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Tropospheric emissions: Monitoring of pollution (TEMPO)

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ABSTRACT

TEMPO was selected in 2012 by NASA as the first Earth Venture Instrument, for launch circa 2018. It will measure atmospheric pollution for greater North America from space using ultraviolet and visible spectroscopy. TEMPO measures from Mexico City to the Canadian tar sands, and from the Atlantic to the Pacific, hourly and at high spatial resolution (~2 km N/S×4.5 km E/W at 36.5°N, 100°W). TEMPO provides a tropospheric measurement suite that includes the key elements of tropospheric air pollution chemistry. Measurements are from geostationary (GEO) orbit, to capture the inherent high variability in the diurnal cycle of emissions and chemistry. The small product spatial footprint resolves pollution sources at sub-urban scale. Together, this temporal and spatial resolution improves emission inventories, monitors population exposure, and enables effective emission-control strategies.

TEMPO takes advantage of a commercial GEO host spacecraft to provide a modest cost mission that measures the spectra required to retrieve O_3, NO_2, SO_2, H_2CO, $C_2H_2O_2$, H_2O, aerosols, cloud parameters, and UVB radiation. TEMPO thus measures the major elements, directly or by proxy, in the tropospheric O_3 chemistry cycle. Multi-spectral observations provide sensitivity to O_3 in the lowermost troposphere, substantially reducing uncertainty in air quality predictions. TEMPO quantifies and tracks the evolution of aerosol loading. It provides near-real-time air quality products that will be made widely, publicly available. TEMPO will launch at a prime time to be the North American component of the global geostationary constellation of pollution monitoring together with European Sentinel-4 and Korean GEMS.

Keywords: Urban and regional atmospheric pollution, tropospheric composition and chemistry, tropospheric transport, atmospheric aerosols

1. INTRODUCTION

TEMPO will be delivered in 2017 for integration onto a NASA-selected GEO host spacecraft for launch as early as 2018. TEMPO and its Asian (GEMS) and European (Sentinel-4) constellation partners make the first tropospheric trace gas measurements from GEO, building on the heritage of six spectrometers flown in low-earth-orbit (LEO). These LEO instruments measure the needed spectra, although at coarse spatial and temporal resolutions, to the precisions required for TEMPO and use retrieval algorithms developed for them by TEMPO Science Team members and currently running in operational environments. This makes TEMPO an innovative use of a well-proven technique, able to produce a revolutionary data set.

TEMPO provides much of the atmospheric measurement capability recommended for GEO-CAPE in the 2007 National Research Council Decadal Survey, Earth Science and Applications from Space: National Imperatives for the Next Decade and Beyond. GEO-CAPE is not planned for implementation this decade. However, instruments from Europe (Sentinel 4) and Asia (GEMS) will form parts of a global GEO constellation for pollution monitoring later this decade, with a major focus on intercontinental pollution transport. TEMPO will launch at a prime time to be a component of this constellation.

2. THE TEMPO SCIENCE MISSION

2.1 Executive Summary

TEMPO's measurements from geostationary orbit (GEO) of tropospheric ozone, aerosols, their precursors, and clouds create a revolutionary dataset that provides understanding and improves prediction of air quality (AQ) and climate forcing, satisfying many of the atmospheric requirements of the NRC Decadal Survey mission GEO-CAPE. TEMPO measures pollution over North America, from Mexico City to the Canadian tar sands, and from the Atlantic to the Pacific (Greater North America, GNA), hourly and at high spatial resolution.

