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NOAA Technical Report OAR CPO-8

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https://doi.org/10.25923/1s4s-t405

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Climate Program Office
Silver Spring, MD
October 2020

Commissioned by the NOAA GEO-XO Program

NOTICE FROM NOAA

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Abbreviations and Acronyms

ABI	Advanced Baseline Imager
AC	atmospheric composition
AHI	Advanced Himawari Imager
AIRS	Atmospheric Infrared Sounder
AMI	Advanced Meteorological Imager
AOD	aerosol optical depth
AQI	Air Quality Index
ARL	Air Resources Laboratory
BUV	backscatter ultraviolet
$C_2H_2O_2$	glyoxal
C_5H_8	isoprene
CAAA	Clean Air Act Amendments
CAMS	Copernicus Atmosphere Monitoring Service
CDC	Centers for Disease Control
CEOS	Committee on Earth Observation Satellites
CH_2O	formaldehyde
CH_4	methane
CIRES	Cooperative Institute for Research in Environmental Sciences
CMR	Copernicus Market Report
CO	carbon monoxide
CO_2	carbon dioxide
CONUS	continental United States
COVID-19	corona virus disease 2019
CrIS	Cross-track Infrared Sounder
CSD	Chemical Sciences Division
CSL	Chemical Sciences Laboratory
CTBTO	Comprehensive Nuclear-Test-Ban Treaty Organization
DAO	Department Administrative Order
DOC	Department of Commerce
DOI	Department of the Interior
DOT/FHWA	Department of Transportation’s Federal Highway Administration
DS2007	National Academies of Sciences, Engineering and Medicine’s 2005-2015 Decadal Survey
DS2017	National Academies of Sciences, Engineering and Medicine’s 2017-2027 Decadal Survey
DSCOVR/EPIC	Deep Space Climate Observatory Earth Polychromatic Imaging Camera
ESM	Earth System Model
ECMWF	European Centre for Medium-Range Weather Forecasts
EPS	Enhanced Polar System
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
EV	Earth Venture
FAA	Federal Aviation Administration
FCI	Flexible Combined Imager
FEMA	Federal Emergency Management Agency

FIREX-AQ	Fire Influence on Regional to Global Environments and Air Quality
FRERP	Federal Radiological Emergency Response Plan
FRP	fire radiative power
GBD	Global Burden of Disease
GEFS-Aerosols	Global Ensemble Forecast System with Aerosols
GEMS	Geostationary Environment Monitoring Spectrometer
GEO-CAPE	Geostationary Coastal and Air Pollution Events
GeoCARB	Geostationary Carbon Observatory
GEOSS	Global Earth Observation System of Systems
GeoTASO	Geostationary Trace Gas and Aerosol Sensor Optimization
GEO-XO	geostationary and extended orbits
GGGRN	Global Greenhouse Gas Reference Network
GHGs	greenhouse gases
GLM	Geostationary Lightning Mapper
GOCART	Goddard Chemistry Aerosol Radiation and Transport
GOES	Geostationary Operational Environmental Satellite
GOME	Global Ozone Monitoring Experiment
GOSAT-1/2	Greenhouse gases Observing Satellite 1/2
IAGOS	In-Service Aircraft for a Global Observing System
IASI	Infrared Atmospheric Sounding Interferometer
IAVW	International Airways Volcano Watch
ICAO	International Civil Aviation Organization
ICSU	International Council of Scientific Unions
IEOS	US Integrated Earth Observations System
IR	infrared
JPSS	Joint Polar Satellite System
LAM	Limited Area Model
LEO	low Earth orbit
MAIA	Multi Angle Imager for Aerosols
MetOp-SG	Metop-Second Generation
MODIS	Moderate Resolution Imaging Spectroradiometer
MOPITT	Measurements of Pollution in the Troposphere
MRW	medium-range weather
N_2O	nitrous oxide
NAAQS	National Ambient Air Quality Standards
NAQFC	National Air Quality Forecast Capability
NASA	National Aeronautics and Space Administration
NASEM	National Academies of Sciences, Engineering and Medicine
NCEP	National Centers for Environmental Protection
NEI	National Emissions Inventory
NESDIS	National Environmental Satellite, Data, and Information Service
NGGPS	Next Generation Global Prediction System
NH_3	ammonia
NIH	National Institutes of Health
NIR	near-infrared
NMFS	National Marine Fisheries Service
NO_2	nitrogen dioxide
NOAA	National Oceanic and Atmospheric Administration

NO_x	nitrogen oxides
NPS	National Park Service
NRF	National Response Framework
NWS	National Weather Service
OAR	Office of Oceanic & Atmospheric Research
OCO-2/3	Orbiting Carbon Observatory 2/3
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapping and Profiler Suite
OSE	observation system experiment
OSSE	observation system simulation experiment
ppmv	parts per million by volume
R2O	research-to-operations
RSMC	Regional Specialized Meteorological Center
S2S	subseasonal-to-seasonal
SBUV	Solar Backscatter Ultraviolet
SIGMETs	Significant Meteorological Information warning messages
SIP	Strategic Implementation Plan
SO_2	sulfur dioxide
SPP	President's Security and Prosperity Program of North American Initiative
SRW	Short Range Weather
Suomi NPP	Suomi National Polar-orbiting Partnership
SWIR	shortwave infrared
TEMPO	Tropospheric Emissions: Monitoring Pollution
TES	Tropospheric Emission Spectrometer
TIR	thermal infrared
TOAR	Tropospheric Ozone Assessment Report
TROPOMI	Tropospheric Monitoring Instrument
UFS	Unified Forecast System
UNFCCC	UN Framework Convention on Climate Change
US	United States
US EPA	United States Environmental Protection Agency
USDA	United States Department of Agriculture
USFS	United States Forest Service
USGS	United States Geological Survey
UVN	ultraviolet-visible-near-infrared
UV-VIS	ultraviolet-visible
VAA	Volcanic Ash Advisories
VAACs	Volcanic Ash Advisory Centers
VIIRS	Visible Infrared Imaging Radiometer Suite
VIS	visible
VIS-IR	visible-infrared
VOC	volatile organic compound
WCRP	World Climate Research Programme
WDC	World Data Centers
WFO	Weather Forecast Offices
WMO	World Meteorological Organization

1. Executive Summary

1.1 Purpose

This document assesses the value of atmospheric composition products from the next generation of the National Oceanic and Atmospheric Administration (NOAA) operational geostationary and extended orbits (GEO-XO) satellites to be launched between 2030 and 2050. Atmospheric Composition (AC) encompasses the vertical and geographical distribution of all gas phase trace chemical constituents (i.e., <<1% by number or mass of the atmosphere) and aerosols. AC plays pivotal roles in air quality, weather, and climate, both directly and via complex Earth System feedbacks. Further, as the month-long dust storms, record-breaking wildfires, and COVID-19 pandemic related mobility restrictions in 2020 have made startlingly evident, AC can dramatically affect life and property.

This report leverages NOAA's and the greater scientific community's decades of experience in measuring AC in situ and from space and translating this knowledge into research and operational capabilities used by various stakeholders. This report also builds on recent studies examining the benefits of geostationary AC observations. Reflecting the assessment of a large team of NOAA scientific, technical, and operational experts, the report is the starting point for a longer-term, comprehensive examination of the value of AC observations for NOAA's operational GEO capabilities. We identify NOAA mission requirements, stakeholder mandates, and seven science and operational application areas that will benefit from one or more GEO satellite instruments providing AC products at high temporal frequency and spatial resolution. NOAA's AC observations and prediction guidance inform forecasts and warnings that save lives and protect property. Extending NOAA's AC observational capability through GEO-based observations of AC is fundamental to NOAA's mission, responsive to national calls for continued AC observations, and necessary to support a wide spectrum of operational applications.

1.2 Motivations

GEO observations of AC are essential to fulfilling NOAA's numerous, long-standing legislative, executive, and international mandates for AC forecasting, monitoring and scientific research. Stakeholders for NOAA's AC capabilities span all levels of government, academia, the private and non-profit sectors, and the public. Quantitative understanding of the current state and trends in AC is absolutely critical to NOAA's Mission Service Areas—particularly for Aviation, Climate, Healthy Oceans, and Weather—and ensuring that the public has access to high quality air quality information is part of NOAA's Weather Mission. For example, changes to AC impact solar and terrestrial radiative forcing and cloud formation, making AC a key component of comprehensive coupled Earth System Models for weather and climate prediction. AC is fundamental to understanding changes in air quality, the stratospheric ozone layer, and climate, as well as their corresponding impacts on human health and natural and engineered ecosystems.

Ensuring NOAA's capabilities for space-based AC observations through GEO-XO coincides with the National Academies of

Sciences, Engineering and Medicine's 2017-2027 Decadal Survey (DS2017), which recommends that NOAA prioritize observations that inform the spatial distribution of trace gases and aerosols and the factors that cause temporal changes in these components. The DS2017 clearly highlights the importance of GEO objectives for AC, particularly with respect to weather, air quality, and climate, and recommends accomplishing them via a range of existing and new missions.

A GEO-XO AC capability will benefit from the National Aeronautics and Space Administration's (NASA's) Geostationary Coastal and Air Pollution Events (GEO-CAPE) mission, which carried out a decade of pre-formulation studies investigating potential GEO AC instrument concepts and numerous observation system simulation experiments (OSSEs) to demonstrate GEO instrument capabilities. GEO-CAPE also developed a novel mission implementation strategy featuring commercial hosting of instruments on one or more GEO satellites to reduce mission risk and potentially total mission cost.

