TEMPO Green Paper: Chemistry experiments with the Tropospheric Emissions: Monitoring of Pollution instrument

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TEMPO is required to spend much of its observing time scanning the full field of regard (FOR) each hour, for as much of the daylight portion of the diurnal cycle as we can arrange (but certainly to 70° solar zenith angle). However, some observing time, perhaps as much as 25%, is available for non-standard observations. Non-standard operations simply mean observing a portion of the FOR (an East/West slice, as North/South is fixed) at higher temporal resolution.

Non-standard observations may be of two types: First, events, which might include volcanic eruptions, forest fires, dust outbreaks, significant storms. Second, "chemistry experiments" which use the world's highest chemistry set to inform atmospheric pollution science in general and satellite retrievals of pollution (especially for TEMPO) in general. Note that:

- 1. Image Navigation and Registration (INR, think "pointing") is likely to be slightly worse in the first hour of daylight and also in the Easternmost several hundred km of the FOR.
- 2. Research scans may need supplemental hand registration to take full advantage of the spatial resolution.
- 3. We do not yet know at what time of the year we will be launched and thus what time of year we will be in commissioning phase. It is reasonable to think that some experiments will be done in commissioning phase but they are not required to be.
- 4. We hope as we fully retire instrument risk to add SO₂, aerosol, C₂H₂O₂ back as operational products and provide validation for them. However, they are always in the spectra, so they can perfectly reasonably be included in chemistry experiments.
- 5. If we do our job of insuring that command sequences are pre-loaded, about 1-hour notice is required to initiate a special sequence.
- 6. Discussion of special observations now hopefully ensures that flexibility remains when operations become more fully developed.

For purposes of discussion we are assuming that special operations have 10-minute time resolution and 1000 km E/W swath but they don't have to be. For oversampling studies, for example, they could be quicker and narrower. Anything down to step and stare (with several km jitter) should be possible.

Normal time resolution studies

Air quality and health

TEMPO is targeted at improving monitoring, assessment, and chemical understanding of air quality over Greater North America. Current observation of air quality from space has been limited so far by the sparseness of LEO satellite data and low sensitivity to near-surface ozone. TEMPO's hourly measurements allow better understanding of the complex chemistry and dynamics that drive air quality on short timescales. The density of TEMPO data is ideally suited for data assimilation into chemical models for both air quality forecasting and for better constraints on emissions that lead to air quality exceedances. Planning is underway to combine TEMPO with regional air quality models to improve EPA air quality indices and to directly supply the public with near real time pollution reports and forecasts through website and mobile applications. The dense spatial coverage of TEMPO will also offer valuable information for epidemiological studies to understand health effects. Hourly temporal resolution offers benefits for cloud slicing to separate lower-mixed layer concentrations from those aloft. The ability to observe and attribute air pollution events over the entire TEMPO field of regard has great policy and societal benefits. There is existing communication with air quality managers through programs such as the NASA Health and Air Quality Applied Sciences Team (HAQAST) that will assist in exploitation of TEMPO data for air quality applications.

Ultraviolet exposure

An ultraviolet index retrieval using O_3 amounts and surface reflectance will enable us to employ different action spectra for erythemal exposure of skin, vitamin D synthesis, DNA damage, and plant response.

Biomass burning

Emissions from biomass burning can vary greatly both regionally and from event to event, but previous work has been unable to fully explain this variability. Of particular interest is the unexplained variability in ozone production from fires. The primary emissions from burning and the chemistry in fire plumes evolve on hourly and daily timescales, making observations from TEMPO especially valuable for investigating these processes. The suite of NO₂, H₂CO, C₂H₂O₂, O₃, H₂O, and aerosol measurements from TEMPO is well suited to investigating how the chemical processing of primary fire emissions effects the secondary formation of VOCs and ozone. Ongoing efforts are working to address complications for trace gas retrievals in forest fires due to high aerosol loading. TEMPO measurements should not only increase understanding of the chemical emissions from biomass burning but also be a powerful tool for monitoring and assessing the impact of burning on human health and climate change. For particularly important fires it is possible to command special TEMPO observations at even shorter than hourly revisit time, probably as short as 10 minutes.