TEMPO's tropospheric trace gas, aerosol, and cloud measurements have the temporal and spatial sampling and precision to resolve diurnal cycle emissions, chemistry, and radiative forcings, monitor pollution at urban scales, and provide for monitoring the inflow and outflow of pollution over GNA. TEMPO will launch at a prime time to be the U.S. component of a global GEO constellation for pollution monitoring. TEMPO's innovative measurements from GEO are built on the heritage of five spectrometers flown in low Earth orbit (LEO),[1-23] which make the proposed measurements at the TEMPO-required precisions using algorithms developed for them by TEMPO Science Team members and running operationaly.[24,25] The LEO measurements lack the ground-breaking time resolution TEMPO offers. As described by Fishman *et al.*,[4] TEMPO observes the tropospheric ozone (O_3) cycle to understand the oxidizing capacity of the atmosphere and the distribution and evolution of air pollution. Tropospheric nitrogen dioxide (NO_2), derived from visible spectra,[8,26-30] is essential to this. With current LEO observations, there are large gaps in our knowledge of the diurnal cycle of emissions, photochemistry, and dynamical transport coupling air quality and climate. Time-resolved measurements during the day-lit period of photochemical conversion and the resultant diurnal cycle are most notably lacking. TEMPO measures the ultraviolet and visible (UV-Vis) spectra to retrieve tropospheric O_3, NO_2, sulfur dioxide (SO_2), formaldehyde (H_2CO), glyoxal ($C_2H_2O_2$), aerosols, cloud parameters, and the UVB surface irradiance and erythemal dose (UVB).[31-38] TEMPO measurements directly relate to four of the six EPA criteria air pollutants (O_3, particulate matter, nitrogen oxides, and SO_2).

2.2 Scientific Goals and Objectives

2.2.1 TEMPO Goals and Objectives and Relevance to Community Goals

TEMPO scientific goals and objectives are strongly focused to provide data for answering key AQ and climate-related questions. The science questions discussed in this section flow from the NASA 2010 Science Plan[39] and the 2007 National Research Council (NRC) Decadal Survey.[40] TEMPO addresses two of the NASA Science Focus Areas for Earth Science:[39]

1) TEMPO provides measurements of atmospheric composition, directly including AQ, improves the ability to forecast AQ, and creates a dataset for examining the societal impacts of AQ.

2) TEMPO measurements address climate forcing by measuring pollution pathways, particularly the details of tropospheric O_3 and aerosol production, transport, and relation to sources.

2.2.2 TEMPO Science Questions

The TEMPO science questions are drawn in large part from work done by the GEO-CAPE Atmospheric and Oceanic Science Working Groups (ASWG and OSWG)[41] with TEMPO Science Team Members as part of the ASWG.

Science Question 1: *What are the temporal and spatial variations of emissions of gases and aerosols important for AQ and climate?*

Providing information on both natural and anthropogenic emissions of aerosols, and of O_3 and aerosol precursors is a major objective of TEMPO. From the NRC: "Based on networks of surface sites, the current system for observation of AQ is patently inadequate to monitor population exposure and to relate pollutant concentrations to their sources or transport. Continuous observation from a geostationary platform will provide the necessary data for improving AQ forecasts through assimilation of chemical data, monitoring pollutant emissions and accidental releases, and understanding pollution transport on regional to intercontinental scales."[40]

Monitoring and predicting AQ requires high spatial and temporal resolution measurements of at least a minimal set of tropospheric gases and aerosol properties: O_3, NO_2 (the standard proxy for odd-nitrogen, NO_x pollution),[8] H_2CO (the standard proxy for volatile organic carbon (VOC) pollution),[17] $C_2H_2O_2$ (a secondary proxy for VOCs),[2] tropospheric SO_2,[16] and aerosol optical depth (AOD) and single scattering albedo (SSA).[32,33] Climate assessments and AQ management are limited by uncertainties in traditional "bottom-up" emission inventories based on application of emission factors to activity rates. Inverse modeling of satellite observations provides "top-down" constraints on emissions inventories of NO_x,[8,9] VOCs,[20] aerosols,[42] and SO_2.[43] For example, Ozone Monitoring Instrument (OMI) NO_2 observations are used to examine the interannual variation in soil NO_x emissions over the central U.S.[44] and to understand NO_x sources in Houston.[45] NO_2 observations from SCIAMACHY provide timely updates to bottom-up emission inventories.[12] NO_2, the photolytic source of tropospheric O_3, varies rapidly in polluted regions, requiring hourly measurements for quantification, as demonstrated for Houston by Fishman et al.[4] OMI H_2CO measurements reveal that at sufficiently high resolution anthropogenic VOC signals can be discerned in addition to biogenic sources.[22]

The value of TEMPO: Hourly measurements at spatial resolution much improved over current LEO sensors and at the precisions already achieved by those sensors, provide much needed insight into the spatial and temporal distributions of criteria pollutant emissions.