Space-based GEO and low Earth orbit (LEO) platforms are necessary to extend the spatial and temporal reach of NOAA's ground- and aircraft-based AC observations, which are quality assured through rigorous calibration processes and are used to verify satellite observations. There is a rich heritage and mature technology for satellite-platform instruments with passive and active measurement capabilities and validated retrievals of AC gaseous and aerosol species. Tropospheric trace gas, aerosol, and cloud measurements in GEO have the temporal and spatial sampling to: resolve diurnal cycles in emissions, chemistry, and radiative forcings; monitor pollution at urban scales; and observe the inflow and outflow of pollution over the United States (US). The level of application of these space-based measurements is strongly dependent on the precision of the measurements to detect changes of the temporal and spatial scales relevant to the process and application, including the sensitivity of the measurement in the lowermost atmosphere, which is the region with substantial variability and the most relevant for air quality.

Without GEO-XO, the US's planned GEO AC capabilities are far more limited than our European and Asian partners, threatening the nation's long-term strategy for leadership in Earth system observation and prediction. The Advanced Baseline Imager (ABI) on NOAA's Geostationary Operational Environmental Satellite (GOES)-R series of spacecraft provides information about dust storms, wildfires and agricultural burning, all major contributors to air pollution in the US. ABI also produces an aerosol optical depth (AOD) product, an integrated measure of the abundance and optical properties of aerosols, along with the ability to distinguish whether those aerosols result from fires or dust storms. In the next few years, NASA will deploy two GEO instruments, Tropospheric Emissions: Monitoring Pollution (TEMPO) and Geostationary Carbon Observatory (GeoCARB), capable of retrieving trace gas distributions and providing additional information to complement ABI's aerosol products. However, TEMPO and GeoCARB are both research instruments intended for demonstration and risk reduction, and their nominal mission lifetimes end by the late 2020s. Outside of this NOAA GEO-XO effort, there are no plans to develop an operational US GEO AC capability. In this regard, the US lags activities in Europe and East Asia, where operational multi-instrument GEO AC measurements and applications are already in place and follow-on operational missions are being planned. GEO-XO is the opportunity for the US to implement an operational GEO AC capability that will match or exceed that of any other nation and serve NOAA's mission to save lives and protect property.

1.3 NOAA Application Areas and GEO-XO Atmospheric Composition Observables

This paper examines seven NOAA application areas that will benefit from a GEO-XO AC capability. This section summarizes key aspects of each application area and its need for specific GEO-XO AC observables, which are listed in *Table 1*.

Air Quality Forecasting. About 100,000 premature deaths annually in the US result from poor air quality, far exceeding the several hundred lives lost each year nationally due to extreme weather events. Through its National Air Quality Forecast Capability (NAQFC), part of the Unified Forecast System (UFS), NOAA issues forecast guidance used as a basis for official air quality forecasts. GEO-XO observations will significantly improve NAQFC forecast guidance, through enhanced evaluations, better constraints on emissions inventories, and better initialization by chemical data assimilation. More accurate air quality forecasts over the US facilitated by new GEO-XO capabilities will help to save lives and improve health outcomes as a result of reduced exposure to severe air pollution events.

Weather and Climate Forecasting. Aerosols and trace gases affect weather and climate directly through their radiative impacts and, in the case of aerosols, indirectly through changes to cloud microphysics. Accurate weather and climate forecasts within the UFS must therefore account for atmospheric composition. The UFS aims to provide daily to seasonal predictions for the globe and hourly predictions for the US. GEO-XO AC observations will help verify and initialize UFS forecasts of aerosols and trace gases, improve the quality of atmospheric state retrievals such as temperature and water vapor, and more accurately simulate diurnally varying incoming shortwave solar radiation.

Fire Weather Forecasting. Poor air quality in much of the US is a result of wildfires, which are increasing in severity as the climate changes. GEO data will enable the highly variable diurnal behavior of fires to be much more accurately represented in NOAA's UFS, which relies heavily on GEO and LEO data. The GEO perspective can provide earlier detection of fires and fill in data gaps between LEO sensors. Fire information from a GEO-XO imager in the 3.9 μm band at 1 km or better spatial resolution will be essential to future NOAA fire weather forecasting efforts. GEO-XO trace gas and aerosol data measured throughout a diurnal cycle will provide critical constraints on fire emissions and downwind smoke chemistry.

Hazards Forecasting. NOAA is responsible for forecasting episodic, high-risk events, including dispersion of ash emissions from volcanic eruptions and of chemical, toxic, and radioactive material. Volcanic Ash Advisories (VAAs) that are critically important to the aviation community combine observations from multiple satellites with model forecasts, and in the future will require more quantitative information on ash concentrations and SO_2. The high temporal frequency of GEO-XO products will be critical to future volcanic ash predictions and could aid in tracking releases of hazardous material from refinery fires, railroad derailments, oil spills, and other industrial accidents. Hazard dispersion also benefits from GEO-XO improvements to weather forecasts.

Stratospheric Ozone Monitoring. Stratospheric ozone (O_3) protects all life on Earth from harmful ultraviolet radiation (UV). Stratospheric O_3 plays an important role in atmospheric structure and large-scale circulation, impacts weather on seasonal to sub-seasonal time scales, and may be impacted by pollutant convection from volcanic eruptions and intense fires, while transport to the troposphere can also be associated with turbulence and its effects on aviation safety. NOAA is mandated by the Clean Air Act and the Montreal Protocol to monitor, assess, and report on the state of the stratospheric O_3 layer, including mandatory stratospheric O_3 measurements. Episodic, rapidly changing stratospheric events can be sampled by GEO-XO backscatter UV (BUV) measurements at high spatial resolution and temporal coverage. Combining GEO-XO BUV with a GEO-XO high-spectral resolution infrared (IR) sounder and in-situ stratospheric O_3 measurements would provide continuous O_3 climate data records. Co-located GEO-XO O_3 and aerosol measurements inform assessments of the impacts of possible future climate intervention approaches.

Greenhouse Gas Monitoring. NOAA's long-term global monitoring of greenhouse gases (GHGs) provides the observational basis for climate forecasting that requires accurate representation of anticipated carbon-climate feedback mechanisms. Sustained atmospheric GHG observations are needed by the US to inform its mandatory reporting, to track the efficacy of its anticipated emissions mitigation efforts, and for understanding potential future climate intervention. GEO-XO shortwave IR (SWIR) observations of GHGs with at least 1-km horizontal resolution would expand spatial and temporal coverage of NOAA's current GHG monitoring strategy that relies heavily on ground-based, tower, and aircraft sampling. GEO-XO thermal IR (TIR) measurements would provide information about GHG vertical distributions. GEO-XO SWIR GHG measurements would increase opportunities for cloud- and aerosol-free observations, could provide unique insights into day-to-day and diurnal variations of large fluxes, and could detect sporadic high emissions events. Simultaneous GEO-XO UV-visible (UV-VIS) spectrometer and VIS-IR imager measurements of a suite of air quality trace gases and aerosols could provide powerful constraints for separating biospheric influences from anthropogenic and fire sources.

Air Quality Monitoring. A robust space-based NOAA air quality monitoring capability provides complementary measurements to existing surface networks and emission monitoring operated by national, tribal, state and local regulatory agencies. NOAA's air quality monitoring is important for evaluating air quality emissions inventories, is useful for the evaluation of the NAQFC, and will inform future NAQFC data assimilation efforts. GEO-XO high spatial and temporal resolution UV-VIS and near-IR (NIR)/TIR spectrometer measurements are sensitive to abundances and changes of these gases and aerosols in the planetary boundary layer. Species of highest priority are:

- O_3. Multi-spectral retrievals could better constrain regional O_3 analyses.
- *Nitrogen dioxide (NO_2)*. The standard proxy for nitrogen oxides (NO_x) pollution.

- *Formaldehyde (CH_2O)*. The standard proxy for volatile organic compound (VOC) pollution.
- *Glyoxal ($C_2H_2O_2$)*. A secondary proxy for VOCs.
- *Carbon monoxide (CO)*. A tracer for fossil fuel combustion and wildfires.
- *Sulfur dioxide (SO_2)*. A tracer for coal combustion and volcanos.
- *Ammonia (NH_3)*. A tracer for agricultural emissions.

A GEO-XO VIS-IR imager would provide information on fires and would measure aerosol type and optical depth, needed for co-monitoring trace gases and their precursors.

Table 1. Recommended GEO-XO AC observables, with the spectral coverage needed and the NOAA application areas that will benefit from each observable (with this report's relevant section numbers).

GEO-XO AC Observable	Spectral Coverage	NOAA Application Area
Trace gases		
Ozone (O_3) (column, profile, stratosphere, troposphere)	UV-VIS Near IR Thermal IR	Stratospheric ozone monitoring *(3.2.1)* Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)* Greenhouse gas monitoring *(3.2.2)*
Nitrogen dioxide (NO_2)	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)* Greenhouse gas monitoring *(3.2.2)* Hazards forecasting *(3.1.4)*
Carbon monoxide (CO)	Shortwave-IR Mid-IR Thermal IR	Air quality monitoring *(3.2.3)* Greenhouse gas monitoring *(3.2.2)* Air quality forecasting *(3.1.1)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)*
Methane (CH_4)	Shortwave-IR Mid-IR Thermal IR	Greenhouse gas monitoring *(3.2.2)* Weather and climate forecasting *(3.1.2)* Hazards forecasting *(3.1.4)* Air quality monitoring *(3.2.3)*
Carbon dioxide (CO_2)	Shortwave-IR Mid-IR Thermal IR	Greenhouse gas monitoring *(3.2.2)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)*
Sulfur dioxide (SO_2)	UV-VIS Thermal IR	Air quality monitoring *(3.2.3)* Hazards forecasting *(3.1.4)*

We define the following spectral regions by radiation wavelength: UV < 0.3 μm, 0.3 μm < VIS < 0.7 μm, 0.7 μm < Near-IR < 1 μm, 1 μm < Shortwave IR < 3 μm, 3 μm < Mid-IR < 5 μm, 2.5 μm < Thermal IR < 14 μm. "Thermal IR" indicates IR radiation emitted by the Earth, in contrast to direct or reflected Solar radiation.

