) ASCAT and WindSat; temperature and ozone profiles from EOS *Aura* MLS; total column ozone from EOS *Aura* OMI; bending angle from GPSRO; microwave and infrared sounding radiances from ATOVS on *NOAA-19*, *MetOp-A*, and *MetOp-B*; microwave sounding radiances from ATMS on *SNPP*; hyperspectral infrared radiances from IASI on *MetOp-A* and *MetOp-B* and from CrIS on *SNPP*; and geostationary radiances from MSG SEVIRI and Geostationary Operational Environmental Satellites (*GOES-11*, *GOES-13*, and *GOES-15*) (Gelaro et al, 2017).

5.0 TEMPO Validation Portal

Initial validation efforts will rely on existing data archives for observational data and models discussed in this document. The initial validation portal will leverage Earthdata Search to create a portal that only includes the data products that will be used for TEMPO validation activities. A group will also be created so that only users of that group can download and access the TEMPO data products until they are publicly released.

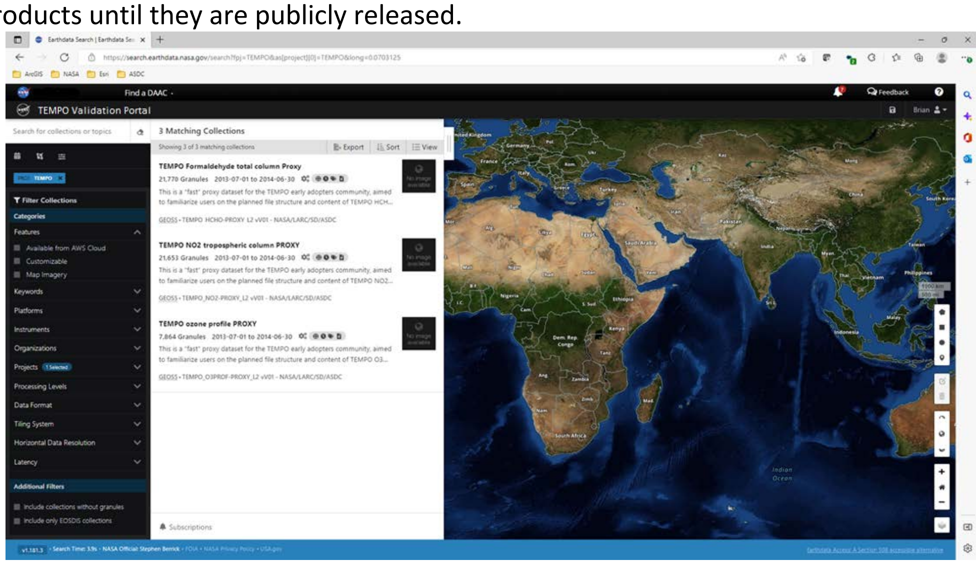

Figure 5-1 Initial TEMPO Validation Portal

This next phase would leverage the Spatial Statistics Toolkit and PaRameter Uncertainty ViEwer (PRUVE), initially developed by the NASA Prediction of Worldwide Energy Resources (POWER) team. The Spatial Statistics Toolkit includes common statistics and visualization functions to produce community accepted plots to be driven by a statistics API, delivered through an interactive map-based user interface. These tools will be generalized and submitted for open source to be scalable and adoptable for TEMPO as well as other future missions.