Quantitative understanding of NO_2 source attribution and plume dynamics requires spatial sampling of 4-12 km, depending on source type.[46] To adequately distinguish enhanced/polluted events from background scenes, tropospheric NO_2 precision of 1×10^{15} molecules cm^{-2} is required for hourly measurements at high spatial resolution (product resolution of 4×4 km^2 baseline and 8×8 km^2 threshold, GEO-CAPE STM.)[41] Screening of cloudy observations is also improved with high spatial resolution and hourly sampling.[47] The other TEMPO gas measurements have similar temporal and spatial requirements to isolate emission sources and distinguish polluted areas and chemical sources of aerosols, and to follow diurnal development from photochemical processes including heterogeneous processes forming aerosols from their precursors. Sensitivity to lower tropospheric and surface O_3 is enhanced over that obtained by UV measurements alone[7] by combining the UV-Vis (Hartley-Huggins and Chappuis band) measurements.[48]

Science Question 2: *How do physical, chemical, and dynamical processes determine tropospheric composition and AQ over scales ranging from urban to continental, diurnally to seasonally?*

Minimal spatial requirements to follow processes are determined by both the urban scale (several km^2) and the scales of dispersion and plume dynamics[46] vs. photochemical transformation. From the ASWG, an appropriate minimal scale for baseline measurements is 4 km$\times$4 km for gases and aerosols.

The value of TEMPO: The TEMPO spatial resolution to meet baseline requirements, at 8×4.5 km^2, is an order of magnitude improvement in area over current LEO sensors. However, TEMPO retrievals will be done at native spatial resolution of 2×4.5 km^2 for most of the products except for ozone profile product, which is normally limited by data quantity and algorithm throughput to the baseline spatial resolution. The maximum scale is the entire GNA field of regard (FOR), allowing for studies of pollution inflow and outflow.

Diurnal processes are resolved by measuring O_3, NO_2, and aerosols hourly (ASWG[4]) and the SO_2 and VOC proxy concentrations several times per day (ASWG). Observations over a year allow examination of seasonal influences of pollution. Combined UV-Vis measurements improve knowledge of O_3 in the lowermost troposphere.[48,49]

Science Question 3: *How do episodic events, such as wild fires, dust outbreaks, and volcanic eruptions, affect atmospheric composition and AQ?*

Significant quantities of gases, aerosols, and volcanic ash are input to the atmosphere by events including wildfires, volcanic eruptions, and industrial catastrophes with considerable alteration of atmospheric composition and large impacts on AQ and potentially to climate.[50]

The value of TEMPO: TEMPO nominally measures at high native spatial resolution, which can be used to enable analysis of these special enhanced pollution episodes. Such data will facilitate the characterization of trace gases and aerosol loading during wild fire events that have a distinct diurnal cycle in not only smoke emission, but also smoke injection when coupled with boundary layer processes.[51] TEMPO can be commanded to measure part of the FOR at a higher temporal frequency, but reduced longitudinal coverage if required for such events.

Science Question 4: *How does air pollution drive climate forcing and how does climate change affect AQ on a continental scale?*

AQ species, especially O_3, aerosols and their precursors are short-lived climate radiative forcers. According to the Intergovernmental Panel on Climate Change they, may exert more forcing on climate change in the next 20 years than increased carbon dioxide (CO_2).[52]

Climate effects on AQ include increased production of tropospheric O_3 and particulate matter, including black carbon, dust and secondary organic aerosols. Increased O_3 can occur due to temperature effects on both O_3 chemistry and increased emissions of precursors.[53] Increased particulates come from more forest fires, dust storms, and VOC emission increases from heat stress on vegetation.[54]

The value of TEMPO: TEMPO retrieved products can be used to compute instantaneous radiative forcing for various types of AQ conditions, as has been demonstrated with OMI,[55,56] but here with increased spatiotemporal sampling. TEMPO AQ data also facilitate quantification of climate change influence on AQ.