Table 1 Con't. Recommended GEO-XO Atmospheric Composition observables, with the spectral coverage needed and the NOAA application areas that will benefit from each observable (with this report's relevant section numbers).

GEO-XO AC Observable	Spectral Coverage	NOAA Application Area
Trace gases con't		
Formaldehyde (CH_2O)	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Glyoxal ($C_2H_2O_2$)	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Nitrous oxide (N_2O)	Shortwave-IR Mid-IR Thermal IR	Greenhouse gas monitoring *(3.2.2)* Weather and climate forecasting *(3.1.2)* Stratospheric ozone monitoring *(3.2.1)*
Ammonia (NH_3)	Mid-IR Thermal IR	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Isoprene (C_5H_8)	Mid-IR Thermal IR	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Aerosols		
Absorbing aerosol optical depth	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol optical depth in UV-VIS	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol optical depth in VIS	VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Single scattering albedo	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol layer height/mixing height	VIS Near-IR	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol type, single scattering albedo	UV-VIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Key quantities related to AC		
Fire detection and characterization (burned area, fire radiative power, fire temperature, fire size)	Mid-IR Thermal IR	Air quality monitoring *(3.2.3)* Fire weather forecasting *(3.1.3)* Weather and climate forecasting *(3.1.2)*
Lightning	Near-IR	Air quality monitoring *(3.2.3)* Fire weather forecasting *(3.1.3)* Weather and climate forecasting *(3.1.2)*

We define the following spectral regions by radiation wavelength: UV < 0.3 µm, 0.3 µm < VIS < 0.7 µm, 0.7 µm < Near-IR < 1 µm, 1 µm < Shortwave IR < 3 µm, 3 µm < Mid-IR < 5 µm, 2.5 µm < Thermal IR < 14 µm. "Thermal IR" indicates IR radiation emitted by the Earth, in contrast to direct or reflected Solar radiation.

1.4 Next Steps and Additional Recommendations

This paper states the motivation for GEO-XO AC capabilities in seven NOAA application areas and represents an initial assessment of their value. Future efforts can build on this work by developing valuation use cases that demonstrate the enormous benefit-to-cost ratio of GEO-XO for these AC applications. These valuation efforts would ideally consider a set of complete AC payloads, each including an imager and one or more spectrometers covering the TIR to UV regions of the spectrum, designed to last 20 years. These quantitative valuation cases should consider both the economic and societal benefits in terms of lives saved, improved health outcomes and corresponding impacts on productivity, property protected, and the potential for generating new products in the global Earth observation market.

Future GEO-XO AC valuation estimates can build on existing science and application value assessments carried out in the US and by its international partners, including by NASA’s GEO-CAPE mission, the teams developing the Geostationary Environment Monitoring Spectrometer (GEMS), TEMPO, GeoCARB and Sentinel-4 ultraviolet-visible-near-infrared (UVN) instruments, and by the Committee on Earth Observation Satellites. Future valuation efforts benefit enormously from GEO-XO’s ongoing user engagement that is garnering user community feedback and helping identify new stakeholders. Experts on GEO-XO’s AC observation capabilities and the applications of GEO-XO AC products will likely work with the staff of NOAA chief economist’s office to derive quantitative valuation estimates. The time and effort required for such analyses should not be underestimated; similar efforts for the Weather applications of GEO-XO instrumentation have taken years. We recommend investment of adequate time and funding to bring together a team of experts on GEO-XO AC instruments, development of resulting operational products, and detailed economic and societal analyses needed to complete credible quantitative valuation estimates.

Future GEO-XO AC capability analyses will likely focus on specific cases within the broad application areas described in this paper. We have shown that GEO-XO’s AC capabilities are likely to produce substantial improvements to NOAA’s future fire weather and air quality forecasts. Air pollution from wildfires and human activity is strongly linked to negative impacts on health, economic output, and quality of life. Fire weather and air quality forecasting are therefore two areas likely to demonstrate the value of GEO-XO AC observations.

These GEO-XO AC quantitative valuation analyses will be pioneering; we could identify no previous estimates of the economic benefits of GEO AC observations. As economic analyses of air pollution regulations and Earth observations carried out in the US and Europe demonstrate, the benefits of efforts aimed at improving air quality and its consequent human health and economic outcomes far exceed their costs. We are confident that similarly high benefit-to-cost ratios would be found for a GEO-XO AC capability.

Our international partners are already demonstrating the feasibility and applications of GEO AC capabilities. The GEO-XO AC valuation studies will assess the benefit of these capabilities for the Nation and fulfill NOAA’s mission to save lives and protect property.

2. Background and Motivation

AC is defined as the distribution of all chemical compounds present in the atmosphere in trace amounts (i.e., at levels much less than 1% by number or mass). These chemical components span all lifetimes, from seconds to centuries. They exist in the gas, aqueous, and solid (particle) phase. These components may undergo rapid, slow, or no chemical transformation in the atmosphere. They are emitted from the terrestrial and marine biosphere, and many components may also be deposited after emission or atmospheric chemical transformation. Atmospheric chemical components are also produced from all manner of anthropogenic activity, especially the burning of fossil fuel or biomass. In most cases of NOAA's operational use and applications, the atmospheric chemical components of interest are trace gases and aerosols with varying lifetimes and a wide variety of chemical activity. Shorter-lived air pollutants such as reactive trace gases and aerosols affect life and property, while radiatively important trace gases and aerosols affect weather and climate.

For AC, the burden of demonstrating a capability to observe and use satellite measurements for air quality, weather, and climate originally fell on research agencies such as NASA and the European Space Agency (ESA). Responsibility for research capabilities, however, are increasingly transitioning to operational agencies such as NOAA and the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), both for technology to launch satellites with similar capabilities and for data utilization in numerical weather and air quality prediction models. *Section 2* of this white paper takes this shifting burden into account, starting with NOAA's mandates regarding AC and a discussion of the need for a US space-based AC capability. We then document the current AC observational capabilities from space, their limitations, and future plans in the broad context of a constellation of satellites from NOAA and its national and international partner agencies. Finally, we detail some comparative advantages of GEO as well as examples which illustrate the necessity for multi-spectral GEO AC capabilities. The background and motivations discussed in this white paper should thus frame the scope for GEO-XO AC capabilities.

2.1. NOAA's Mandates for Atmospheric Composition

2.1.1. NOAA's Legislative and Executive Mandates

There are numerous mandates for NOAA's AC research, monitoring and operational activities and its unbiased assessments of the information generated by these efforts and by other entities. These drivers include a variety of legislation, orders and programs of the executive branch, and agreements and treaties between the US and other nations and international bodies. A list of many of these mandates is shown in *Table 2*. Here we discuss mandates relevant to NOAA's AC capabilities overall, which direct NOAA to observe, monitor, forecast and act in a wide range of AC-relevant application areas. *Section 3* of this report provides the particular drivers for each of the specific application areas of NOAA's AC capabilities. For each of the AC application areas, *Section 3* will also highlight which products are most impactful and how these products would be improved by a GEO capability.

Table 2. List of NOAA's mandates relevant to AC.

Legislative
Direct Congressional appropriations *E.g., H.R.2157 - Additional Supplemental Appropriations for Disaster Relief Act, 2019*
Clean Air Act 1990 Title IV and Title VI, 42 U.S.C. *Ozone depletion: § 7401 et seq.* *Lake/coasts deposition: § 7412(m)* *Ecosystems: § 7403(e)* *Acid deposition program: § 7403(j)*
Global Change Research Act of 1990, 15 U.S.C. § 2921 et seq
Global Climate Protection Act of 1990, 7 U.S.C. § 6701 et seq.
Weather Research and Forecasting Innovation Act of 2017, Pub.L. 115–25, H.R. 353
National Climate Program Act, 15 U.S.C. § 2901-2908, at 2904(d) (4), et seq.
Geophysical Surveys: Improvement of methods, etc.; investigations & research, 33 U.S.C. §883(d)
National Weather Service Organic Act, 15 U.S.C. § 313
Federal Records Act as amended, 44 U.S.C. §3101 et seq.
Data Quality Act, Public Law 106-554, Section 515, 2001
36 C.F.R., Chapter XII National Archive and Records Administration (NARA) Records and Guidelines
Coastal Zone Management Act (CZMA) of 1972, 16 U.S.C. 1450 et seq. (amended 1990 and 1996)
Consolidated Appropriations Act, 2005, Public Law No. 108-447
Executive
Numerous interagency agreements: Federal, state/local/tribal (S/L/T)
National Response Framework (NRF): Annexes assigned dispersion prediction responsibilities for smoke and radioactive and hazardous materials to NOAA.
Federal Radiological Emergency Response Plan (FRERP): NOAA is primary Dept. of Commerce agency to assist Federal, State, local orgs. responding to a radiological emergency.
Strategic Plan for the US Integrated Earth Observations System (IEOS), USGEO Report, 2005
President's Security and Prosperity Program of North America Initiative (SPP), 2005
US Ocean Action Plan/ Charting the Course for Ocean Science for the United States for the Next Decade (2007)
Department Administrative Order (DAO) 212-2 Information Technology Handbook
International
UN Framework Convention on Climate Change (UNFCCC)
Montreal Protocol on Substances that Deplete the Ozone Layer (and subsequent amendments)
Global Earth Observation System of Systems (GEOSS)
International Council of Scientific Unions (ICSU) guidelines/policy regarding World Data Centers (WDC)

Congressional appropriations and many laws drive NOAA's AC efforts. One goal of NOAA's AC mission is tracking the efficacy of various public laws. Legislation as diverse as the Clean Air Act and its 1990 Amendments to the Weather Research and the Forecasting Innovation Act of 2017 direct NOAA to carry out work in a variety of specific AC application areas. These applications include conducting research on and develop forecasting capabilities for air quality, quantifying the impacts of atmospheric composition on weather and climate predictions, monitoring stratospheric O_3 depletion and the recovery of the stratospheric O_3 layer, and more generally, understanding the state of AC and how it changes with time, in order to improve NOAA's forecasts and protect lives and property.

