

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 (i.e., standard operations), 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. The commissioning phase is scheduled for June – September 2023. 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, a notice of 2-3 hours is required to initiate a special sequence.
6. Special operations can 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.

7. Discussion of special observations now hopefully ensures that flexibility remains when operations become more fully developed.

Standard 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

Changes in clouds, aerosols and the stratospheric ozone layer modulate biologically harmful ultraviolet (UV-B and UV-A: 290-400nm) radiation reaching the Earth's surface and penetrating to ecologically significant depths in natural waters. Current operational LEO satellite algorithms for mapping of hyperspectral UV irradiance at the Earth's surface (Krotkov et al., 1998; Krotkov et al., 2002a; Tanskanen et al., 2006) and at different depths underwater (Vasilkov et al., 2001; Vasilkov et al., 2005) assume "frozen cloud transmittance," estimated from the measured UV reflectivity at the time of LEO satellite overpass (Krotkov et al., 2001; Krotkov et al., 2002b). A spectral surface ultraviolet (UV) irradiance retrievals using TEMPO hourly O₃ amounts and cloud and surface reflectances will enable us to account for diurnal changes in cloudiness and produce hourly targeted UV indices and accurate daily exposures, employing different action spectra for erythral 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. The unexplained variability in ozone production rate from fires is of particular interest. 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 affects the secondarily formed compounds such as volatile organic compounds (VOCs), ozone and secondary organic aerosols. Ongoing efforts are working to address algorithmic complications for trace gas retrievals in forest fires

from high aerosol loadings. TEMPO measurements will not only increase understanding of the chemical emissions from biomass burning, but will also be a powerful tool for monitoring and assessing their impact on human health and the environment.

There is growing evidence on the consequences on soil, soil biota, soil chemistry, indigenous plant life, and fauna of not letting fire-adapted ecosystems burn. The accumulated dry fuels caused by suppressing wildfires can be partially moderated by prescribed fires. These controlled activities can be monitored by TEMPO to assure minimal short-term air pollution impact on humans, while being able to restore natural unperturbed ecosystem components. For particularly important fires it is possible to command special TEMPO observations as special operation, revisiting at 10-minute frequency.

Synergistic GOES-16/17 Products

As TEMPO will use NOAA GOES-16/17 advanced baseline imager (ABI) data for INR, GOES ABI products can be easily used for TEMPO applications. GOES cloud information is of particular interest for improving and using TEMPO products. A wealth of GOES cloud information such as clear sky mask (i.e., cloud classification), cloud optical depth, geometrical cloud fraction, cloud-top height, cloud-top phase, and temperature is available at TEMPO sub-pixel level. These cloud products can be mapped to TEMPO spatial pixels and can be used to improve TEMPO cloud, aerosol and trace gas retrievals, and assist in screening cloud-contaminated TEMPO data. In addition, other GOES products including radiances, aerosol detection/optical depth, fire/hot spot characterization, and snow/ice cover can also be mapped to TEMPO footprints to help improve the retrievals and analysis of 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 (Jaeglé et al. 2004; Jaeglé et al. 2005). 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.

Mapping NO₂ and SO₂ dry deposition at high resolution

TEMPO measurements of NO₂ and SO₂ can be used in combination with high-resolution model calculations of deposition velocity to map NO₂ and SO₂ dry deposition to soil, water and vegetation. Previous studies have used space-based observations of NO₂ and SO₂ from low Earth orbit to map regional and global deposition (Jia et al., 2016; Kharol et al., 2018; Nowlan et al., 2014), but at coarser spatial resolutions than those available from TEMPO. As deposition changes greatly between surface types and with local meteorology, the high spatial resolution of TEMPO should allow improvements in our spatial quantification of dry deposition, and in the resulting nitrogen and sulfur deposition budgets. With only one or fewer observations per day, previous studies needed to make model-based assumptions of the diurnal cycles of surface NO₂ and SO₂ concentrations. The hourly TEMPO products will allow improved constraints on time-dependent deposition.

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 (McGrath et al., 2015), and much more worldwide. Collateral effects include changes in water and carbon exchange. TEMPO will measure 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 smaller by oversampling (Zhu et al., 2014; Sun et al., 2018). Such studies can contribute to optimized agricultural choices. Forest studies can contribute to improved prevention of human-induced wildfires.

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 ground-based 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 (Simpson et al., 2015). 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. TEMPO measurements of BrO over the coastal areas and salt lakes can also provide better understanding of Br contribution from short-lived species to stratospheric Br budget and their effect on ozone hole recovery.

Air pollution from oil and gas fields

TEMPO measurements of O₃, NO₂, H₂CO, C₂H₂O₂, 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 (Zhang et al., 2019)

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, drilling platform plumes, and other concentrated sources

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. Especially for the drilling platform plumes, higher temporal measurements may improve detection limits and measurement precisions enough to make measurements for significantly fainter platform sources than can now be done. It will likely be possible to measure NO_x emissions from highways and aircraft routes as well.