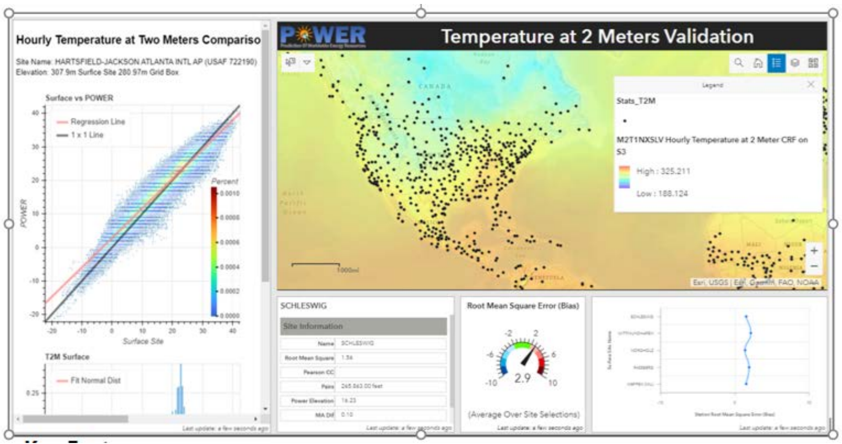

Figure 5-2 POWER PaRameter Uncertainty ViEwer (PRUVE) User Interface

The TEMPO Validation team will additionally ensure a feedback loop with our mission partners to help contribute to the improvement of the next versions of data and assist in capturing statistical requirements driving public, private, and non-governmental application initiatives. Key features to include, but not limited to: Single feature service provides the underlying uncertainty statistics; Minimal coding using Esri Operations Dashboard; Prototype includes 3,000 surface sites; Dynamic data visualization available for each site; Creates maps, plots, and conducts spatial analysis on the fly; Automatically displays referenced statistical content; and Integrated image service as a backdrop. Version 1 will support generating statistics for select air quality, meteorology, climate and solar radiation parameters based on the following data products.

Table 5-1 [1]Geophysical Correlative and Auxiliary Data Sets for Validation

Acronym	Network Description	Website
AERONET	AErosol RObotic NETwork: global network of inter-calibrated multispectral sun-photometers measuring aerosol optical depth and several other aerosol characteristics.	https://aeronet.gsfc.nasa.gov
AirNow	In situ near-real-time measurements across the U.S. of O_3 and NO_2.	https://docs.airnowapi.org/
AQS	In situ monitoring regulatory networks across the U.S. which includes SLAMS, CASTNet, and PAMS - O_3, NO_2, HCHO	https://aqs.epa.gov/aqsweb/documents/data_api.html
IAGOS	In-service Aircraft for a Global Observing System: European Research Infrastructure for global observations of atmospheric composition from commercial aircraft. In situ sensors on measuring along-route O_3, CO, CO_2, CH_4, NO_x, NO_y, H_2O, aerosols and cloud particles. Successor of MOZAIC programme.	https://www.iagos.org

GAW	World Meteorological Organization's Global Atmosphere Watch programme: in situ monitoring networks and contributing networks like NDACC, SHADOZ and TCCON.	http://www.wmo.int/pages/prog/arep/gaw/gaw_home_en.html
MPLNET	NASA's Micro-Pulse Lidar Network: a federated network of lidar systems designed to measure aerosol and cloud vertical structure, and boundary layer heights. Most MPLNET sites are co-located with AERONET sites. MPLNET is also a contributing network to the GAW Aerosol Lidar Observation Network (GALION).	https://mplnet.gsfc.nasa.gov/
NDACC	Network for the Detection of Atmospheric Composition Change: global network of remote sounding research stations with a variety of instruments: Brewer and Dobson spectrophotometers (O_3), DOAS UV-Visible spectrometers (Zenith-sky: O_3, NO_2, BrO, OClO; Multi-axis: NO_2, HCHO, SO_2…), FTIR spectrometers (CH_4, CO, N_2O, CFCs, H_2O…), lidars (stratospheric and tropospheric O_3, H_2O, temperature, aerosols), millimeter wave radiometers (O_3, H_2O, ClO), UV spectral irradiance instruments, ozone sondes, and aerosol backscatter sondes.	http://ndacc.org
PGN	Pandonia Global Network: Network of inter-calibrated Pandora instruments (UV-vis spectrometers) measuring a variety of species (NO_2, HCHO, O_3, and SO_2);.	http://pandonia-global-network.org
SHADOZ	NASA's Southern Hemisphere ADditional Ozonesondes programme: ozonesonde stations operating in the tropics, subtropics, and in the southern hemisphere in general, with coordinated launches and a central archive. Network operating since 1998.	https://tropo.gsfc.nasa.gov/shadoz
TCCON	Total Carbon Column Observing Network: global network of Fourier Transform near-infrared Spectrometers recording direct solar spectra for the measurement of atmospheric CO_2, CH_4, N_2O, HF, CO, H_2O, and HDO.	http://tccon.caltech.edu/
TOLNet	Tropospheric Ozone Lidar Network: North-American network of ground-based lidar instruments for profiling of tropospheric ozone.	https://www-air.larc.nasa.gov/missions/TOLNet
GO3OS/ WOUDC	WMO's Global Ozone Observing System / World Ozone and Ultraviolet Radiation Data Centre: centrally archived global network of total ozone column instruments: Brewer and Dobson spectrophotometers, ozonesondes, Russian UV filter radiometers, stratospheric ozone lidars, Umkehr O3 profiling, UV-visible DOAS spectrometers.	http://woudc.org