Similarly, NOAA is part of numerous agreements with other Federal agencies and with state, local and tribal governments to provide AC information. For example, NOAA issues air quality forecast guidance through the NAQFC. NOAA's guidance is used as a basis for official air quality forecasts and air pollution alerts issued by the US Environmental Protection Agency (US EPA) and state and local regulatory agencies to protect groups sensitive to poor air quality. NOAA plays a lead role in issuing smoke forecasts used by first responders who fight wildfires and protect people and property in harm's way. NOAA is the primary agency to issue dispersion forecasts for chemical fires, radiological accidents and other emergency events that release hazardous pollutants into the atmosphere.

NOAA plays a key role in demonstrating US compliance with international agreements and treaties. For example, NOAA has a lead role in the Montreal Protocol on Substances that Deplete the Ozone Layer and its subsequent amendments. NOAA's ongoing measurements of the stratospheric O_3 layer demonstrate that the O_3 layer is recovering from depletion that began several decades ago. NOAA's long-term observations of a variety of compounds that deplete O_3 provide confirmation that the Montreal Protocol's bans on these substances are actually working. One example of the sensitivity of NOAA's observations was a report (Montzka et al., 2018) of unexpected increases in emissions of a banned O_3-depleting substance, CFC-11, that were later attributed to sources in China.

2.1.2. NOAA's Mission Service Areas

Quantitative understanding of the current state and trends in AC is critical to all of NOAA's Mission Service Areas, highlighted in *Figure 1*. NOAA's AC capabilities include volcanic ash forecasts to ensure safer air travel and fire weather predictions that protect first responders and residents in the path of wildfires. Changes to AC impact solar and terrestrial radiative forcing and cloud formation, making AC a key component of comprehensive coupled Earth System Models for weather and climate prediction. AC is fundamental to understanding changes in air quality, the stratospheric O_3 layer, and climate, as well as their corresponding impacts on human health and natural and engineered ecosystems. Protecting marine and coastal ecosystems requires the capacity to predict the current state of AC and its changes over time. While the specifics are discussed in more detail in *Section 3*, overall AC's synergies with NOAA mission activities such as weather forecasting and oceans monitoring mean that strengthening NOAA's AC capabilities through GEO-XO results in down-the-line improvements for a multitude of NOAA mission activities across multiple line offices.

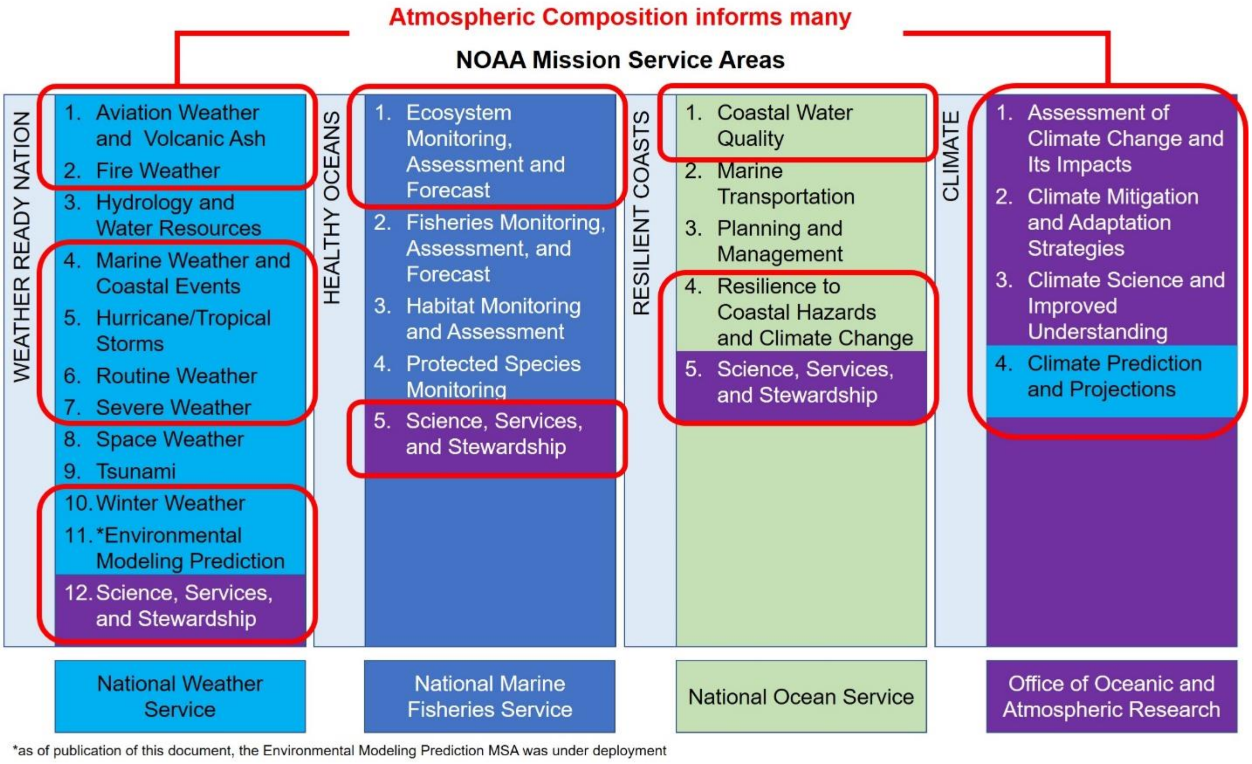


Figure 1. NOAA's Mission Service Areas.

2.2 The Need for a US Space-Based Atmospheric Composition Capability

2.2.1. 2017-2027 Decadal Survey

At the request of NASA, NOAA, and the USGS, the Committee on the Decadal Survey for Earth Science and Applications from Space of the National Academies of Sciences, Engineering and Medicine (NASEM) Space Studies Board, Division on Engineering and Physical Sciences released the 2017-2027 Decadal Survey, "Thriving on Our Changing Planet: A Decadal Strategy for Earth Observations from Space" (NASEM, 2018, hereafter referred to as "DS2017"). The survey looks ten years into the future, prioritizing research areas, observations, and notable missions in order to make those observations feasible. An overarching theme of the assessment is that satellite-based observations have and will continue to play a key role in the discovery, understanding, and monitoring of key chemical species in the atmosphere.

The future poses several challenges in the realm of earth observations, most being closely related to the monitoring of atmospheric chemical variables. These areas of concern include: the improvement of weather forecasts (e.g. further developments in assimilation and modeling), protection against solid earth hazards (e.g. volcanic ash), mitigation of the adverse impacts of climate change (e.g. quantifying present-day regional carbon sources and sinks), the protection of ecosystems, and the improvement of human health (e.g. examining how environmental factors relate to patterns of morbidity and mortality).

In regards to applications and priorities related to AC, the DS2017 recommends that NOAA, NASA, and the US Geological Survey (USGS) pursue the following key science areas: the influence of Earth surface variations on weather and air quality; impacts of aerosols on global warming; impacts of carbon cycle variations on climate and ecosystems; long-term air pollution and impacts; processes influencing tropospheric O_3 and its impacts; methane (CH_4) variations and impacts on tropospheric composition and chemistry; and, cloud microphysical property dependence on aerosols and precipitation.

New observations recommended by the DS2017 consider both observations that are not currently made and also impending gaps in observations. It was assumed that currently operating and planned satellite missions, referred to as the Program of Record, would proceed as planned over the decade. With this context, new observing system priorities from the DS2017 highlight the need for observations on aerosol properties, CO_2 and CH_4 fluxes and trends, vertical profiles of O_3 and trace gases, as well as vertical and temporal profiling of the planetary boundary layer, temperature, and heights. The DS2017 also contains clear statements of the ongoing importance of GEO objectives for AC and recommends accomplishing them via a range of existing and new missions. The importance of GEO atmospheric science goals is highlighted in DS2017 “Weather and Air Quality” and “Climate Variability and Change” priorities. Air quality is a “Most Important” Science and Applications Priority (Table 3.3, Question W-5) and part of two other “Most Important” priorities (Questions W-1, W-2). Methane measurements are part of the “Most Important” priorities for greenhouse gas measurements (Questions C-2d, E-3a, and E-4a). While the existence of the TEMPO and GeoCARB missions in the Program of Record *(see Section 2.2.2)* precluded recommendations for new GEO AC missions in the 2017-2027 period, these “Most Important” priorities indicate that continuity of such measurements will be a high national priority in the GEO-XO era.

Given the DS2017’s clear statements on the importance of GEO objectives for AC, ensuring AC capabilities through GEO-XO illustrates that NOAA is giving NASEM’s recommendations full consideration. The GEO-XO AC capabilities detailed in this white paper will provide the operational continuity to extend the DS2017’s Program of Record measurements of trace gas and aerosol products in order to address these DS2017 priorities into the 2030’s through 2050’s.