Water vapor studies

TEMPO water vapor and pollution measurements (Wang et al., 2019) will contribute to understanding the extent that corn sweat worsens heat waves and air pollution in the U.S. Midwest. There is significant short-term variability in water vapor columns due to land moisture fluxes from evapotranspiration, atmospheric turbulence and large-scale horizontal motions. The high temporal resolution of the TEMPO water vapor product will be a valuable top-down constraint on surface moisture fluxes, or the vertical mass column. GOES-16/17 provides high

resolution water vapor maps based on IR bands (6.2-7.3 μm), but they are usually applicable for qualitative analyses. TEMPO will offer an hourly quantitative measurement of water vapor that can mathematically be incorporated into models. Synergistic use of GOES cloud and aerosol products will provide better scattering corrections to the TEMPO water vapor product, allowing cloudy scenes to be incorporated in to data assimilation systems. 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. A considerable number of severe rainfall incidents in southern U.S. occur during frontal passages, which are mainly a result of discontinuity and rapid changes in density and wind velocity between two different air masses (cold and dry vs. warm and moist). TEMPO provides the high temporal water vapor measurements for assimilation into weather models to bolster the capabilities of operational models to produce better forecasts before a front enters a specific region.

Volcanoes

The FOR of TEMPO includes several active volcanoes including Popocatépetl and Fuego de Colima in Mexico, and the emissions from Soufrière Hills in Montserrat and the downwind area of several volcanos in Alaska. TEMPO will provide detailed understanding of the pollution produced by dispersed volcanic ash (VA), sulfur dioxide (SO_2), and sulfate (H_2SO_4) particles and how they are transformed and transported. BrO/SO_2 ratios can be calculated downwind of craters at different distances to determine their evolution and, in combination with meteorological data, estimate hourly fluxes. TEMPO also will provide information about volcanic BrO injection into the lower stratosphere. Volcanic eruptions can inject significant amounts of SO_2 , VA, and H_2SO_4 particles into the atmosphere at commercial aircraft cruising altitudes. The ash clouds, in particular, pose a substantial risk to aviation safety due to the potential ingestion of silicate ash into jet engines. Present regulations dictate a zero ash tolerance policy for jet aircraft, which in case of uncertain VA location, could lead to prolonged flight cancellations that have a ripple effect on the airline industry's economy and personal travel as happened in the aftermath of the 2010 Eyjafjallajökull (Iceland) eruption. TEMPO's frequent volcanic SO_2 and ash measurements will complement GOES-16 and -17 infrared VA observations and could be used by NOAA/NESDIS Washington VA Advisory center to issue VA advisories for North American airspace (Krotkov et al., 2010)

Socio-economic studies

TEMPO will perform quantitative studies of pollution that inform the state of developing economies such as Cuba, as pollution and economic activity are often highly correlated. TEMPO will be able to evaluate the horizontal inhomogeneity of pollutants in megacities such as Los Angeles and the Mexico City Metropolitan Area, illustrating not only health hazards in different neighborhoods, but linking pollution to demographics and socio-economical levels. Combining TEMPO observations with ancillary information on economic activity it will be possible to obtain information about the effect on air quality of different economic activities in urban areas.

National pollution inventories

Space- and time-resolved TEMPO measurements of NO_2 and SO_2 will provide information about point and mobile sources and significantly contribute to National Pollution Inventories. LEO satellite pollution (NO_2 , SO_2) plume tracking and "top-down" point source emission estimates

have been proved valuable reducing latency and improving accuracy of traditional “bottom-up” emissions inventories. TEMPO will drastically improve number of measurements over North American point pollution sources (e.g., power plants, refineries, cities) reducing statistical uncertainties and improving time resolution of the top-down emissions estimates, which will be assimilated into the next generation of chemical weather forecast models (Beirle et al., 2011; Valin et al., 2013; de Foy et al., 2014; Liu et al., 2016; Streets et al., 2013).

Regional and local transport of pollutants

TEMPO will provide unique hourly information, never available before, to conduct research on local and regional transport of aerosols and pollutants. TEMPO can be used (coupled with meteorological datasets) to determine the impact of agricultural practices on the air quality of recipient areas (such as urban areas where biomass burning is not common). In turn, the impact of emissions from urban areas (coupled with meteorological datasets) over suburban or rural areas can be determined using a similar approach.

Sea breeze studies

TEMPO will be able to examine daytime sea breeze transport into the mainland of maritime, biomass burning, and other anthropogenic aerosols from industrial and populated cities located along the coasts. Cuba (Fonte and Antuña, 2011; Estevan et al., 2011; Barja et al., 2011; Antuña et al., 2012; Barja et al., 2013; Estevan et al., 2014; Garcia et al., 2015) and the Florida peninsula are two natural laboratories for studying the contribution of aerosols to cloud formation produced by the sea breezes converging from their coasts using TEMPO synergistic cloud products combined with advanced aerosol products. Since Cuba has few surface stations conducting air quality monitoring in the country, TEMPO will make an additional contribution by filling information gaps on these data. Validation of the broadband aerosol optical depth (BAOD) measurements at four Cuban stations conducting solar radiation measurements with TEMPO AOD observations will contribute to the improvement of the Cuban BAOD dataset dating back in some stations more than 30 years and extend existing comparisons performed with MODIS AOD (Antuña-Marrero et al., 2018).

Transboundary pollution gradients

TEMPO can explore whether there are significant gradients in the air quality of contiguous urban areas extending on both sides of national borders, the impact of different air quality regulations, and how the transport of people and goods across borders affects air quality. TEMPO will be able to measure whether there are areas where systematic transport of pollution across the border occurs. TEMPO spatial and temporal resolution will be able to address these issues in areas of the U.S./Mexico border (e.g., San Diego/Tijuana, El Paso/Juárez) and the U.S./Canada border (e.g., Detroit/Windsor).