UCN	Unified Ceilometer Network: dedicated Ceilometer observations and derived continuous Planetary Boundary Layer Heights primarily located at air quality monitoring stations within the U.S.	https://www.ucn-portal.org

1 Adopted from CEOS Geostationary Satellite Constellation for Observing Global Air Quality: Geophysical Validation Needs, Version 1.1, 2 October 2019

6.0 COMMUNITY PARTICIPATION IN VALIDATION

TEMPO is a novel air quality satellite mission and a promising asset to the atmospheric chemistry and air quality community with an overall goal of providing novel space-based observations of key air quality pollutants and surrogates to inform innovative air quality science and applications. For the Operations Phase this document presents a series of best effort validation activities which is expected to result in episodic and routine assessment of TEMPO L2 data products and traceable data quality as related to the product maturity levels.

As such this document presents information on product validation needs, requirements, methods and tools. Potential future Announcements of Opportunity (AO) calls may be considered to broaden community participation in TEMPO validation activities. For any future AO call this document may serve as a reference for validation of geophysical requirements.

As an outcome of the 2022 TEMPO Science Team meeting attendees were provided with an opportunity to express interests in validation activities. Appendix A provides the input received from the individuals or research groups.

7.0 SUMMARY

TEMPO's field of regard extends from the latitudes of Mexico City and Cuba to north of the Alberta Canada tar sands and across North America and adjacent coastal regions. TEMPO will participate in a triad of international geostationary platforms comprising the South Korean GEMS over Asia, TEMPO over North America, and Sentinel 4 over Europe. TEMPO observation repeat times range from a few minutes to one hour, which will allow TEMPO to provide unique observations for a broad range of atmospheric chemistry and related investigations. Validation over the wide range of viewing geometries and species distributions will require judicious implementation of many correlative instrument observations. Because TEMPO's goals are to obtain species concentrations at higher temporal and spatial resolution than previous satellites, TEMPO validation requires extensive quantification of spatio-temporal gradients using validation techniques that are more sophisticated than traditional intercomparisons.

This validation plan describes a variety of interdependent TEMPO validation activities to fulfill not only the mission requirements (three Pandora instruments over a rather limited time span), but also activities to assess the more complex spatial and temporal distributions of trace gases. We plan to use the full network of Pandora instruments within the field of regard and to use a variety of time-dependent correlative measurements in a cohesive model coordinate system that is essential for effective use of both the measurements and theoretical calculations of complex trace gas distributions and chemical processes. As part of this process, TEMPO will use existing air-quality models to assist interpretation of the disparate measurements.

This validation plan prescribes three levels of validation increasing from an initial Beta Validation to a Provisional Validation that will be available during early phases of the mission and, finally, a Full Validation over the life of the TEMPO mission. As part of the TEMPO mission, validation results will be published in the peer-reviewed literature.

Other than fixed-based measurements, two validation approaches include 1) Focused campaigns of large numbers of instruments deployed in a specified area for a short time (about 1 month) and 2) High-frequency TEMPO revisit observations (about 10 minutes) over selected targets of opportunity. Include a table of validation Green Paper (cite) experiments. The spaceborne instruments, hourly data from EPIC on DSCOVR at L1, and 10 LEO platforms (e.g., OMPS, TropOMI, MODIS), will provide broad spatial coverage of baseline O_3, NO_2, and HCHO and non-baseline H_2O, SO_2, BrO, and CHOCHO for estimation of spatial gradients (accounting for different footprint sizes), mean differences and variances. Airborne ozone and aerosol profiles by HSRL2/DIAL and SeaRey insitu measurements will focus on validating Planetary Boundary Layer (PBL) ozone. Because airborne GCAS and GeoTASO spectrometer measurements most nearly simulate TEMPO observations, these instruments will focus on validating the spatial-temporal distributions of all TEMPO measured gas columns. Additional in situ airborne measurements of many gases measured by multiple instruments will provide both flightpath data and useful reference context for chemistry-dynamics model calculations.