2.2.2. GEO-CAPE, TEMPO, and GeoCARB

The NASEM 2005-2015 Decadal Survey (DS2007) recommended the GEO-CAPE mission, a NASA-led effort in 2009-2018 to advance the science of both coastal ocean biophysics and atmospheric-pollution chemistry and to help determine the readiness of these conceptual GEO missions to begin the formulation phase (Fishman et al., 2008). The GEO-CAPE mission study team completed several white papers and other documentation reporting results of their pre-formulation studies (GEO-CAPE Team, 2018).

While GEO-CAPE studies confirmed the DS2007 recommendations for a GEO mission was at a high level of technology readiness, the DS2007 cost estimate of $550 million for a dedicated GEO mission was low by a factor of two to three. The GEO-CAPE study team developed a novel mission implementation strategy featuring commercial hosting of instruments on one or more GEO satellites to reduce mission risk and potentially total mission cost, while providing programmatic flexibility by allowing smaller components of the mission to be individually initiated as NASA funding profiles allowed. Other GEO-CAPE deliverables included developing science traceability matrices to express measurement requirements, conducting field campaigns and other science studies to affirm and refine these requirements, and multiple synergistic activities with NASA's Earth Sciences Division programs. GEO-CAPE team members at the same time pursued Earth Venture (EV) opportunities, the only means of initiating GEO-CAPE satellite observations in a constrained budgetary environment.

The selection of the TEMPO mission through NASA's EV Instrument 1 solicitation was the first step toward the GEO-CAPE distributed implementation strategy. TEMPO will meet many of the GEO-CAPE atmospheric science objectives and is a pathfinder for the hosted payload mission strategy. TEMPO is a UV-VIS hyperspectral spectrometer covering the spectral region from 290 nm to 740 nm with 0.2 nm resolution with a gap between 490 nm to 540 nm. The spatial resolution for derived AC products will be approximately 2 km by 4.5 km at the center of the field of regard with the satellite positioned at 100 degrees west longitude. The standard products from TEMPO will be NO_2, O_3, and aerosols at hourly resolution and H_2CO, $C_2H_2O_2$, and SO_2 at least three times during the day. TEMPO is optimized for trace gas retrievals. Without a cloud camera and coverage in SWIR, an optimized suite of aerosol products can be derived in synergy with other instruments in GEO such as ABI.

The study team determined that the remaining atmospheric GEO-CAPE measurement objectives could be met by an instrument of comparable cost to TEMPO that makes measurements in IR wavelengths, as defined in the GEO-CAPE atmospheric science traceability matrix, and use of data from the ABI on the GOES-R/S series satellites. The GeoCARB mission, selected in December 2016 via the EV Mission 2 solicitation, will likely partially meet remaining GEO-CAPE atmospheric science requirements associated with infrared measurements, pending its final configuration and observing strategy, and also demonstrates an alternative partnering strategy for a commercial hosted payload mission.

The GEO-CAPE final report recognizes that all of GEO-CAPE objectives could be met in a cost-effective manner by completing NASA missions in the Program of Record (i.e., TEMPO and GeoCARB), investing in fused data products using observations from these missions and those of NOAA and international space agencies, and capturing future EV and Explorer opportunities (primarily to fulfill GEO-CAPE's coastal waters objectives). The value of GEO-CAPE observations will be amplified by being embedded within an integrated observing strategy featuring similar geostationary observations from missions over other parts of the globe combined with LEO observations to provide full global context. GEO-CAPE study team members are key participants in international activities to implement this potential under the auspices of the Committee on Earth Observation Satellites (CEOS), and as members of mission science teams in Europe and Korea. Data harmonization activities featuring common validation strategies will be essential for providing truly interoperable data products from these satellite constellations. GEO-CAPE study activities helped define and begin building the modeling capabilities necessary for realizing these visions.

There are several additional GEO-CAPE recommendations planned over the coming decade via NOAA, NASA, and US EPA investments which will provide mature, well-validated GEO AC products with a broad user base. First, fulfill the Program of Record missions for TEMPO, GeoCARB, and Multi Angle Imager for Aerosols (MAIA) and maintain close coordination among these missions and partner missions in operation (GOES ABI, Sentinel-5 Precursor Tropospheric Monitoring Instrument [TROPOMI], Suomi National Polar-orbiting Partnership [NPP], Joint Polar Satellite System [JPSS], Enhanced Polar System [EPS]) to meet the science and applications priorities expressed in the DS2017. Second, fully exploit these improved air quality monitoring data over North America by sustaining ongoing activities to improve retrieval algorithms, chemical data assimilation capabilities, inverse modeling capabilities for constraining emissions estimates, and integrated observing system frameworks (such as observation system simulation experiments), including synergistic aerosol retrievals using GEO observations from TEMPO, ABI, and potentially GeoCARB. Third, continue collaborations with partners such as the US EPA and regional air quality organizations to further implement and maintain long-term ground sites combining continuous in-situ and remote-sensing measurements (e.g., Pandora and lidar) many times per hour. Data from such sites are critical for validation of the geostationary measurements, science and applications data utilization, and stakeholder uptake of the satellite data. Fourth, continue to mature mechanisms for engaging end-users to aid early adoption of TEMPO and other GEO-CAPE related observations, including participation in collaborative regional field campaigns. Fifth, create a formal Constellation Science Team for Air Quality, supported by stable funding for US members, to collaborate with national and international partners in order to mature harmonized, consistent, well-validated interoperable data products from the constellations of GEO and LEO satellites now in orbit and those in advanced planning stages.

The GEO-CAPE report's final recommendation was that, as highly time-resolved observations are the next frontier of Earth science from space, we should build on the lessons learned from the communal GEO-CAPE study activities by continuing to work with all stakeholders to jointly identify priorities and develop advocacy for sustainable future highly time-resolved observations. A decade from now, any GEO-XO AC mission would sustain the capabilities, products, and user base described above.

2.3. Existing LEO and GEO Atmospheric Composition Capabilities

There are numerous AC observables available on current and planned space-based platforms. *Table 3* summarizes these products and the instruments that measure these observables in GEO and LEO currently, or will within the next few years, along with the NOAA application areas that benefit from each observable.

Table 3. AC observables from space, spectral coverage needed for each, current and planned capabilities to measure the observable in GEO and LEO orbit, and the relevant NOAA application areas that benefit from the observable (with report section numbers). Orange entries indicate the GEO platforms observing the US.

Observable	**Spectral Coverage**	**Current / Planned Capabilities** **Heritage GEO**	 **Heritage LEO**	**Application Area**
Trace gases				
Ozone (O_3) (column, profile, stratosphere, troposphere)	UV-VIS Near-IR Thermal IR	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP	Stratospheric ozone monitoring *(3.2.1)* Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)* Greenhouse gas monitoring *(3.2.2)*
Nitrogen Dioxide (NO_2)	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)* Greenhouse gas monitoring *(3.2.2)* Hazards forecasting *(3.1.4)*
Carbon monoxide (CO)	Shortwave-IR Mid-IR Thermal IR		MetOp IASI JPSS CrIS Aqua AIRS MOPITT	Air quality monitoring *(3.2.3)* Greenhouse gas monitoring *(3.2.2)* Air quality forecasting *(3.1.1)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)*
Methane (CH_4)	Shortwave-IR Mid-IR Thermal IR	GeoCARB	MetOp IASI JPSS CrIS Aqua AIRS OCO-2 TROPOMI GOSAT	Greenhouse gas monitoring *(3.2.2)* Weather and climate forecasting *(3.1.2)* Hazards forecasting *(3.1.4)* Air quality monitoring *(3.2.3)*

We define the following spectral regions by radiation wavelength: UV < 0.3 μm, 0.3 μm < VIS < 0.7 μm, 0.7 μm < Near-IR < 1 μm, 1 μm < Shortwave IR < 3 μm, 3 μm < Mid-IR < 5 μm, 2.5 μm < Thermal IR < 14 μm. "Thermal IR" indicates IR radiation emitted by the Earth, in contrast to direct or reflected Solar radiation.

Table 3 con't. AC observables from space, spectral coverage needed for each, current and planned capabilities to measure the observable in GEO and LEO orbit, and the relevant NOAA application areas that benefit from the observable (w/ section numbers). Orange indicates the GEO platforms observing the US.

Observable	Spectral Coverage	Current / Planned Capabilities		Application Area
		Heritage GEO	Heritage LEO	
Trace gases con't				
Carbon dioxide (CO_2)	Shortwave-IR Mid-IR Thermal IR	GeoCARB	OCO-2 GOSAT Metop IASI JPSS CrIS Aqua AIRS	Greenhouse gas monitoring *(3.2.2)* Weather and climate forecasting *(3.1.2)* Fire weather forecasting *(3.1.3)*
Sulfur Dioxide (SO_2)	UV-VIS Thermal IR	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Hazards forecasting *(3.1.4)*
Formaldehyde (CH_2O)	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Glyoxal ($C_2H_2O_2$)	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Nitrous oxide (N_2O)	Shortwave-IR Mid-IR Thermal IR		JPSS CrIS	Greenhouse gas monitoring *(3.2.2)* Weather and climate forecasting *(3.1.2)* Stratospheric ozone monitoring *(3.2.1)*
Ammonia (NH_3)	Mid-IR Thermal IR		JPSS CrIS Metop IASI Aqua AIRS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Isoprene (C_5H_8)	Mid-IR Thermal IR		JPSS CrIS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)*
Aerosols				
Absorbing aerosol optical depth	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol optical depth in UV-VIS	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*

We define the following spectral regions by radiation wavelength: UV < 0.3 μm, 0.3 μm < VIS < 0.7 μm, 0.7 μm < Near-IR < 1 μm, 1 μm < Shortwave IR < 3 μm, 3 μm < Mid-IR < 5 μm, 2.5 μm < Thermal IR < 14 μm. "Thermal IR" indicates IR radiation emitted by the Earth, in contrast to direct or reflected Solar radiation.