Synergistic Cloud Products

As TEMPO will use GOES-R data for INR, GOES-R products can be easily used for TEMPO applications. Especially, GOES-R cloud information is of particular interest for improving and using TEMPO products. A wealth of GOES-R cloud information such as cloud optical depth, geometrical cloud fraction, cloud-top height, cloud-top phase, and temperature are available at TEMPO sub-pixel level. These cloud products can be mapped to TEMPO spatial pixels and can

be used to improve TEMPO clouds, aerosol and trace gas retrievals and used to screen cloudcontaminated TEMPO data.

Advanced aerosol products

As the first geostationary satellite to measure ultraviolet and visible spectra over North-America, TEMPO provides a unique opportunity to develop new research algorithms for aerosol retrievals by taking advantage of its hourly observations and its synergy with other geostationary satellites that measure the radiation in the visible, shortwave infrared and thermal infrared. TEMPO may be used together with the Advanced Baseline Imager instruments on the NOAA GOES-16 and GOES-S satellites for aerosol retrievals. A combination of 3 shortwave bands from GOES-R (470, 640, and 860 nm) and 4 bands from TEMPO (340, 380, 470, and 640 nm) can improve the retrieval of both AOD and fine-mode AOD accuracy; comparing to the retrieval from the single sensor, the joint retrieval reduces AOD and fine model AOD uncertainties respectively from 30% to 10% and from 40% to 20%. In addition, radiances in the spectral regions of O₂-O₂ and O₂ absorption (*e.g.*, O₂ *B*, O₂ γ) can be used to retrieve the aerosol plume height. Furthermore, multiple measurements taken for the same pixel (from same viewing angle but multiple solar zenith angle and therefore scattering angles) can provide information on aerosol shape. TEMPO observations of aerosol precursors will offer information on aerosol production processes.

Soil NO_x after fertilizer application and after rainfall

U.S. and Central American inventories of soil NO_x due to nitrogen fertilization are uncertain by more than 100%. There is an underestimate of NO release by nitrogen-fertilized croplands as well as an underestimate of rain-induced emissions from semiarid soils. TEMPO measures greater North America croplands hourly and so is able to follow the temporal evolution of NO_x emissions from croplands after fertilizer application and from rain-induced emissions from semi-arid soils. Should even higher temporal resolution over selected regions be useful, that may be accomplished by special observations.

Solar-induced fluorescence from chlorophyll

TEMPO measurements of solar-induced fluorescence from chlorophyll may be made over both land and ocean. Land measurements can be used for studies of primary productivity, the length of carbon uptake period, drought responses, and tropical dynamics. These apply both to agriculture and forests. Ocean measurements can be used to detect red tides and to conduct studies on the physiology, phenology, and productivity of phytoplankton.

Foliage studies

TEMPO will be capable of measuring spectral indices for estimating foliage pigment contents and concentrations applied generally to leaves but not the full canopy. A single spectrally invariant parameter, the Directional Area Scattering Factor, relates canopy-measured spectral indices to pigment concentrations at the leaf scale.

Crop and forest damage from ground-level ozone

Ozone damages vegetation by entering through the stomata and oxidizing chemicals that perform the photosynthetic process. This damage amounts to several billion dollars per year in the U.S. alone, and much more worldwide. Collateral effects include changes in water and carbon exchange. TEMPO will measure the ozone as well as water vapor, permitting quantitative studies of the detailed correlation of vegetation damage for various crop types and cultivars at the TEMPO pixel scale or (by oversampling) smaller. Such studies can contribute to optimized agricultural choices. Forest studies can contribute to improved wildfire prevention.