Ground-based approaches include the primary validation measurements: Pandora instruments in the Pandonia Global Network (PGN), TOLNet ozone and aerosol lidars, Dobson and Brewer spectrometers, and Fourier-transform infrared spectroscopy (FTIR) instruments. The PGN instruments measure the same gases as TEMPO with similar sensitivity but with ground-up inverse geometry making them more sensitive to the lower-altitude distribution. The TOLNet lidars, Dobson, and Brewers all measure ozone columns. The lidars also measure the vertical distribution of the ozone column to provide validation of TEMPO's tropospheric and PBL ozone estimates. In the context of model-assimilated meteorology, the time series of these ground-based instruments provide excellent temporal validation that are useful for Lagrangian model spatial-validation information. Validation will pay notable attention to measurements from wide-spread ground-based observations (e.g., MPL, AQS, AirNow, BEACON, et al.)

The primary validation challenge will be to accurately compute the comparable TEMPO column (or partial column) aided by the correlative measurements. The high-time-resolution Pandora measurements (seconds) will most closely correspond 3-second integration time during hourly TEMPO measurements repeat cycles and will provide a useful reference for time variation of species concentrations at specific locations. If these measurements match, then that agreement will provide confidence in the concentration variations over the entire TEMPO field of regard.

Short-term single point in situ measurements from balloons or aircraft will provide the greatest challenge for integration into the validation data set.

The major correlative networks appear in Table 5-1 with links to their locations. The Langley Atmospheric Science Data Center LaRC ASDC will host the TEMPO validation data activities in addition to those provided elsewhere. The NASA/MSFC Short-term Prediction Research and Transition Center (SPoRT) project will manage the Green Paper special operations including those operations related to validation.

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9.0 **Appendix A.** TEMPO Validation Activities Survey results from the 2022 TEMPO STM

Investigator or Research Group	**TEMPO L2 Products:**	**Methodology/data**	**Anticipated timeline to provide analysis**	**Resources (Existing vs Need)**
Cohen, UCB	NO2, O3, aerosol	Use BEACO2N observations in the SF Bay Area, LA and Providence, RI http://beacon.berkeley.edu/about/ to evaluate pixel to pixel variation and time of day variation in NO2 ozone and aerosol.	Work will start when TEMPO data is available	Some of each
Herman, GSFC	O3 Total Column + Trop Column, AOD and UV Aerosol Index, provide surface UVB Algorithm developed for EPIC + Validation. Work with the Pandora team to supply O3 and NO2 validation products from selected sites.	Use of DSCOVR/EPIC and pandora		No extra resources are required

Lamsal, GSFC	NO2 - total column, strat. column, trop. column* plus NO2 slant column and auxiliary information such as NO2 scattering weights (or averaging kernel)	Our team at NASA Goddard has been developing consistent multi-satellite NO2 products by applying OMI NO2 V4 algorithm to GOME-2 (2007-present) and TROPOMI (2018-present). Could apply NO2 algorithm to TEMPO L1B data and perform end-to-end comparison with the operational TEMPO NO2 retrievals. Involved in retrieving NO2 from air-borne sensors: GCAS and GeoTASO. New remote sensing instrument, CHAPS-D, being developed (JHU-APL & NASA GSFC, PI: William Swartz); available for air-borne deployment in 2023-2024. Used Pandora NO2 data.	Our validation activities will start as soon as the preliminary data become available to us. We will share our findings with the retrieval teams. We anticipate that our analysis results will be available in summer of 2024.	Leverage existing resources on best effort basis until dedicated funds become available
Li, GSFC	SO2 - total columns assume different a priori profiles (PBL/pollution SO2, volcanic SO2)	Use retrievals using different techniques (e.g., PCA, DOAS, COBRA) from LEO sensors (OMI, OMPS, TROPOMI) for direct comparisons with our TEMPO PCA SO2 retrievals. Will compare TEMPO PCA SO2 retrievals with available ground-based measurements from PANDORA and MAX-DOAS. Will compare TEMPO PCA SO2 retrievals with available in situ measurements from aircraft and sondes.	June 2024	Leverage OMI and OMPS resources but would require other resources for sustained effort
CSL, NOAA	O3 profile, trop. column, free trop, 0-2 km; NO2 trop.	Flight camping AEROMMA summer of 2023 (https://csl.noaa.gov/projects/aeromma/). The NASA DC-8 will aim for 4-5 flights over	AEROMMA field campaign are expected to finalized by September 1, 2024 and will be archived on the NOAA CSL website (https://csl.noaa.gov/projects/aeromma/data.html).	Resource in place