Transatlantic dust transport

Degraded air quality in the Greater Caribbean Basin (GCB), including Small Island States, is often linked to transatlantic transport of Saharan dust (Prospero and Mayol-Bracero, 2013). TEMPO dense spatial and temporal observations are well suited to characterize these synoptic-scale events, the dispersion of dust throughout the northern part of the GCB, the uptake of tropospheric O₃ by dust particles, and the correlation between dust particles, diesel particulate matter with enhanced NO₂ concentrations. Saharan air masses can also act to suppress the

formation of tropical storms and hurricanes (Dunion and Velden, 2004). TEMPO will provide continuous measurements of aerosols and water vapor that will enhance our understanding of the microphysical processes governing storm formation/suppression.

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 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 representativeness 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 in North American cities

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 at intra-urban scales. This experiment will use TEMPO NO₂ vertical columns to quantify, explain, and make policy recommendations on the causes of NO₂ air pollution within cities.

Examining impacts of warehouse density on Inland Empire Air Quality

San Bernardino, CA and surrounding regions have well documented air quality issues, with summertime ozone exceeding the National Ambient Air Quality Standards (NAAQS) for months at a time. In recent years, the logistics industry has greatly expanded in this region to accommodate increases in online shopping. This increase is associated with further declines in air quality throughout the region, but existing surface monitoring networks lack sufficient density to fully quantify these impacts. TEMPO data will be used to examine columns of NO₂ and HCHO in the vicinity of extensive warehouse developments that are prolific throughout the Inland Empire, east of Los Angeles. Ratios of HCHO to NO₂ will be used to characterize ozone production regimes in these regions. The high spatial resolution and hourly data will allow for detailed comparisons of these pollutants in the vicinity of industrial sites with the surrounding area and quantification of impacts of logistics industry expansion on regional air quality.

Assimilating High Spatiotemporal Resolution Observations of Atmospheric Composition for Regional Air Quality Forecasting with Dynamic Emissions Adjustment

Poor air quality (AQ) is one of the most important environmental issues facing the U.S. AQ managers use AQ forecasts (and other tools) to better understand, plan for, and mitigate poor AQ events. Accurate AQ forecasts depend, in part, on high spatiotemporal near-real-time (NRT)

observations to initialize chemical transport models and dynamically adjust the emissions. TEMPO will provide high spatiotemporal AQ observations that will revolutionize AQ forecasting and emissions adjustment in the U.S. In anticipation of the TEMPO launch, in collaboration with researchers at NASA, NOAA, and various universities, we are using WRF-Chem/DART with regional domain resolutions of 12 km, 4 km to assimilate synthetic TEMPO observations together with conventional meteorological, AQ *in situ*, and AQ remote-sensing (ground-based profilers and/or satellites) observations in observing system simulation experiments (OSSEs) and retrospective forecast/assimilation/verification experiments with dynamic emissions adjustment to determine the benefit of TEMPO for improving: (1) AQ forecast skill and predictability; (2) anthropogenic emission estimates, and (3) wildfire emission estimates.

Our development of forward operators for assimilating OMI, TROPOMI, and TEMPO retrievals and our current experiments make it feasible to assimilate TEMPO retrievals immediately upon availability. Once TEMPO retrievals are available in NRT, we will assimilate those observations in true AQ forecast/assimilation experiments to demonstrate the associated improvements in forecast skill, predictability, and emissions estimation. We plan to collaborate with NOAA to apply WRF-Chem/DART for NRT AQ forecasting with meteorological/chemical data assimilation and dynamic emissions adjustment during the Atmospheric Emissions and Reactions Observed from Megacities to Marine Areas (AEROMMA) and the NASA Synergistic TEMPO Air Quality Science (STAQS) field programs: in mid-2023. During these campaigns, we would prepare 12- to 24-hour forecasts (with longer lead times if necessary) for flight and data collection planning. After the campaigns, we would use the AEROMMA and STAQS data to improve and validate our chemical data assimilation/dynamic emissions adjustment algorithms. We would assimilate available TEMPO data in both of those tasks.

Spatial inhomogeneities of NO₂ and HCHO over urban areas

Spatial inhomogeneities of NO₂ and HCHO have been identified in the Mexico City Metropolitan Area (MCMA) using ground-based MAX-DOAS measurements. The identified inhomogeneities are more pronounced for HCHO than for NO₂ and are variable during the day. Specifically, for HCHO it has been identified that at some of the MAX-DOAS stations located in the MCMA, early in the morning vertical column densities (VCDs) measured at different viewing directions are comparable, however from 11 in the morning or noon (depending on the station), VCDs measured towards the western part of the MCMA are higher than the ones measured towards the eastern side. By using TEMPO data, the objective is to study more deeply the possible inhomogeneities, with hourly time resolution (or better, if useful), in the MCMA as well as other metropolitan areas in Mexico such as Monterrey and Guadalajara.