Science Question 5: *How can observations from space improve AQ forecasts and assessments for societal benefit?*

The GEO-CAPE AQ objective is "to satisfy basic research and operational needs related to AQ assessment and forecasting to support air-program management and public health; emission of precursors of O_3 and aerosol, including human and natural sources; pollutant transport into, across, and out of North, Central, and South America."[40]

ASWG objectives flowing from this include: 1) Using measurements to improve modeling of atmospheric processes; 2) Improving AQ forecasts by providing data with sufficient temporal and spatial resolution to improve data assimilation; 3) Enhancing the overall AQ observing system by combining data from satellites and ground-based locations; 4) Providing measurements for monitoring hazards, *e.g.*, volcanoes, dust storms, fires, pollution episodes and UV exposure.

The sparseness of surface measurements limits the ability to provide nationwide AQ index (AQI) maps and forecasts,[50] so that 36 million Americans (~40% of the CONUS) do not receive current AQ information, despite the Environmental Protection Agency's (EPA) establishment of the AIRNow program[57] that provides real-time and forecasted AQ information to alert the public to AQ health effects.

The value of TEMPO: TEMPO high spatiotemporal resolution measurements will be incorporated into the AIRNow Satellite Data Processor system for improved coverage of four of the five AQI maps and forecasts (O_3, SO_2, NO_2 and PM2.5). This will be done in coordination with TEMPO Co-I J. Szykman. In addition, near-real-time (NRT) maps of O_3, NO_2, SO_2, AOD and UVB will be directly available from TEMPO, with web and smart phone display applications.

The improved spatiotemporal resolution of the TEMPO measurements is ideally suited for constraining regional AQ prediction systems employing global chemical data assimilation systems developed to utilize LEO trace gas data.[58-62] These prediction systems will benefit significantly from TEMPO's multiple observations of a given region each day at a horizontal resolution that is commensurate with regional AQ prediction. Additionally, TEMPO UV-Vis measurements of tropospheric O_3[7,48] can substantially improve the analysis and assimilation of surface O_3 concentrations, reducing errors by 50%.[49]

TEMPO's high spatiotemporal resolution allows a more detailed assessment of emission inventories, *e.g.* urban scale and large power plant NO_2 emissions and mobile emissions that show significant spatial and temporal variations due to urban transit patterns, than is possible with LEO observations.[44,63,64]

TEMPO observations benefit epidemiologic studies of AQ and UV exposure health effects. High density observations provide statistics to resolve air pollution related health effects, *e.g.* increased heart failure and cardiopulmonary symptoms produced by increased exposure to smoke.[65]

TEMPO research will use operational hourly derived aerosol properties to improve estimates of surface PM2.5 by adapting an existing near-UV algorithm.[33,66] In addition, TEMPO and GOES-R data can be combined as is currently done with MISR- and ATSR-2-type aerosol retrievals.[67-69] Further advances are possible with TEMPO owing to potential retrievable information on aerosol size distributions.[70,71]

Science Question 6: *How does intercontinental transport affect AQ?*

The international Committee on Earth Observation Satellites (CEOS) coordinates civil space-borne Earth observations.[72] CEOS recommends development of an international constellation of geostationary pollution monitors. This includes the European Sentinel-4, on Meteosat Third Generation, the Korean GEMS on MP-GEOSAT, and GEO-CAPE. A Canadian program of two satellites (PHEOS, on PCW) flying in highly elliptical orbits is also envisaged to measure high northern latitudes. All non-U.S. instruments are planned (Sentinel-4 and GEMS) or proposed (PHEOS) to launch in the

2017/2018 time frame. GEO-CAPE will not launch until more than a decade from now, leaving the constellation without a U.S. component. TEMPO fills this gap, providing for improved coverage of the northern hemisphere to better elucidate intercontinental transport of pollution.

The value of TEMPO: TEMPO can resolve O_3 sources spatially and temporally. This helps to distinguish transport sources arriving within the FOR from stratosphere-troposphere exchange[7,73]. Aerosol and trace gas data at high temporal resolution from TEMPO can also be used to constrain model boundary and initial conditions[74] through assimilation techniques. This improves forecasts of aerosol and gas transport[75]. Aerosol associated with fire emissions, such as transport of Central American/Canadian smoke to the U.S., has distinct diurnal variations[76] and can significantly degrade U.S. AQ. Long range pollution transport from East Asia and dust transport from East Asia and Africa also impacts U.S. AQ.