	Column; HCHO trop. Column; SO2 trop. Column; AAOD, AOD, layer height; C2H2O2 trop. Column; BrO total column; HNO2, IO, NO3 (twilight conditions)	Tier 1 cities (Los Angeles, New York City, and Chicago), including vertical profiling. The DC-8 aircraft will coordinate with NASA G-V equipped with GCAS (NO2 and HCHO) and HSRL-2 (aerosol and ozone profiles), NASA G-III equipped with AVIRIS-NG (GHGs), and NOAA Twin Otter equipped with a MAX-DOAS and Doppler Wind Lidar. See submitted response for map aircraft planned and DC-8 payload. Plan to use these observations to evaluate TEMPO L2 products of NO2, O3, HCHO, CHOCHO and aerosols within the WRF-Chem model. Other trace gas products can be added to evaluation pending needs of the TEMPO STM. We will also leverage our experience with evaluating TEMPO L2 products along with polar-orbiting satellites including for Suomi-NPP/OMPS/CrIS/VIIRS, NOAA-20/OMPS/CrIS/VIIRS, Sentinel-5P/TROPOMI and Aura/OMI.	Once observational data are archived and finalized, WRF-Chem modeling efforts will begin and ensue for the following 1-2 years.	
Ortega, NCAR	O3 total column, strat. column, trop. Column; NO2 total column, strat. column, trop. Column; HCHO trop. Column; H2O total column & profiles;	The FTIR system was upgraded and joined NDACC; (2) In 2021, acquired a PANDORA instrument, joined PGN a few months after initial observation in August 2021; (3) an AERONET Cimel sun photometer; (4) possible in situ NO2 drone observations to explore boundary layer; (5) possible in situ NO2 at Foothills lab.	Data products from NDACC ground-based observations are retrieved near-real-time and analysis can be carried out as desired, data are posted online at NCAR. Pandora & AERONET are operational, available online.	Currently no resources for TEMPO validation, optimistic that we can participate and will contribute on a best effort basis.

	Aerosols – AOD; additional products derived from the FTIR (e.g., wildfire tracers, among others)			
Pierce, SSEC-UW	NO2 total column, strat. column, trop. Column; HCHO trop. Column; AAOD, AOD, layer height	Continue to support Midwest PANDORA deployments including Chiwaukee Prairie, WI. Deployment of CL61 ceilometer and/or WindPro Lidar. Participate in ozone season Wisconsin DNR Enhanced Ozone Monitoring program. Potential deployment of AERI instrument onboard Viking Expedition vessel in Summer 2023. SSEC HSRL Lidar for aerosol layer height. Real-time air quality forecasting support for field campaigns. Indirect validation using high-resolution air quality model as transfer standard between non-coincident validation measurements (airborne, ground based, polar orbiting). Data assimilation studies using both polar orbiting (TROPOMI, OMPS) and geostationary (TEMPO, GEMS) satellite data. Use of analysis increments to intercompare satellite measurements.	Standup WRF-Chem regional air quality forecast system over Midwest by Summer 2023. High-resolution WRF/CMAQ air quality simulations over Chicago, Ill and Western shore of Lake Michigan in 2024	NASA FINESSE for high resolution WRF/CMAQ AQ summer 2023 simulations. Some funding available through No Cost Extension of current SAO contract for TEMPO Science Team

Pusede, UVA	NO2 total column, strat. column, trop. column	Evaluate use of TEMPO for describing neighborhood-level inequalities using a combination of aircraft, ground-based, and other datasets. This includes determining how well TEMPO resolves census tract and block group spatial scales and when/where TEMPO columns reflect surface distributions. Builds on past research using TROPOMI.	As soon as the data are available	Have funding but could make more progress if additional funds become available