Special 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. 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 $6 \pm 2 \text{ Tg N y}^{-1}$ from lightning (Martin et al., 2007). Assimilation of satellite observations of these species into a global model (Miyazaki et al., 2014) has yielded similar values of $6.3 \pm 1.4 \text{ TgNy}^{-1}$. Direct analysis of satellite NO₂ observations in relation to observed lightning flashes has also been conducted to estimate NO_x production per flash (Bucsela et al., 2010; Pickering et al., 2016; Bucsela et al., 2019; Allen et al., 2019), yielding generally smaller values of production per flash than implied by the global modeling approach. In addition, a demonstration of the potential synergy between TEMPO and the Geostationary Lightning Mappers (GLM) on GOES 16 was conducted with the Geo-CAPE Airborne Simulator (GCAS) UV/Vis spectrometer on NASA ER-2 aircraft flights over thunderstorms in Spring 2017 (Allen et al., 2021b). High time resolution (e.g., 10 minutes) TEMPO measurements, including tropospheric NO₂ and O₃, can be made for time periods and longitudinal bands (~1000 km width) selected to coincide with large thunderstorm activity, including outflow regions, with fairly short notice. The experiments will be Lagrangian in nature, following the evolution of lightning NO_x plumes as storms develop and evolve, and outflow is transported downwind. Planning for these experiments will be based on the NOAA/NCEP/Storm Prediction Center's Convective Outlooks issued for 3-days, 2-days, and 1-day in advance. On the experiment day, NCEP High Resolution Rapid Refresh (HRRR) model forecasts for 15-minute intervals will be used along with observed radar data to determine exact storm locations. The TEMPO NO₂ observations will be analyzed together with flash rates from the GLM instruments on GEOS 16 and 17 to estimate NO_x production per flash. Doing so, we 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. Tropospheric columns of NO_x will be determined by dividing the TEMPO tropospheric slant columns of NO₂ over deep convective pixels (high cloud radiative fraction and low optical centroid pressure) by specially-derived AMFs appropriate for thunderstorms. AMFs may be taken from the GEOS-CF model and would include use of model NO_x/NO₂ ratios. Careful consideration of background NO_x will be necessary to estimate the amount from recent lightning. High temporal 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. Experiments for lightning NO_x should be conducted on multiple days throughout the May to August period, such that a variety of storm types, storm regions, and lightning flash rates can be analyzed. An excellent addition to the TEMPO experiments would be to include aircraft transects of storm anvils and downwind outflow for TEMPO lightning NO₂ validation and for quantification of the NO_x/NO₂ ratio.

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 special 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 special 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 (Oikawa et al., 2015; Almaraz et al., 2018; Sha et al., 2021). 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 NO₂ and O₃ 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 PM_{2.5} concentrations, as well as odor for areas downwind. These precursor NO_x and ammonia emissions chemically transform in the atmosphere to particulate form and become an important source of PM_{2.5}, 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 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 currently in the planning stages. The proposed meteorological and chemical measurements from ground sites and aircraft will be synergistic with geostationary remote sensing observations from TEMPO. 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.

High resolution scanning over the NYC Area

After reviewing preliminary data from the Long Island Sound Tropospheric Ozone Study 2018, it is apparent that the area around NYC emits noticeably larger amounts of NO₂ on days that monitor elevated ground level ozone. The TROPOMI satellite images verify that the NYC area NO₂ emissions stand out among the other major cities from Washington DC, to Boston. Higher resolution images from the NASA GCAS flights were able to pin-point specific NO₂ plumes to point source electrical generating units (EGUs). Because Connecticut continues to monitor the highest ozone design values on the East Coast, it is vital that the source, strength, and timing of the ozone precursors be determined, especially during the ‘ozone season,’ which typically occurs between May 1 and September 30. Although the TEMPO spatial resolution will not match the 250 meter resolution of the GCAS images, the instrument will be able to scan more frequently (e.g., 10 minutes) and produce spatial resolution images greater than the nominal 2.1 km x 4.7 km pixel size. In addition to the point source EGU plumes, it would be useful to determine contributions from mobile source emissions (NO₂, H₂CO, and C₂H₂O₂) along major highways and from marine vessels in shipping channels and along the land/water interface. Furthermore, with the geostationary TEMPO measurements, it would be highly informative to track NO₂ emissions activity over time in the study area during daylight hours spanning multiple days of a high ozone episode.

Monitoring Volcanic Activity, Emissions, and Air Quality Impacts from Mexican Volcanoes

Volcanoes can inject a mixture of ash particles and gases, including SO₂, CO₂, H₂O, and hydrogen sulfide (H₂S), into the atmosphere. Both ash and the formation of fine-grained sulfate aerosols (SO₄) from SO₂ gas-to-particle conversion can contribute to the amount of volcanic particulate matter (PM) in the atmosphere. Heterogeneous reactions in the volcanic plume during daylight can also produce bromine monoxide (BrO), especially in conditions of high ozone concentrations. This experiment focuses on the Mexican volcanoes of Popocatepetl and Fuego de Colima, with Popocatepetl actively emitting ash and gases in 2022 and Colima last erupting in 2019. Popocatepetl is of particular interest in terms of impacts on air quality due to its proximity to the densely populated area of Mexico City.

This experiment plans to utilize the special observations from TEMPO for rapid monitoring of volcanic emissions and air pollutant concentrations during Popocatepetl and Colima eruptions. SO₂ and BrO observations from TEMPO will provide detailed information on gas emissions, transformation, and transport within the volcanic plume. Changes in BrO/SO₂ ratios could offer critical awareness on the eruptive activity of the volcanoes, as low BrO/SO₂ ratios have been linked to high explosive activity. TEMPO aerosol products of AOD, Aerosol Layer Height (ALH), and UV Aerosol Index (UVAI) will help characterize the PM composition and concentration within the volcanic plume. Altogether, the SO₂, BrO, and aerosol products from the special scan operations of TEMPO will provide new insights on the temporal evolution of air

pollutants within volcanic plumes, which can cause major disruptions in air traffic and impact air quality and human health.