Halogen oxide studies in coastal and lake regions

The atmospheric chemistry of halogen oxides (*e.g.*, BrO and IO) over the ocean, and in particular in coastal regions, can play important roles in ozone destruction, oxidizing capacity, and dimethylsulfide oxidation to form cloud condensation nuclei. The budgets and distribution of reactive halogens along the coastal areas of North America are poorly known. Therefore, providing a measure of the budgets and diurnal evolution of coastal halogen oxides is necessary to understand their roles in atmospheric photochemistry of coastal regions. Previous groundbased observations have shown enhanced levels (at a few pptv) of halogen oxides over coastal locations with respect to their background concentrations over the remote marine boundary layer. Previous global satellite instruments lacked the sensitivity and spatial resolution to detect the presence of active halogen chemistry over mid-latitude coastal areas. TEMPO observations together with atmospheric models will allow examination of the processes linking ocean halogen emissions and their potential impact on the oxidizing capacity of coastal environments of North America.

TEMPO also performs hourly measurements of one of the world's largest salt lakes: the Great Salt Lake in Utah. Measurements over Salt Lake City show the highest concentrations of BrO over the globe. Hourly measurement at a high spatial resolution can improve understanding of BrO production in salt lakes.

Air pollution from oil and gas fields

TEMPO measurements of O_3 , NO_2 , H_2CO , $C_2H_2O_2$, and aerosols will contribute to understanding and quantifying the emission from oil and gas fields, and to understanding the chemical evolution of air pollution (*e.g.*, wintertime high ozone episodes) near oil and gas production regions,

Night light measurements resolving lighting type

TEMPO offers the possibility of collecting spectra of nighttime lights when the sun is >60° from its boresight or when the sun is fully eclipsed by the Earth. Many different types of outdoor lighting are used across the U.S., including Hg vapor, high and low-pressure Na lamps, and LEDs, which should be classifiable by virtue of their spectral signatures. With a 10 s dwell time, TEMPO can map such lights with adequate SNR over greater North America in a single scan of ~3 hours near the winter solstice (Carr et al., 2017); the domain can be covered piecemeal in several days during other time periods. Weaker signals within a small region can be detected with even longer dwell time. While not specifically intended for nighttime collections, TEMPO provides an interesting capability for studying nightlights as markers for surface aerosol pollution, human activity, energy conservation, and compliance with outdoor lighting standards intended to reduce light pollution.

Ship tracks and drilling platform plumes

TEMPO will be able to monitor pollution over ship tracks and from drilling platform plumes, *e.g.*, in the Gulf of Mexico and off the coast of California. For the drilling platform plumes in particular, higher temporal measurements may improve detection limits and measurement

precisions enough to make measurements for significantly fainter platform sources.

Water vapor studies

TEMPO water vapor and pollution measurements will contribute to understanding the extent that corn sweat contributes to making heat waves and air pollution in the U.S. Midwest worse. The tails of land-falling atmospheric rivers over the west coast can be captured by TEMPO. Land-falling hurricanes from the Atlantic and the Gulf of Mexico can be monitored after they move into the FOR.

Volcanoes

TEMPO will provide detailed understanding of the pollution produced by volcanoes, and how SO₂ and ash are transformed and transported.

Economic studies

TEMPO will perform quantitative studies of pollution that inform the state of developing or receding economies, *e.g.*, for North American regions and for Cuba, as pollution and economic prosperity are generally highly correlated.

Tropical cyclones

There remains a large gap in understanding the impact of gas-aerosol-cloud interaction processes on tropical cyclones in the Earth system. Tropical cyclones frequently interact with dust aerosols transported from the Sahara Desert and sea salt over the Atlantic Ocean. While approaching the North American landmass, smoke and anthropogenic aerosols from biomass burning and urban emission sources can also interact with tropical cyclones. The synergy of TEMPO and the Advanced Baseline Imager (ABI) aboard the GOES-16 and 17 Series will provide unprecedented detail on the spatiotemporal evolution of trace gases, aerosols, and cloud processes in the vicinity of tropical cyclones. This high-temporal information will enable robust studies on the trace gas emissions and transport and chemical processes that can govern aerosol formation and interactions with tropical cyclones. Single scatter albedo and aerosol layer height from TEMPO observations will aid in characterizing the evolution of aerosols. The high-time (less than 60 min) microwave observations from the TROPICS (Time-Resolved Observations of Precipitation structure and storm Intensity with a Constellation of SmallSats, launch date 2021) mission will provide key information on the diurnal evolution of the temperature, humidity, and precipitation structure of tropical cyclones. Altogether, the complementary TEMPO, ABI, and TROPICS data will advance the state of knowledge on how gas and aerosol processes can influence the diurnal evolution of tropical cyclones.