Table 3 con't. AC observables from space, spectral coverage needed for each, current and planned capabilities to measure the observable in GEO and LEO orbit, and the relevant NOAA application areas that benefit from the observable (w/ section numbers). Orange indicates the GEO platforms observing the US.

Observable	**Spectral Coverage**	**Current / Planned Capabilities**		**Application Area**
		Heritage GEO	**Heritage LEO**	
Aerosols con't				
Aerosol optical depth in VIS	VIS	GOES-R ABI Himawari AHI G2A AMI	Aqua MODIS Terra MODIS JPSS VIIRS	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Single scattering albedo	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI OMPS-NP Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol Layer height/Mixing height	VIS Near-IR	TEMPO Sentinel-4 UVN	S5P TROPOMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Aerosol type, single scattering albedo	UV-VIS	GK-2B GEMS Sentinel-4 UVN TEMPO	S5P TROPOMI Aura OMI	Air quality monitoring *(3.2.3)* Air quality forecasting *(3.1.1)* Fire weather forecasting *(3.1.3)*
Key quantities related to AC				
Fire detection and characterization (burned area, fire radiative power, fire temperature, fire size)	Mid-IR Thermal IR	GOES-R ABI Himawari AHI GK-2A AMI	JPSS VIIRS Sentinel-3	Air quality monitoring *(3.2.3)* Fire weather forecasting *(3.1.3)* Weather and climate forecasting *(3.1.2)*
Lightning	Near-IR	GOES-R GLM		Air quality monitoring *(3.2.3)* Fire weather forecasting *(3.1.3)* Weather and climate forecasting *(3.1.2)*

We define the following spectral regions by radiation wavelength: UV < 0.3 µm, 0.3 µm < VIS < 0.7 µm, 0.7 µm < Near-IR < 1 µm, 1 µm < Shortwave IR < 3 µm, 3 µm < Mid-IR < 5 µm, 2.5 µm < Thermal IR < 14 µm. "Thermal IR" indicates IR radiation emitted by the Earth, in contrast to direct or reflected Solar radiation.

Air quality related trace gas observations at high spatial resolution (5.6 km x 3.5 km) from Sentinel 5P TROPOMI are revolutionizing the use of satellite data in air quality monitoring, such as the investigation of NO_x emissions' changes due to COVID-19 related economic shutdown in 2020 *(Figure 2)*. Similar observational capabilities from a geostationary orbit are or soon will be in place for GEOKOMPSAT-2B GEMS, Sentinel-4 UVN, and TEMPO (Lahoz et al., 2012; Quesada-Ruiz et al., 2020). GEMS was launched on February 18, 2020 and is already in orbit and is beginning to provide its first measurements of spatially and temporally resolved tropospheric column amounts of trace gases and aerosols for air quality. The diurnal variation of trace gases such as NO_2, CH_2O, SO_2, aerosols etc. driven by time of the day dependent emissions (e.g., rush hour vehicular emissions) and photochemistry will be observed routinely over a regional domain covering most of East Asia. The soon to be launched Sentinel-4 (potential launch date 2023) and TEMPO (potential launch date 2022) covering Europe and much of north America including all the continental United States (CONUS), respectively, combined with GEMS over Asia are expected to form a geostationary constellation of satellites for air quality and atmospheric composition (*Figure 3*, taken from CEOS, 2019).

The research satellite missions such as TEMPO traditionally offer a window into the measurement capabilities such as product accuracy etc. and how the products can be used in a variety of applications. However, research missions are not designed to have a long lifetime and are built for demonstration and risk reduction. An operational capability needs to evolve from the research demonstration, especially when the products in question meet the needs of operational agencies such as NOAA, USDA, USFS, FEMA, and US EPA. Such operational capabilities are already being implemented in Europe with the two-satellite Sentinel-4 series (15 years) and East Asia with GEMS (10 years) and a follow-on in preliminary planning. Historically, in the US, there has been a precedent for transition from NASA research missions to NOAA operations; with AC instruments such as TEMPO or a similar instrument on GEO-XO, the tradition will continue.

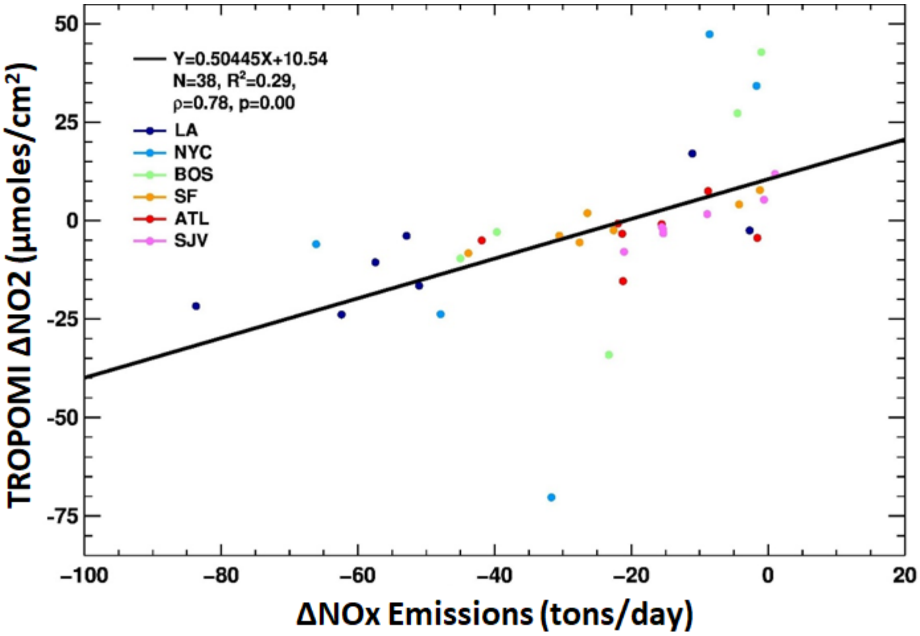


Figure 2. Changes in TROPOMI tropospheric column NO_2 due to lockdown measures in March 2020 shown to correlate well with changes to NO_x emissions measured from ground for various cities in the US. The positive correlation shows that changes in traffic patterns/emissions can easily be tracked using TROPOMI NO_2 observations.

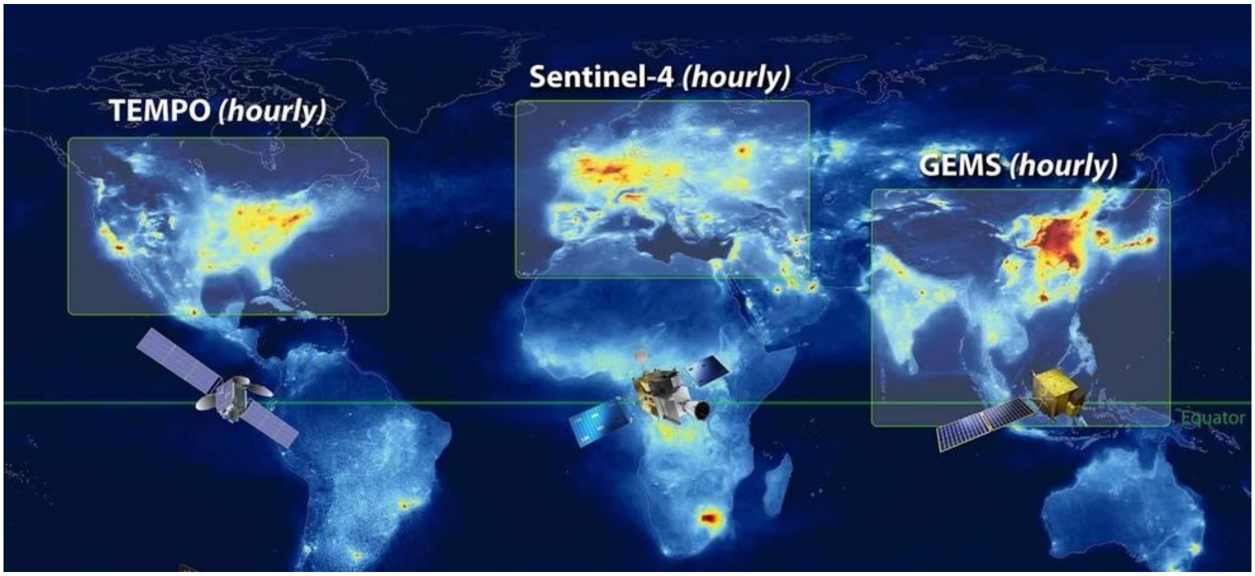


Figure 3. A pioneering new constellation of three space-based instruments has started to take shape to advance global air quality science and monitoring (Credits: NASA).

The geostationary constellation for air quality will provide hourly (tropospheric) trace gas and aerosol observations derived from algorithms similar to those applied to TROPOMI measurements. By the time the GEO constellation is in place, a follow-on to TROPOMI is expected to fly on the operational EUMETSAT Sentinel 5 platform. The polar-orbiting Sentinel 5, flying underneath the three GEOs (at some point over the US) and deriving the same observables, is expected to become a transfer standard for cross calibration. The current TEMPO mission lifetime does not extend to 2030, after which the international constellation will be missing its US component unless a GEO-XO UV-VIS instrument replaces TEMPO.