TEMPO Validation during the May-June 2024 Satellite Coastal and Oceanic Atmospheric Pollution Experiment 2 (SCOAPE-II) Gulf of Mexico Cruise

The May 2019 Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE; <https://asdc.larc.nasa.gov/project/SCOAPE>) collected coastal and shipboard in-situ, remotely-sensed, and profile atmospheric composition data for the Bureau of Ocean Energy Management (BOEM) to examine air quality in the Gulf of Mexico (GOM) near oil and gas (ONG) operations. BOEM seeks to understand GOM air quality and evaluate their ONG emissions inventories (principally NO₂), because they are mandated to ensure that these operations do not significantly impact the air quality of any US State. Results published in Thompson et al. (2020) and Thompson et al. (2023, in review) found that satellite NO₂ measurements from OMI and TROPOMI are generally of sufficient accuracy (within ~10%) to monitor air quality over the GOM, but that overall levels of pollution are highly dependent on meteorological conditions (e.g., wind and source regions), potentially masking the signal from ONG emissions. With TEMPO in mind, BOEM has funded a SCOAPE-II GOM cruise, tentatively planned for a two-week period during May-June 2024. The SCOAPE-II cruise will carry much of the same instrumentation as SCOAPE, including the Pandora spectrometer, in-situ O₃, NO₂, CO, CH₄, and CO₂, VOC canisters, a ceilometer, ozonesondes, and standard meteorological instruments, to further examine GOM air quality near ONG operations and evaluate TEMPO's ability to monitor and quantify ONG emissions. The cruise will also be coordinated with NASA aircraft measurements of NO₂ and HCHO (GCAS) and CH₄ (AVIRIS) over the GOM. The SCOAPE-II cruise is an ideal validation opportunity for TEMPO. It will offer a wealth of in-situ and remotely-sensed data over a wide range of conditions, i.e., relatively clean and over-water to coastal gradients to intense point source emissions. More frequent ~10 minute TEMPO scans will allow for tracking of NO₂ plumes emitted from individual platforms, particularly those that are flaring excess natural gas product. Furthermore, SCOAPE-II will allow optimization of TEMPO retrievals over an often challenging marine environment where no routine surface monitoring is possible. Thus, TEMPO will benefit greatly from targeted viewing of the GOM during the May-June 2024 SCOAPE-II cruise.

TEMPO High-Temporal-Resolution Aerosol & Gas Observations of Central American Volcanic Plumes

If any of the many volcanoes situated just south of the nominal TEMPO FOR were to erupt during the TEMPO mission, there would be scientific and likely also disaster-response value to acquiring TEMPO data of the event. None of these volcanoes is well monitored from suborbital platforms, and high-temporal-resolution aerosol and gas measurements would provide insight into the eruptive style, as well as details of volcanic plume composition, transport, and evolution. The combination of high-quality gas and aerosol measurement would likely provide a unique dataset for exploring volcanic plume processes. The data could also help inform aviation and downwind populations of potential hazards. For disaster response, the data would be used to inform the VAAC about plume composition: a sulfate/water dominated plume would pose a downwind air quality hazard, whereas an ash-rich plume would in addition represent a risk to aviation. Further, constraints on volcanic plume height would be used to initialize the models that simulate plume dispersion, helping provide more accurate aviation and downwind

population hazard warnings.

Formation of ozone along the Colorado Front Range due to interactions between regional meteorology, urban pollution, and Oil and Gas extraction operations adjacent to the Denver Metro area

Along the Front Range of Colorado, the South Platte River (Platte) flows northward out of Denver, CO into Weld County, eventually reaching Greeley, CO where it joins other rivers as it turns to continue eastward toward Nebraska. This confluence of waterways acts as a low spot along the terrain of the northern Front Range. Just to the west of the South Platte, I-25 runs north-to-south connecting the many cities and towns that lie to the north of the Denver Metro area; and further west of this is the major topographic barrier of the Rocky Mountains. Another topographic barrier, the Palmer Divide, lies to the south of the Denver Metro area. While the Palmer Divide is lower in elevation than the greater Rocky Mountains to the west, this rise in terrain also acts to limit the movement of surface pollutants and contributes to the accumulation of air pollution in this region. Also situated along the I-25/Platte corridor is the Denver-Julesburg Basin (D-J Basin); a region of highly concentrated oil and gas (O&G) extraction, storage, and transport operations.

The features described above, are all encompassed within the Northern Colorado Front Range Ozone Nonattainment Area (NAA). The designation for the NAA has been downgraded several times, most recently reaching ‘Severe’ nonattainment. The persistence and prevalence of ozone pollution in the NAA is due to interactions between terrain and its influence on local meteorology, urban emissions from the Front Range urban corridor, and emissions from the O&G operations of the D-J Basin. Although Greeley is situated at the low-spot of the region and amidst the wells of the D-J Basin, the highest concentrations of ozone are typically found in the western and southwestern portions of the Denver Metro area. The explanation for this surrounds the complexities of the ‘slosh’ of pollutants along the Platte and the Front Range urban corridor. Further documentation of the processes contributing to the ‘slosh’ of pollutants will lead to greater understanding of the timing, spatial extent, and severity of air pollution episodes when they occur. Use of TEMPO special operations can be employed to observe trace gasses and ozone precursors, and follow the evolution as they convert to ozone and accumulate along the Colorado Front Range.

Air Quality Impacts at NPS units and Surrounding Communities from Oil and Gas Activities Across Multiple Basins in the Western U.S.