2.3 Baseline Data Products

TEMPO will measure as standard baseline data products the quantities listed in Table 1 for Greater North America. H_2CO, SO_2, and $C_2H_2O_2$ meet precision requirements up to 50° solar zenith angle (SZA). All other products meet precision requirements up to 70° SZA. The spatial and temporal resolutions and SZA constraints are for meeting the requirements only. Operational retrievals will be done hourly at native spatial resolution ($\sim 2 \times 4.5$ km^2) during the day-lit period except for ozone profile retrievals at spatial resolution of $\sim 8 \times 4.5$ km^2.

Table 1. TEMPO Baseline Products

Species/Products		Typical Value[1]	Required Precision[1]	Expected Precision[2]	
				Worst[1]	Nominal[1]
O_3 Profile	0-2 km (ppbv)	40	10	9.15	9.00
	FT (ppbv)[3]	50	10	5.03	4.95
	SOC[3]	8×10^3	5%	0.81%	0.76%
Total O_3		9×10^3	3%	1.54%	1.47%
NO_2[*]		6	1.00	0.65	0.45
H_2CO[*] (3/day)		10	10.0	2.30	1.95
SO_2[*] (3/day)		10	10.0	8.54	5.70
$C_2H_2O_2$[*] (3/day)		0.2	0.40	0.23	0.17
AOD		0.1 - 1	0.05	0.041	0.034
AAOD		0 - 0.05	0.03	0.025	0.020
Aerosol Index (AI)		-1 - +5	0.2	0.16	0.13
Cloud Fraction		0 - 1	0.05	0.015	0.011
Cloud Top Pressure (hPa)		200 - 900	100	85.0	60.0
Spatial resolution: 8×4.5 km^2 at the center of the FOR. Time resolution : Hourly unless noted. [1]Units are 10^{15} molecules cm^{-2} for gases and unitless for aerosols and clouds unless specified. [2]Expected precision is viewing condition dependent. Results are for worst and nominal cases. 3FT = free troposphere, 2km – tropopause; SOC = stratospheric O_3 column. [*]= background value. Pollution is higher, and in starred constituents, the precision is applied to polluted cases.					
Threshold products are at 8×9 km^2, at 80 minute time resolution.					

2.4 Secondary Data Products

Secondary products (non-baseline, but proven, and provided on a best effort basis) are surface UV-B, bromine oxide (BrO), H_2O, and volcanic SO_2 (column amount and plume altitude). Research products developed by the Science Team include improved AOD, absorbing aerosol index (AAI), and aerosol absorption optical depth (AAOD) all having reduced cloud contamination using a larger number of native pixels for cloud clearing, aerosol size, and aerosol plume altitude. Diurnal out-going shortwave radiation and cloud forcing is now being tested and implemented for OMI (J. Joiner private comm., 2012). Additional cloud/aerosol products are possible using the O_2-O_2 collision complex and/or the O_2 *B* band. Nighttime "city lights" products (similar to visible-earth.nasa.gov), which represent anthropogenic activities at the same spatial resolution as air quality products, will be produced twice per day (late evening and early

morning) in NRT as a research product. Meeting TEMPO measurement requirements for NO_2 (visible) implies the sensitivity for city lights products over the CONUS within a 2-hour period at 2×4.5 km^2 to 1.1×10^{-8} W cm^{-2} sr^{-1} μm^{-1}.