By the early 2030s when GEO-XO is in orbit along with similar satellite missions from partner agencies in Europe and Asia, the retrieval science and innovative product application areas will have evolved. The synergistic use of products or the synergistic retrieval of a suite of products by combining measurements from different instruments (e.g., imager and spectrometer) may become the norm. Testing of these approaches is beginning now with polar-orbiting satellites making measurements that will become operational on geostationary platforms in the era of GEO-XO. For example, combining observations from different sensors (imager + high-spectral resolution sounder, active + passive, GEO+GEO, GEO+LEO) can help to constrain particulate pollution levels. This can be made possible by developing aerosol algorithms to combine measurements from a geostationary satellite visible imager and a geostationary satellite UV spectrometer in the same field of regard (i.e., geographic coverage). Early on, the Himawari-8 Advanced Himawari Imager (AHI) and GEOKOMPSAT-2B GEMS can be used as a test bed and expand the methodology to the combination of ABI/TEMPO over the US and Flexible Combined Imager (FCI)/UVN over Europe. The imager/spectrometer combination will provide simultaneous retrievals of AOD, aerosol layer height, aerosol composition, and aerosol single scattering albedo. This suite of aerosol products can be applied in obtaining the near-surface particulate pollution information needed for air quality monitoring/human health applications *(Figure 4)*.

A host of applications will become possible in the next decade with the geostationary constellation for air quality. These include deriving top-down anthropogenic emissions on hourly time scales and enhanced monitoring of hourly particulate matter of 2.5 µm or less (PM2.5) observations globally. Taking the recent COVID-19 related economic shutdown as an example, where we were able to track the decreased mobility (and corresponding reduced vehicular emissions) using TROPOMI NO_2 measurements, the current limitation is this LEO instrument's once-daily coverage.

There is a diurnal cycle to NO_2 associated with emissions from traffic peaking in the morning and evening as well as photochemistry. This diurnal cycle is not captured from single-satellite LEO observations, and it is not known if emissions reductions due to the pandemic shutdown are fully represented by a polar-orbiting satellite observing at 1:30 PM local equator crossing time. These emissions changes observed by TROPOMI will likely help improve air quality models, but the hourly variations, which can only be provided by a geostationary platform, will still be lacking.

Another area for synergy is the use of the cloud mask product developed from one sensor in an algorithm to derive products for another sensor. Most geophysical parameters including aerosols and trace gases require a cloud mask to remove cloud contamination of the retrievals. For UV-VIS spectrometers that do not carry infrared wavelengths, it is difficult to derive a cloud mask just based on visible wavelengths. An example of such synergy currently exists between Suomi NPP Visible Infrared Imaging Radiometer Suite (VIIRS) and Sentinel 5P TROPOMI. The VIIRS cloud mask is used by some TROPOMI trace gas and aerosol retrieval algorithms. A similar synergistic approach could use a GEO-XO imager to remove cloud contamination in a GEO-XO UV-VIS spectrometer retrieval.

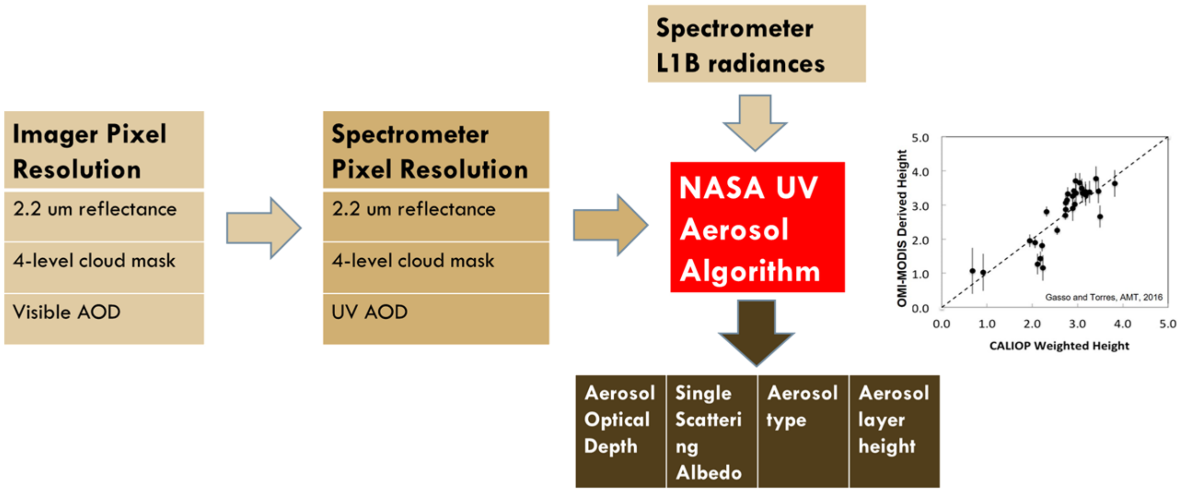


Figure 4. Schematic of a synergistic approach to retrieve a suite of aerosol products by combining measurements made by an imager and a spectrometer, either on the same platform or different platforms but viewing the same geographic location.

2.4. Advantages of GEO Observations for Atmospheric Composition Applications

AC applications in general will greatly benefit from increased temporal resolution geostationary measurements. A significant disadvantage of LEO is that it limits monitoring of fire emission dynamics, formation of photochemical smog, and how atmospheric transport and planetary boundary layer dynamics impact tropospheric composition. However, the benefit of GEO is not uniform across all AC products, and there may be tradeoffs in regard to vertical resolution between LEO and GEO. Thus, the overall improvement needs to consider all aspects of LEO versus GEO products.

Overall, GEO measurements promise an improvement in regards to fields that are useful when looked at in two dimensions and continuously across the day, including removing cloud contamination while measuring total columns and profiles of a number of trace gases, and retrieving aerosol properties. GEO allows observation while clouds pass underneath, providing many more opportunities for cloud free data collection. This is especially important for persistently cloudy regions and for techniques that are extremely sensitive to cloud contamination (e.g., measurement of SWIR in reflected sunlight for total column CO_2 and CH_4 as developed for GeoCARB).

These are characteristics of AC that will most benefit from a geostationary platform:

- Measuring O_3, aerosol, and aerosol precursors (e.g., NO_2, CH_2O), which have strong diurnal cycles in emissions and photochemical production.
- Fire/smoke evolution/injection height requires hourly to sub-hourly resolution or better.
- Net radiation, energy budget, and boundary layer dynamics vary diurnally, influencing transport of pollutants, wind speed and direction, cloud evolution, and other processes influencing AC.
- Products for the energy production sector on shorter timescales (minutes to 24 hours) including shortwave radiation (direct and diffuse) and wind speed and direction.
- Increased sampling in general decreases chances of data loss to clouds.
- Unique detailed information about spatial gradients and the evolution of plumes that can be used to infer emissions from urban areas and large point sources, e.g. for tracking accidental release of hazardous chemicals.

2.5. A Multi-spectral GEO Approach to Atmospheric Composition

Global observational capabilities of AC from polar-orbiting satellites are being met from the current missions (e.g., Sentinel series) and are expected to continue for the next 50 years with extensive planning by EUMETSAT with its Metop-SG (Second Generation) program. Additionally, plans are underway for geostationary AC measurements covering Europe and Asia. Unless GEO-XO folds in capabilities for AC instruments, the US will not have a comparable capability, especially after TEMPO ceases to make measurements. It should be emphasized that even assuming a successful launch and execution of TEMPO mission, it is still a NASA research instrument built with two years' life expectancy with an end date well before 2030.

Currently, NOAA cannot fully measure AC changes in the planetary boundary layer from space. The Cross-track Infrared Sounder (CrIS), a high-spectral resolution IR sounder instrument onboard Suomi NPP and NOAA-20, measures greenhouse gases such as CO_2 and CH_4 (Liu et al., 2016). However, comparison of these CrIS trace gas to aircraft observations made by NOAA and University of Maryland shows that the CrIS instrument does not have the capability to resolve the presence of these trace gases in the boundary layer/lower troposphere *(Figure 5)*. In order to measure the full tropospheric column of greenhouse gases such as CH_4, a space-based capability must extend beyond the typically measured thermal infrared region into the SWIR region. TROPOMI includes the methane SWIR bands and is able to detect CH_4 in the boundary layer, enabling the use of this LEO instrument for tracking emissions of CH_4 from a variety of sources (de Gouw et al., 2020). One of the many important effects of climate change is changes in fire activity due to changing rainfall patterns and land use and land cover characteristics. Fires emit large amounts of trace gases, of which CO is one of the main pollutants and a precursor for photochemical (O_3) smog. In the analysis of CO from fires for some recent wildfires, comparisons of CrIS with TROPOMI retrievals show that CrIS does not detect the enhancements to CO from intense fires whose plumes remain in the lower troposphere *(Figure 6)*. While globally patterns of CO observed by CrIS and TROPOMI are very similar, CrIS appears to be insensitive to CO changes in the lower layers of the atmosphere.