The widespread air quality impacts from oil and gas (O&G) activity emissions from multiple basins have been observed at National Park Service (NPS) units and their surrounding communities. While regional ozone control strategies have successfully decreased ozone levels across most of the U.S., the Carlsbad, NM area, including Carlsbad Caverns National Park (CAVE), has been struggling with degrading air quality and associated negative health effects on the impacted communities. Additionally, Guadalupe Mountains National Park (GUMO), approximately 40 miles SW of CAVE located in Texas, is now also experiencing similar air quality impacts resulting from O&G emissions in the Permian Basin. Additionally, air quality at Rocky Mountain National Park (ROMO) and Mesa Verde National Park (MEVE) are impacted by energy extraction activities in the Denver-Julesburg and San Juan Basins, respectively. Moreover, sites such as Dinosaur National Monument (DINO), located on the eastern edge of the Uintah Basin, still experience wintertime ozone events resulting from O&G emissions.

As a result of the air quality impacts from O&G activities that exceed the NAAQS at these NPS units and their surrounding communities, we are requesting high-frequency ozone data to supplement the ground-based ozone and meteorological measurements at these sites. It would be useful to have 1-10 minute resolution TEMPO data over our locations to couple with the 1-minute ozone and meteorological data from our ground sites. Additionally, measurements of NO₂, HCHO, C₂H₂O₂, SO₂ and aerosols will aid significantly in rapidly identifying the magnitude and extent of pollution events centered on O&G activities in these basins.

Study of Winter Air Pollution in Toronto (SWAPIT)

Toronto is Canada's largest urban area and it continues to grow rapidly with the population of the Greater Toronto Area (GTA) projected to reach 10 million by 2046. Major metropolitan areas like the GTA are sites of concern for air pollution due to their combination of abundant emission sources and dense human populations. In excess of 10,000 premature mortalities are attributed to air pollution exposure in Canada each year, and half of these deaths occur in the most populated 5% of census divisions. This total is an order of magnitude larger in the US.

SWAPIT is led by Environment and Climate Change Canada (ECCC) and aims to improve the state of knowledge about air pollution under conditions relevant to cities in northern climates. Urban air quality research has tended to focus on phenomena relevant to summer when smog formation is facilitated by high temperatures and abundant sunlight. Nonetheless, elevated wintertime pollutant concentrations have been observed and suggest that some air quality issues worsen in colder weather (e.g., SOCAAR, 2019). The winter period has therefore been selected for investigation to create a more balanced view of urban air pollution throughout the year.

The role of TEMPO within the SWAPIT campaign is twofold. TEMPO will assist SWAPIT by providing a regional view of key pollutants such as NO₂ and HCHO, including upwind air masses (e.g., clean air from the north, or aged pollution from US centers) and downwind chemical transformations or deposition. This will place the more detailed SWAPIT ground observations into context and help in its interpretation. In the case of NO₂ (and perhaps other pollutants), TEMPO will be used to determine city-wide NO_x emissions with unprecedented spatial/sectoral/diurnal information, and which will be used to (i) help constrain retrospective high resolution air quality model runs and (ii) compare directly with bottom-up or other top-down emissions data. Additionally, SWAPIT observations will be used to help validate TEMPO data, particularly its ability to capture spatial gradients through the GTA, as well as its ability to capture diurnally variation on timescales of one hour and shorter. Throughout the campaign period there will be intermittent snow cover which provides an excellent opportunity to evaluate the performance of TEMPO for snow/snow-free/mixed conditions.

Higher frequency TEMPO data will help in two regards. It will better match the higher frequency ground and mobile data, generally obtained every minute or so, which would mean less averaging and blurring of gradients in evaluating TEMPO precision and biases.

Also, the higher frequency will enable averaging of level 2 data, when necessary, to obtain higher signal to noise while still maintaining significant temporal resolution. For when deriving NO_x emissions, the additional scans will provide some combination of better precision, spatial, and/or temporal characteristics.

Utah Summer Ozone Study (USOS) 2024

In response to a request from the Utah Division of Air Quality (UDAQ) to provide scientific

information for its State Implementation Plan (SIP), the NOAA Chemical Sciences Laboratory (NOAA CSL) will lead a study of summertime ozone in the Northern Wasatch Front (NWF) region and adjacent areas in the summer of 2024. Measurements of the spatial distribution and speciation of major ozone precursors (NO_x and VOCs), together with additional chemical measurements and meteorological data, will enable better understanding of the factors that lead to high ozone. The NOAA CSL mobile laboratory will conduct drives throughout the region to characterize the spatial distribution of pollutants at surface level. The mobile lab will conduct continuous measurements at a fixed location (to be determined) during non-drive times. The payload will include visible absorbing trace gases such as NO₂, HCHO and O₃, together with detailed measurements of speciated volatile organic compounds, speciated reactive nitrogen, and halogen species. NOAA CSL, in collaboration with the NOAA Air Resources Laboratory (ARL), has submitted a request for time on the NOAA Twin Otter aircraft (pending, to be decided in July 2023) to conduct measurements of meteorology (wind fields from a doppler lidar), in situ NO_x and O₃, and greenhouse gases, and column measurements of visible absorbing trace gases via MAX DOAS (tentative, pending funding decision). The Twin Otter may conduct a small number of mass balance flights examining methane and NO_x emissions in the oil and gas producing Uintah Basin region, immediately east of the NWF. A request has also been made to conduct detailed in situ measurements of nitrogen oxides, ozone, VOCs and other trace gases (tentative, pending funding decision).