Tracking short-term public health outcomes using high-resolution TEMPO data

The Mount Sinai Health System is a large, multi-faceted healthcare system, located predominantly in the greater New York metropolitan area. Mount Sinai has more than 150,000 inpatient, 3.4 million outpatient, and 0.5 million emergency visits each year over eight hospitals and numerous health centers. The health system is integrating and harmonizing health records across all encounters to ensure effective data to improve health outcomes. Near real-time daytime hourly estimates of gaseous air pollutants from TEMPO will be included as acute exposures in epidemiological case-crossover analyses of children's asthma exacerbations. This approach compares exposure before case events (*e.g.* unprompted emergency or urgent care

medical visits and medication adjustments) and control periods for the same participants. Distributed lag non-linear modelling will be used to identify critical exposure windows relative to the time of visit, assigning exposure based on the child's geocoded home address. The richness of our health datasets will allow us to stratify by key variables such as asthmatic subtypes, as they may be differentially susceptible to air pollution levels. Improved exposure assessment within epidemiological studies can provide the evidence base to predict short-term public health outcomes and, consequently, improve healthcare decision-making. For example, changing air pollution levels may lead to notifications or prompts for specific patients to avoid physical exertion or to stay indoors when possible. It can also underscore the importance of effective disease management, whereby individuals who live in areas with chronically higher exposures can be targeted for outreach for checkups and prescription refills.

Consistently understanding the representativeness within the TEMPO FoR of O₃ products using a network of O₃ Lidars and ancillary co-located measurements

There is a lack of current understanding in answering the fundamental question: *How will the TEMPO tropospheric ozone products ozone products, especially the 0-2km column, be evaluated for accuracy and precision?* This effort would focus on a higher temporal frequency sampling of selected scenes of opportunity that intersect with the Tropospheric Ozone Lidar Network (TOLNet) observations at their home institution sites. The emphasis on this effort would be to increase sampling frequency at TOLNet sites to more fully explore the representiveness of the TEMPO O₃ 0-2km products. For instance, how do TEMPO retrievals perform in scenes that are: (1) clean vs polluted (w.r.t ozone and particulate matter); (2) complex scenes such as coastlines or mountainous terrain; (3) high sun angles vs. low angles and different times of the day; (4) cloud-free vs. cloudy; (5) direct zenith retrievals vs. reconstructed products using air mass factors; (6) surface albedo/land type impact.

This effort would further seek to quantify from a "bottom up" approach the statistics and accuracy of TEMPO's measurements and how the SNR varies during several times of the day, which will need to be more fully explored in the age of geostationary observations. To rigorously understand this representativeness, especially in the vertical, a dedicated and consistent data set from existing ground-based ozone lidars and co-located ancillary measurements *(e.g., ceilometer, Pandora spectrometer, ozonesondes)* is needed. These proposed sites could be the 7-8 "home" institutions or deployable assets for intensive field operations.

Observing NO₂ pollution inequality in North American cities

In North American cities, urban air pollution levels are typically higher in neighborhoods where residents are primarily people of color and have lower household incomes. For most atmospheric trace species, especially primary pollutants with short atmospheric lifetimes, spatiotemporal variability within cities cannot be captured using traditional monitoring approaches, even in intensively-monitored cities. The high spatial and temporal resolution of TEMPO observations will provide new insight into the identity and timing of the emission sources and atmospheric drivers of air pollution inequality at intra-urban scales. TEMPO data will improve our ability to not only describe inequalities, but also to eliminate them through air quality policy making. This experiment will use TEMPO NO₂ vertical columns to quantify, explain, and make policy recommendations on the causes of NO₂ air pollution disparities within cities.