3. MISSION IMPLEMENTATION

TEMPO is a dispersive grating spectrometer that measures solar back scattered light in the UV-Vis spectral range to measure trace gases, aerosols, and clouds. The TEMPO instrument draws from low Earth orbit instrument subassembly heritage and adapts them to geostationary GEO operations. A scan mirror steps the spectrometer slit across the FOR from East to West. A three-mirror telescope images the scene onto the slit of an Offner-type spectrometer. Spectra are imaged onto two 2K×1K CCD focal plane arrays. One array measures 2K ground pixels from 290-490 nm and the other from 540-740 nm. The instrument's thermal and structural design ensures stability over full temperature range incurred in the GEO orbit. Instrument control electronics provide all the functionality to operate the instrument, manage data, and interface to the host spacecraft. Figure 1 shows the range of expected Earth radiance spectra to be measured by TEMPO (TEMPO measurements for longer than 740 nm are not planned), expressed as albedos. They are derived from ESA GOME-1 measurements[1,77] and cover the extremes of conditions measured over the Earth (they also serve as a useful guide to the astronomical detection of Earthlike extrasolar planets).
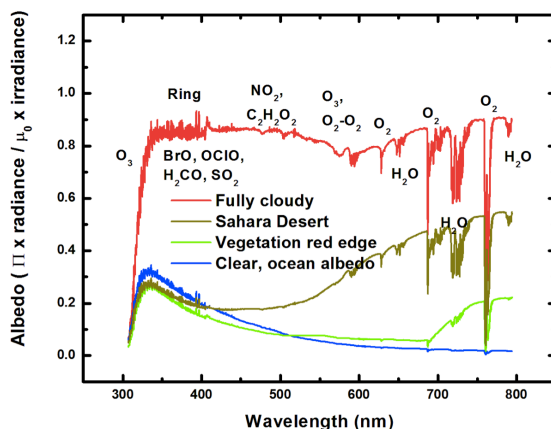

Figure 1. Earth albedo (reflectance) spectra derived from the ESA GOME-1 instrument for the range of conditions to be monitored by TEMPO.

TEMPO is managed by NASA LaRC (Wendy Pennington, Instrument Project Manager, and Alan Little, Mission Project Manager). The instrument is being built by Ball Aerospace & Technologies Corp. The Science Team includes members from NASA LaRC and GSFC, the EPA, NOAA, NCAR, Harvard U., U. California at Berkeley, U. Alabama in Huntsville, U. Nebraska, St. Louis U., and U. Maryland (Baltimore County and College Park), Carr Aeronautics and RT Solutions. International collaborations include Korea, Canada, Mexico, and the European Space Agency.

3.1 Measurement Characteristics

The TEMPO Science Team has performed the radiative transfer modeling and retrieval sensitivity studies to determine the instrument requirements. The retrieval precisions and degrees of freedom[78] for O_3 profiles and the trace gas vertical column densities (VCDs) are directly calculated using the optimal estimation approach for clear-sky scenarios in the CONUS with a minimal surface albedo (0.03). Results for the worst and nominal viewing scenarios are shown in Table 1. Interferences due to surface albedo, other trace gases, and the Ring effect are fully accounted for.[24] Spectroscopic errors are not included. They mainly cause systematic errors and can be reduced in the future. Since retrieved O_3 profiles use a priori information, the precision requirements for O_3 in Table 1 include smoothing errors. O_3 sensitivity analysis indicates that it is necessary to include the visible Chappuis band (550-650 nm) to meet the 0-2 km 10 ppbv precision and the GEO-CAPE objective of sensitivity to the lowest 2 km for surface AQ, shown by the averaging kernels (AVGK) in Figure 2. The spectral range 290-740 nm is therefore selected to cover the relevant absorption features of O_3, other trace gases and aerosol features. A spectral resolution of 0.6 nm, sampled at 0.2 nm to avoid spectral undersampling,[79,80] matches the spectral range to the detector.
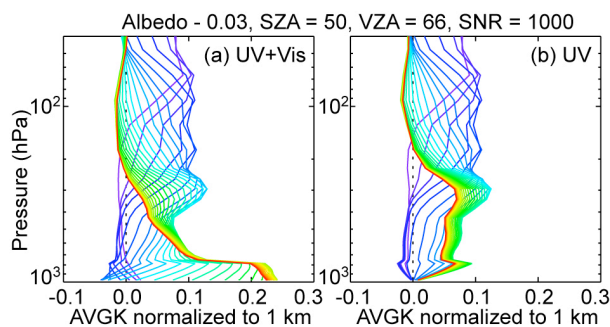
Figure 2. TEMPO UV-Vis observations (a) significantly improve sensitivity to O₃ near the surface compared to using UV only (b), as shown by the retrieval averaging kernels.