The NWF is home to a variety of unique pollution sources that interact through transport processes in complex terrain. Inter-valley transport, lake-land breezes, and up- and down-valley winds at different times of day all contribute to the complex and rapidly changing O₃ concentrations, often on time scales faster than 1 hour. High frequency remote sensing data of the suite of trace gas columns from TEMPO, including NO₂, HCHO, CHOCHO, BrO, SO₂ and O₃, as well as aerosol optical depth, will significantly augment ground based and airborne measurements to characterize the evolution of O₃ and its precursors in this region on a sub-hourly time scale. Major sources of interest that occur in addition to urban pollution include 1) A magnesium refinery on the Great Salt Lake that is the largest single emitter of halogen species in the U.S. and a known source of chlorine and bromine radicals; 2) Mining operations that are thought to be significant sources of nitrogen oxides contributing to regional pollution; 3) Smelting operations and coal fired power generation that have been a historical source of sulfur dioxide; 4) Oil refineries that are a significant source of volatile organic compounds that can be tracked through remote sensing measurements of HCHO and CHOCHO; 5) Periodic impacts from wildfire smoke that affect the entire western United States and that may contribute to substantially enhanced ozone and particulate matter in major urban areas of the intermountain west, such as Salt Lake City; 6) Biogenic emissions from the forested areas of the Wasatch, Oquirrh and other mountain ranges.

Coastal Texas Air Quality Observations

In August and/or September 2023, four weeks of intense monitoring will occur onshore and offshore of Houston, Texas to study the transport and formation of ozone and particulate matter. Three ship-based platforms will include in-situ trace gas (ship-dependent O₃, O_x, NO, NO₂, SO₂, CO, PM_{2.5} size distribution and optical properties, and/or VOCs), meteorology, one Pandora, two ceilometers, and ozonesonde measurements in Galveston Bay and the Gulf of Mexico to study the over-water interaction of atmospheric chemistry and meteorology where surface monitoring sites do not exist. Onshore measurements from a mobile air quality laboratory (O₃, NO, NO₂,

SO₂, CO, VOCs, HCHO, isoprene, PM_{2.5} size distribution and optical properties, meteorology), instrumented drone (O₃ and/or VOCs), Pandoras, stationary sites, and ozonesondes will complement the offshore measurements to evaluate the interaction of the sea/bay breezes and other transport conditions on surface and aloft air quality. The 2023 measurements will follow on the 2021 and 2022 TRacking Aerosol Convection ExpeRiment – Air Quality (TRACER-AQ) field campaigns (Jensen et al., 2022; Judd et al., 2021), providing a unique three-year span of August/September measurements in the Houston area and surrounding waters. The addition of high-frequency TEMPO data in 2023 will enhance the spatiotemporal observations of air quality (including the HCHO/NO₂ ozone formation sensitivity ratios) throughout the Houston area, especially for dynamic atmospheric processes like sea/bay breezes, boundary layer development and mixing of aloft residual layers. The TEMPO observations will provide important validation data for future photochemical modeling used in the State Implementation Plan process. The surface trace gas and Pandora and ozonesonde measurements from the campaign will provide a unique onshore and offshore dataset to evaluate the TEMPO retrievals. TEMPO special operations of the campaign would provide a test during the satellite’s commissioning phase, which would develop confidence in future special ops like the May-June 2024 Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE-II) measuring air quality in the Gulf of Mexico.

Lightning NO_x Generation in Explosive Volcanic Eruption Plumes

Explosive volcanic eruptions can produce abundant in-cloud and cloud-to-ground lightning via several mechanisms. One of these (the ‘dirty thunderstorm’) is analogous to non-volcanic thunderstorms, where the fallout of volcanic ash and ash-rich hydrometeors causes charge separation, and hence is a potential source of lightning NO_x (LNO_x). Observations by the NASA/Aura Ozone Monitoring Instrument (OMI) suggest that some explosive volcanic eruptions might produce significant amounts of ‘volcanic’ LNO_x (hereafter referred to as volcanic lightning NO_x or vLNO_x), detectable within a few hours of eruptions. This vLNO_x could be generated at higher latitudes than conventional LNO_x, which is concentrated in the tropics. However, due to the low temporal resolution of OMI and the relatively short atmospheric lifetime of NO_x, the conditions required for, and the timing and magnitude of, vLNO_x generation in volcanic eruption clouds remain elusive. High-cadence TEMPO observations of volcanic eruptions could potentially confirm and provide new insight into the generation of vLNO_x in volcanic eruption plumes. Specifically, high frequency TEMPO observations of volcanic SO₂ and ash (via the UV Aerosol Index, Optical Depth and Aerosol Layer Height), coupled with NO₂ observations and synergistic TEMPO/GOES-R lightning products (and/or GOES-16/17 Geostationary Lightning Mapper [GLM] data), could elucidate the links between the emission and fallout of volcanic ash, volcanic lightning generation and vLNO_x production. Since volcanic eruptions can evolve on very short timescales, this experiment would require special TEMPO observations (e.g., 10 minute cadence) of a significant explosive eruption within the TEMPO Field of Regard (FoR) close to the volcanic source, most likely in Mexico, the Caribbean, northern Central America (e.g., Guatemala) or Alaska. Such eruptions can occur at any time and are difficult to forecast, but in some cases large eruptions are preceded by precursory activity that may provide some advance warning. Ideally, the targeted eruption would be spatially and/or temporally distinct from other deep convection to avoid contamination with other sources of LNO_x. TEMPO observations would be used to track any observed vLNO_x emissions downwind (along with any volcanic SO₂ and ash) to constrain the vLNO_x lifetime.