High time resolution experiments

Lightning NO_x

Lightning-produced NO is the major NO_x source in the upper troposphere and can lead to substantial tropospheric O₃ production there. Interpretation of satellite measurements of tropospheric NO₂ and O₃, and upper tropospheric HNO₃, in association with a global chemical transport model leads to an overall estimate of 6 ± 2 Tg N y⁻¹ from lightning. Direct analysis of satellite NO₂ observations in relation to observed lightning flashes has also been conducted to estimate NO_x production per flash. High time resolution TEMPO measurements, including tropospheric NO_2 and O_3 , can be made for time periods and longitudinal bands selected to coincide with large thunderstorm activity, including outflow regions, with fairly short notice. These observations can be analyzed together with flash rates from the Geostationary Lightning Mapper onboard the GOES-16 and 17 satellites to estimate NO_x production per flash. Doing so may be able to significantly better quantify lightning NO_x and O₃ production over Greater North America, and determine regional variability of NO_x production per flash. Sophisticated analysis of NO₂ and lightning measurements and coincident meteorology will be necessary due to the substantial lightning NO₂ signal in cloudy scenes. High time resolution TEMPO NO₂ observations will allow evaluation of NO_x lifetime in the near field of deep convection. An understanding of this lifetime is critical in constraining satellite-based estimates of NO_x production per flash.

Morning and evening higher-frequency scans

TEMPO's optimized data collection scan pattern during mornings and evenings provides multiple advantages for addressing TEMPO science questions. The increased frequency of scans coincides with peaks in vehicle miles traveled on each coast, and thus is better able to capture the variability in NO_x and VOC emissions from mobile sources through measurements of NO₂, H₂CO, and C₂H₂O₂. The morning and evening are also of interest for better quantifying the diurnal changes in photochemistry as there is rapid change in the number of available photons. More frequent observations of the morning atmosphere in the Eastern U.S. are of particular benefit since there is usually a rapid rise in ozone concentrations during that time period. Morning NO_x and VOCs are often the primary drivers of peak ozone levels later in the day. More frequent observations lead not only to more accurate quantification of the early morning production of these ozone precursors, but also better characterization of the diurnal patterns of emissions, and better assessment and forecasting of peak ozone air quality levels.

TEMPO can measure pollution development during the morning and evening rush hours at urban scales over non-coastal as well as coastal cities using special observations. TEMPO will also determine how pollution varies during the week and on weekends and determine long-term seasonal and interannual variability. TEMPO will be able to monitor pollution with the resolution to quantify emissions over major highways.

Dwell-time studies and temporal selection to improve detection limits

Possible additional measurements include nitrous acid (early morning measurements are likely necessary), methyl glyoxal, and iodine oxide over coastal areas.

Exploring the value of TEMPO in assessing pollution transport during upslope flows

The Northern Colorado Front Range Metro area (NFRMA) is in non-attainment for the EPA 8-

hour ozone standard (NAAQS). Characterizing and modeling air quality in the NFRMA poses large challenges due to the complex terrain and meteorology as well as the mix of diverse pollution sources including urban sources, power plants, large industrial sources, agricultural activities, oil and gas exploration and also natural sources like wildfires, biogenic VOCs or windblown dust. The transport patterns during upslope events can vary widely in their characteristics and there are still open questions such as how much of the transported pollution is brought back to the NFRMA via return flows or mixed into the free tropospheric westerlies. TEMPO measurements should resolve upslope events and whether the expected vertical resolution of the ozone product would be sufficient to provide information of return flows. They might also allow for a statistical assessment of the impact of upslope pollution transport on remote mountain areas. Such studies would be also of interest for other areas in the U.S. with similar topography, *e.g.*, Salt Lake City and a variety of areas in the Intermountain West.

Tidal effects on estuarine circulation and outflow plumes

TEMPO will resolve tidal effects on estuarine circulation and the pollution outflow plume in the Chesapeake Bay and their relationship to ecosystem variability.