The TEMPO FOR is sampled from East to West in 1250 scans with 2,000 pixels (N/S) in each scan at a native spatial resolution of 2 km N/S×4.5 km E/W over GNA, driven by the requirements of spatiotemporal resolution, coverage, and signal to noise ratio (SNR). The native spatial resolution is defined at the center of the domain, 36.5°N, 100°W, assuming the preferred orbit longitude of 100°W. The TEMPO ground sampled area (GSA) depends on the particular pixel's viewing angle within the FOR and varies because of the Earth's curvature. Users routinely re-grid satellite data for data assimilation and scientific analysis[81,82] to account for these expected variations. The GSA varies by only a factor of <3.0 over the CONUS for a GEO longitude range of 80°W-115°W, compared to the factor of 10 variation across an OMI swath. TEMPO's GSA allows spatial co-adding of four native pixels to the baseline product resolution, which over the CONUS at the preferred GEO longitude will provide a factor of >5 improvement over the best (nadir) resolution of OMI and 50 times that of GOME-2. TEMPO has the added benefit of viewing a given location with a consistent GSA. Measurements are hourly from 2 AM until 10 PM with longer integration times for twilight and nighttime obtained by co-adding temporally.

3.2 Measurement Considerations

The baseline algorithms, all developed by TEMPO Science Team members and applied to OMI and other sensors, have well documented performance and error analyses.[24,25,31] The retrieval algorithms derive all products using TEMPO measurements of solar irradiance and back scattered radiance. The radiance and irradiance required accuracies are achieved by standard prelaunch instrument characterization and calibration plus on-orbit radiometric trending. This approach has been successfully used by OMI, GOME-1 and -2 and SCIAMACHY.[77,83-92]

The trace gas retrievals have minimal sensitivity to absolute radiance values; they exploit relative spectral variations in backscatter spectra as correlated with target molecular absorption spectra. Thus, relative variations in the absorption cross sections of the target molecules are more important than the absolute values. Laboratory measurements of the cross sections are of sufficient accuracy for all target gases and interfering gases.[93-103]

Cai et al.[104] have shown that the polarization state of reflected sunlight can be calculated using existing retrieval forward models to a level sufficient to correct instrument polarization effects that would otherwise adversely affect trace-gas retrievals similar to TEMPO.

3.3 Projected Instrument Performance

Based upon heritage experience with UV-Vis grating spectrometers, TEMPO instrument performance should significantly surpass the requirements for the majority of species. The mapping of this expected instrument performance to baseline science products is given in Table 1.

Retrieval precisions for baseline measurements under worst and nominal viewing scenarios demonstrate that all measurement requirements are met. Retrievals of NO₂, H₂CO, C₂H₂O₂, total, stratospheric, and free tropospheric O₃, aerosols, and clouds can even meet the precision requirements at 2 km×4.5 km for SZA up to 70°.

3.4 Retrieval Algorithms and Heritage of Default Launch Algorithms

Retrievals developed for the GOME, GOME 2, OMI, and SCIAMACHY sensors have all proved the measurement approach of TEMPO. TEMPO level 0-1, level 1-2, and level 2-3 operational algorithms implemented at launch are adapted from current operational algorithms developed by Science Team members at the Smithsonian Astrophysical Observatory (SAO) and the NASA Goddard Space Flight Center (GSFC), with some modifications required to interface with TEMPO data and additional optimizations for TEMPO data. Improved algorithms, particularly for aerosols and clouds will be implemented operationally when they have been fully developed, tested, and validated.

3.4.1 Minor Trace Gas Retrieval Heritage

SAO has developed trace gas algorithms for GOME-1, GOME-2, OMI, SCIAMACHY, and OMPS (and performed retrievals on all but OMPS), starting in 1985. Fitting algorithms for level 2 NO_2, H_2CO, $C_2H_2O_2$, SO_2, H_2O, and BrO products are adapted from the operational OMI BrO/H_2CO/chlorine dioxide (OClO) algorithms developed at SAO.[17,79,105-110] Trace gas slant column densities (SCDs) are derived by directly fitting measured radiances within an optimized spectral region through an empirical equation based on the Beer-Lambert law. SAO has initially developed much of the physics and methodology for these algorithms such as wavelength and slit calibration,[111] undersampling correction,[79,80-112] Ring effect correction,[113] high-resolution solar reference spectrum,[114] and improvement in trace gas absorption cross sections,[101,115,116] which have been widely used in other operational and research algorithms. SCDs are then converted to VCDs through air mass factors calculated with the VLIDORT[117,118] radiative transfer model and trace gas profiles from GEOS-Chem chemical transport model simulation.[108,119] In the current OMI BrO algorithm, wavelength-dependent air mass factors are multiplied with BrO cross sections to directly derive VCDs in one step; this method can be applied to improve the retrievals of other trace gases. Extensive climatologies of wavelength-dependent scattering weights have now been developed, making this one-step process an option for TEMPO. The trace gas-fitting algorithms are generic and can be applied to the different trace gases. The major changes are algorithm inputs (*e.g.*, spectral range, fitting parameters) or interface to read the level 1 data.