Supporting local government public health and air quality decision-making with a sub-city scale air quality forecasting system from data fusion of models, satellite, in-situ measurements, and low-cost sensors

Sub-city scale air quality estimates and forecasts are a critical need for areas that are disproportionately impacted by poor air quality or intermittent air quality events, such as wildfires. Data fusion approaches that use ground-based networks (e.g., reference grade monitors, low-cost sensor), regional or global air quality forecasts (e.g., GEOS-CF), and satellite retrievals have been proven to be an effective method for quantifying air quality in areas that have historically been under-represented in ground-based monitoring networks which can lead to poor forecasting performance. A team of researchers at NASA, Sonoma Technology, Inc., UNEP, Lamont-Doherty Earth Observatory, Clarity Movement Co., and EPA will use a data fusion approach that uses low-cost sensors, reference grade monitors, CAMS, GEOS-CF, MODIS, VIIRS, TROPOMI, and GOES to develop near real-time (NRT) forecasting of PM_{2.5}, NO₂, and O₃ for four North American regions (southern Mississippi, centered on Gulfport; western Oregon, centered on Eugene; southwestern Idaho, centered on Boise; and central Colorado, centered on Denver). The NRT forecasting will generate an hourly forecast of sub-city scale air quality estimates that will support decision-making needs for end users. The data will be available through a Google Earth Engine (GEE) tool that will ingest these data continually to perform the data fusions.

Use of standard operation (hourly temporal resolution) and/or special operation (sub-hourly temporal resolution) TEMPO measurements of NO₂, O₃, and AOD will be investigated to expand the NRT forecasting capabilities of this effort so that top-down measurements can be better represented within the data fusion approach. The current use of polar-orbiting satellite information for trace gases in our data fusion approach limits its ability to identify sub-model-grid-scale variability in trace gas concentrations at sub-daily timescales. Notably, incorporating the routine hourly TEMPO measurements into our data fusion methodology will potentially support better spatiotemporal performance of the sub-city air quality forecasting and will allow for enhanced quality assurance. Additionally, higher frequency data sampled during special operations over at least one of our partner cities will allow our team to test the impact such information might have if only available for a relatively short time period (e.g., part of a day to a whole day) or if we would need consistent high frequency data over the full calibration period (a week or more). Preference would be to target poor air-quality events (summertime ozone, wildfire smoke, stratospheric intrusions) as well as some normal background conditions (to serve as a control).

Constraining trace gas emissions from biomass burning with machine learning applications

The new spatial and temporal resolution of TEMPO data will provide an unprecedented opportunity to assess emissions from wildland fire smoke and the effects of aging on smoke composition. Preliminary evidence suggests that the aging of smoke is related to substantial changes in the chemical properties of the smoke, with impacts on ambient concentrations and toxicity of particulate matter and complex interactions with ozone formation. The broad spatial coverage, along with the unique retrievals of ozone, precursors, and aerosols, presents a new opportunity to study the evolution of wildland fire smoke over time.

Wildland fire detections from the latest generation of GOES provide an input data set to understand the progression of wildland fires at high temporal resolution. Combining TEMPO

data on aerosols and other atmospheric constituents at similar high resolution can underpin new research on the evolution of wildfire smoke at very high time resolutions and link emissions and chemistry to burning conditions on the ground. Furthermore, coarse CTMs often fail to capture the behavior of wildland fire smoke. Using detailed meteorological and satellite fire detection data sets, ML models will be developed to downscale and adjust CTM outputs to reflect the localized impact impacted by wildland fire smoke.

Industrial upset emission detection

Industrial manufacturing facilities can emit large quantities of pollution when they are malfunctioning, conducting maintenance, starting up, or shutting down. Regulators consider these so-called “upset emissions” as distinct from routine emissions. Consequently, upset emissions often go unreported and lack the same level of regulatory oversight as emissions from day-to-day operations.

The goal of this experiment is to better characterize the location, frequency, duration, magnitude, and air quality implications of industrial upset emissions. Our objectives are twofold. First, we will examine the spatial and chemical signatures of pollution around industrial facilities before, during, and after known emissions events. Second, we will assess the utility of TEMPO data for detecting and characterizing changes in air pollution around unreported upset emissions events.

Upset emissions can vary substantially over sub-hourly timescales and sub-km spatial scales. Higher frequency data would thus allow us to achieve our first objective by 1) providing a more granular picture of how emissions evolve with time, and 2) offering the flexibility to oversample the data as needed to reduce noise and enhance spatial resolution. Higher frequency data would also contribute to our second objective by helping us to answer questions such as: How do satellite data spatial and temporal resolution impact our ability to detect and characterize upset emissions events? How big does an emissions event need to be in order to be detected using standard-resolution TEMPO data?

DoD Wildfire Science Initiative Fort Stewart Prescribed Fire Campaign

The Fort Stewart experimental campaign will consist of 3 operational scale prescribed (Rx) fires at Fort Stewart in early February 2024. The burns will be about 1000 acres and will be instrumented with under canopy fire intensity measurements, LiDAR as well as a suite of smoke and meteorological measurements to evaluate and tune new management tools for predicting fire behavior (QUIC-Fire), fuels inventory (INTELIMON), and smoke (QUIC-Smoke). Higher frequency TEMPO data (NO_2 , HCHO , O_3) will be valuable for monitoring the rapidly varying emissions and air pollutant processes associated with Rx burns. TEMPO data can help improve Rx fire management through improving the new fire tools, which will result in better forest health, improved Rx fire safety, and better smoke management.

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