Air quality responses to sudden changes in emissions

TEMPO high time resolution could enable monitoring of air quality responses to sudden changes in emissions, such as those that occur during temporary power blackouts.

Cloud field correlation with pollution

TEMPO high time resolution studies may resolve photochemical effects under moving cloud fields.

Agricultural soil NO_x emissions and air quality in California

Although stricter air quality regulations in California have led to significant reductions in NO_x emissions from transportation sources, the state continues to experience air quality exceedances on a regular basis, including in rural agricultural areas. Recent research has indicated that soil NO_x emissions from agricultural areas are likely a major source of pollution and the continued degradation of air quality in the state. However, evaluating contributions of various NO_x emission sources, including fires, mobile sources, and agricultural soils, to pollutant concentrations in California is extremely challenging using observations from the mid-day overpasses from the current fleet of polar-orbiting spectrometers. The suite of hourly trace gas products at high spatial resolution from TEMPO will permit more detailed attribution studies of NO_x emission sources over California. In particular, TEMPO observations of NO_2 and O_3 in the tropospheric layer will be able to monitor rapid variations in pollutants over agricultural areas. The high-resolution TEMPO products will be used in conjunction with soil moisture retrievals from the Soil Moisture Active Passive (SMAP) satellite to assess the diurnal cycle of soil NO_x emissions, in relation to rainfall, irrigation schedule, and temperature, and impact on air quality in California.

Agricultural soil NO_x emissions in the Upper Midwest and air quality forecasting

Recent observations over the past four years have indicated that soil NO_x emissions from the vast agricultural area of the Upper Midwest are likely a contributing source of pollution with some degradation of air quality in the state. Agricultural activities in late fall, such as manure and/or

anhydrous ammonia application to fields after harvest, are a likely contributor to elevated PM2.5 concentrations, as well as odor for areas downwind. These precursor NOx and ammonia emissions chemically transform in the atmosphere to particulate form and become an important source of PM2.5, thus presenting air quality forecast challenges. This experiment aims to utilize a similar approach as the agricultural soil NO_x study over California, which fuses tropospheric NO₂ and O₃ information from TEMPO with soil moisture retrievals from the SMAP satellite to evaluate the impact of soil NO_x emissions on air quality in Minnesota and Iowa.

Wintertime air quality in western U.S. and the Aquarius campaign

Wintertime particulate matter haze is a significant-air quality issue that affects air basins across the western U.S. Persistent cold-air pools, or temperature inversions lower than the surrounding terrain, serve to confine surface emissions during multi-day events characterized by elevated pollutant levels, including NO₂ and PM_{2.5}. These events affect major urban areas across the intermountain west and are particularly severe in the valleys of Great Salt Lake Basin in northern Utah, including Salt Lake City, and the Central Valley of California. AQUARIUS (Air Quality Research in the Western U.S.) is a multi-agency (NSF, NOAA, DOE) field campaign planned for the 2022-23 winter. The proposed meteorological and chemical measurements from ground sites and aircraft will be synergistic with geostationary remote sensing observations from TEMPO that are expected occur shortly after its launch. Dedicated, high-frequency TEMPO measurements during the AQUARIUS campaign would serve to provide validation data for TEMPO and context information for AQUARIUS.

Dust source detection

TEMPO offers a much-needed capability to detect active source areas for windblown dust emissions. Dust storms in North America are mostly short-lived, occurring a few hours before sunset and lasting 2-5 hours (Huang et al., 2015). Such a temporal pattern makes TEMPO a preferred platform for observing dust storms in this region. The high temporal and spatial resolution characteristics of TEMPO observations can be utilized to identify dust sources using several approaches, such as the back-tracking method developed by Schepanski et al. (2007) and an empirical method used by the NOAA Hazardous Mapping System (HMS) team. Similar to the Saharan dust map (Schepanski et al. 2007), a new source map for North America can be derived by analyzing the TEMPO data. TEMPO enables tracking a dust plume backwards to the place where it first appears, i.e., the source area.

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