In addition to the algorithm development at SAO, the GSFC team has developed algorithms to retrieve SO_2 from TOMS[120] and OMI data[121,122] using up to six wavelengths. Recently, several more advanced SO_2 algorithms that combine spectral fitting and radiative transfer calculations have been developed to retrieve both SO_2 VCDs and plume height at both GSFC[15,123-125] and SAO.[16] The GSFC team has also developed OMI operational tropospheric NO_2 VCDs[126,127] using the SCDs derived by the Koninklijk Nederlands Meteorologisch Instituut (KNMI) NO_2 fitting algorithm.

3.4.2 O_3 Profile and Tropospheric O_3 Retrieval Heritage

The TEMPO O_3 profile algorithm will be adapted from the GOME, OMI and GOME-2 algorithms.[7,104,116,128-130] The idea to derive O_3 profile information including tropospheric O_3 from the Hartley and Huggins bands in the UV and Chappuis bands in the visible was first proposed by and has been successfully implemented by the SAO group.[1,48,131] The algorithm derives O_3 profiles by directly fitting the observed radiances in the Hartley/Huggins bands through on-line VLIDORT calculations using the optimal estimation method.[132] The GOME-2 retrievals also implement the inclusion of the Chappuis bands to enhance the sensitivity to near-surface O_3;[133] however, the improvement resulting from this inclusion over retrievals that are constrained to the UV segment of the spectrum have not been quantified due to calibration inconsistencies in three bands in the GOME-2 spectra. The single focal plane approach of TEMPO eliminates this error. This algorithm has also been used to derive SO_2 VCDs and plume height for OMI.[16]

3.4.3 Total O_3 Retrieval Heritage

The level 2 total O_3 algorithm will be adapted from operational algorithms developed by Science Team members at NASA GSFC. Total O_3 column is retrieved with the TOMS V8.5 algorithm,[134] which has been used to derive nearly 40 years of total O_3 record from TOMS, SBUV, and OMI data dating back to 1970s. It uses two wavelengths to derive total O_3: a weakly absorbing wavelength (331.2 nm) to estimate an effective surface reflectivity (or effective cloud fraction), and another wavelength (317.5 nm) with stronger O_3 absorption to estimate O_3. In addition, the O_3 profile algorithm in **3.4.2** also derives total O_3 by utilizing more spectral information.[7,128]

3.4.4 Aerosol Retrieval Heritage

The TEMPO operational aerosol algorithm will be adapted from the TOMS aerosol and OMAERUV algorithms,[32,135-139] which uses two wavelengths (354 and 388 nm) to retrieve AI, AOD, AAOD, and single aerosol scattering albedo based on a predefined set of biomass burning, dust and sulfate aerosol models.

3.4.5 Cloud Retrieval Heritage

The level 2 cloud algorithm will be adapted from the OMI Raman cloud algorithm, which derives optical centroid cloud pressure and radiative cloud fraction from the amount of filling in of solar Fraunhofer lines caused by rotational Raman scattering in the atmosphere.[34,35,140-142] The cloud fraction does not represent true geometrical cloud fraction and the cloud pressure does not represent the physical cloud-top pressure (especially in the case of multiple cloud layers), but a transmittance weighted cloud pressure that we call the Optical Centroid Cloud Pressure (OCCP). However, it better represents enhanced trace gas absorption by multiple scattering inside clouds than the physical-top pressure and is thus better for trace gas retrievals from UV radiances.

3.4.6 UVB Retrieval Heritage

The UVB algorithm will be adapted from the TOMS and OMI operational algorithm. It produces surface UV irradiance, erythemal dose rate (UV index), and the erythemal daily dose from level 2 products of O_3, aerosols, and clouds.[36,143-147]

4. ACKNOWLEDGEMENTS

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