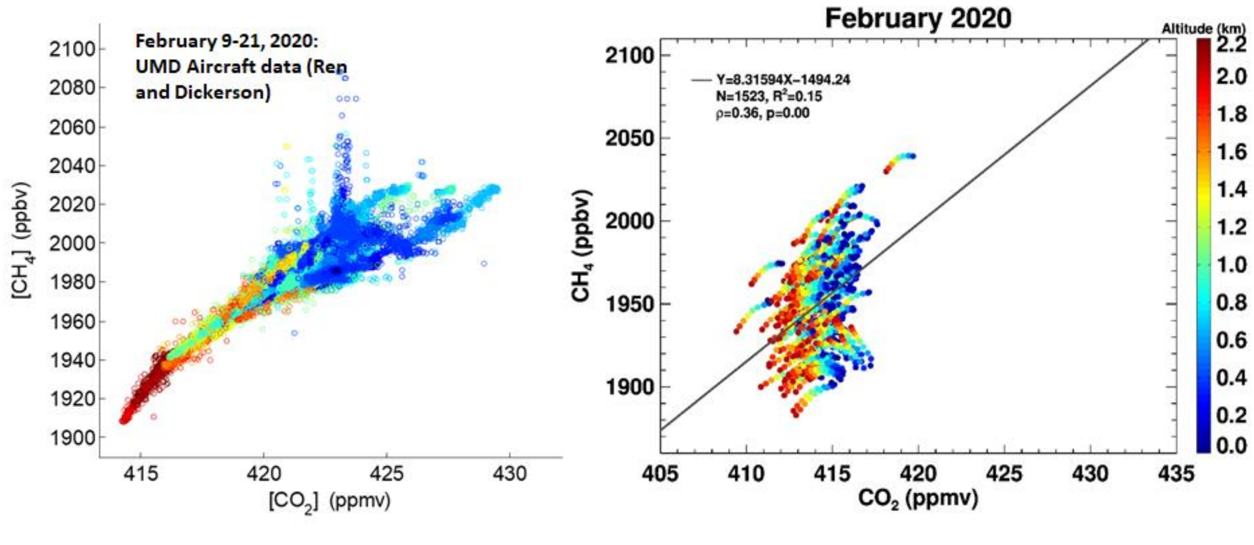


Figure 5. Correlation between CH_4 and CO_2 in the lowest 2.2 km observed by Suomi NPP CrIS during February 2020 in the Washington, DC metropolitan area. The CrIS CO_2 observations do not show the dynamic range and are limited to between 410 and 420 ppmv, while aircraft observations (left panel) show the dynamic range to be between 415 and 430 ppmv. Aircraft observations are courtesy of Russ Dickerson and Xinrong Ren of University of Maryland, College Park, MD, USA.

One of the key capabilities of a spectrometer in the UV-VIS-NIR is to determine aerosol and cloud layer height using oxygen A-band and B-band absorption. Algorithms to retrieve aerosol layer height using oxygen absorption have matured with the development of products from Deep Space Climate Observatory Earth Polychromatic Imaging Camera (DSCOVR/EPIC) and TROPOMI in preparation for TEMPO's launch (Xu et al., GRL 2017). The TROPOMI aerosol layer height is an operational product that is routinely used by users including NOAA to track the altitude at which smoke is being transported. This is critical information for operational air quality forecasters, as this information informs them whether their local/regional air quality will be impacted by long-range transport. The unprecedented fire activity induced by hundreds of lightning strikes in California during the late summer of 2020 released tons of smoke into the atmosphere that made its journey from California to eastern US. The TROPOMI aerosol layer height product *(Figure 7)* shows that while smoke in the vicinity of the fire sources was near the ground, the transport happened between 2 and 4 km, and in some places the transported smoke descended into the boundary layer, likely impacting air quality. The spectral coverage needed for aerosol layer height is in the oxygen bands centered at 764 nm (A-band) and 688 nm (B-band), with reference non-absorption bands nearby *(Figure 8)*. If the GEO-XO imager does not include these bands and the IR sounder covers only the thermal infrared, we will not have a capability to derive aerosol layer height in the GEO-XO era. Although there are some experimental smoke plume height algorithms using the 11-μm brightness temperature that have been applied to ABI using the Lyapustin et al. (2019) technique, the retrievals are made with a lot of assumptions (e.g., plume heights only for AODs > 0.5, plume heights are not accurate when smoke moves away from the source region, etc.) that break down easily.

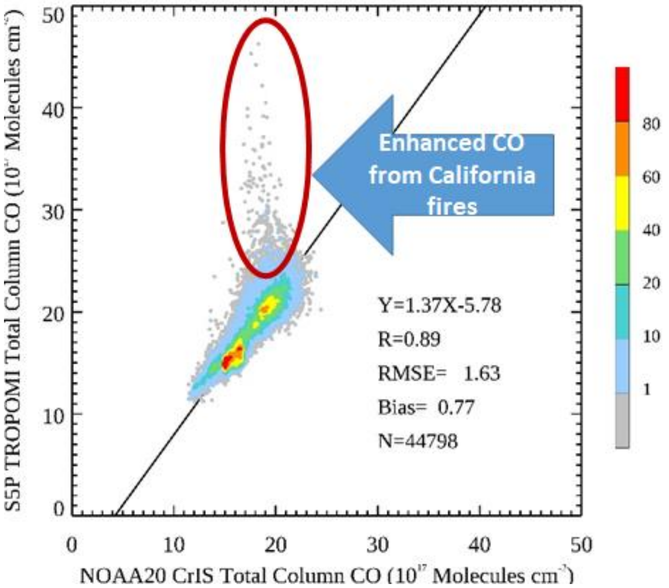


Figure 6. Comparison of NOAA-20 CrIS total column carbon monoxide with Sentinel 5P TROPOMI carbon monoxide for July and August 2018 over CONUS. This time period was marked by extreme fires in California.

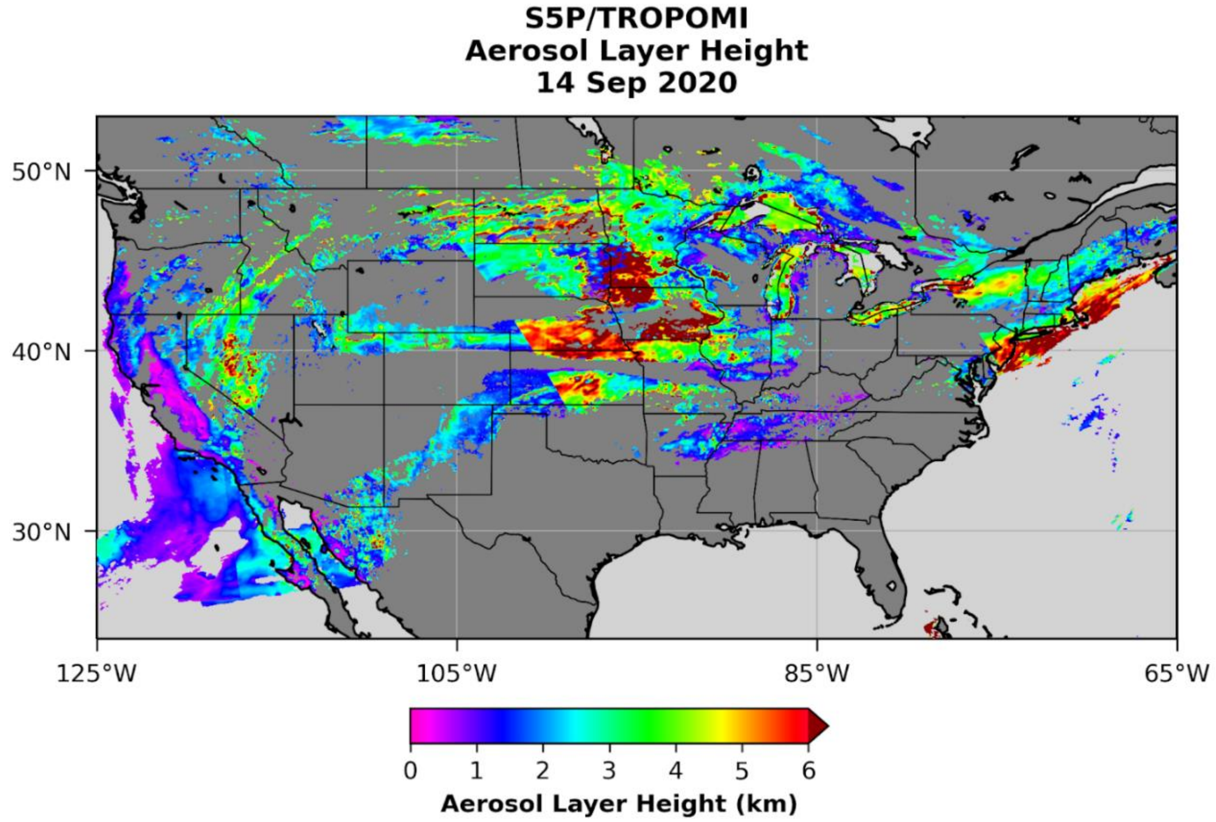


Figure 7. S5P observations of aerosol layer height for California fires on September 14, 2020. The layer height shows that smoke is close to the ground near the fire sources and is aloft when transported downwind. In some downwind regions smoke descended near the surface impacting local air quality.

Though an IR sounder is good for many weather applications (Barnet et al., 2004; Chahine et al., 2006; Wang et al., 2007), it falls short for AC. It can provide distributions of some greenhouse gases and some air quality relevant trace gases, but only in the upper troposphere. A sounder alone would not meet the AC requirements needed for air quality and climate applications. Smoke from fires, dust storms, and anthropogenic pollution changes rapidly and can be driven by weather and chemistry on sub-diurnal scales. This changing air quality and AC can only be monitored accurately with a geostationary satellite. As discussed in detail in *Section 3.2.3*, photochemical smog precursors like NO_2, CH_2O, $C_2H_2O_2$, etc. have a significant diurnal variation. These compounds absorb in the UV-VIS spectral region, and therefore an instrument with spectral coverage in the UV-VIS is essential to monitor these smog-inducing compounds. Asia and Europe are ready for this challenge as they have already identified their AC missions. It is essential for NOAA to join Europe and Asia by adapting NASA's TEMPO or ESA's TROPOMI as an AC instrument for GEO-XO.

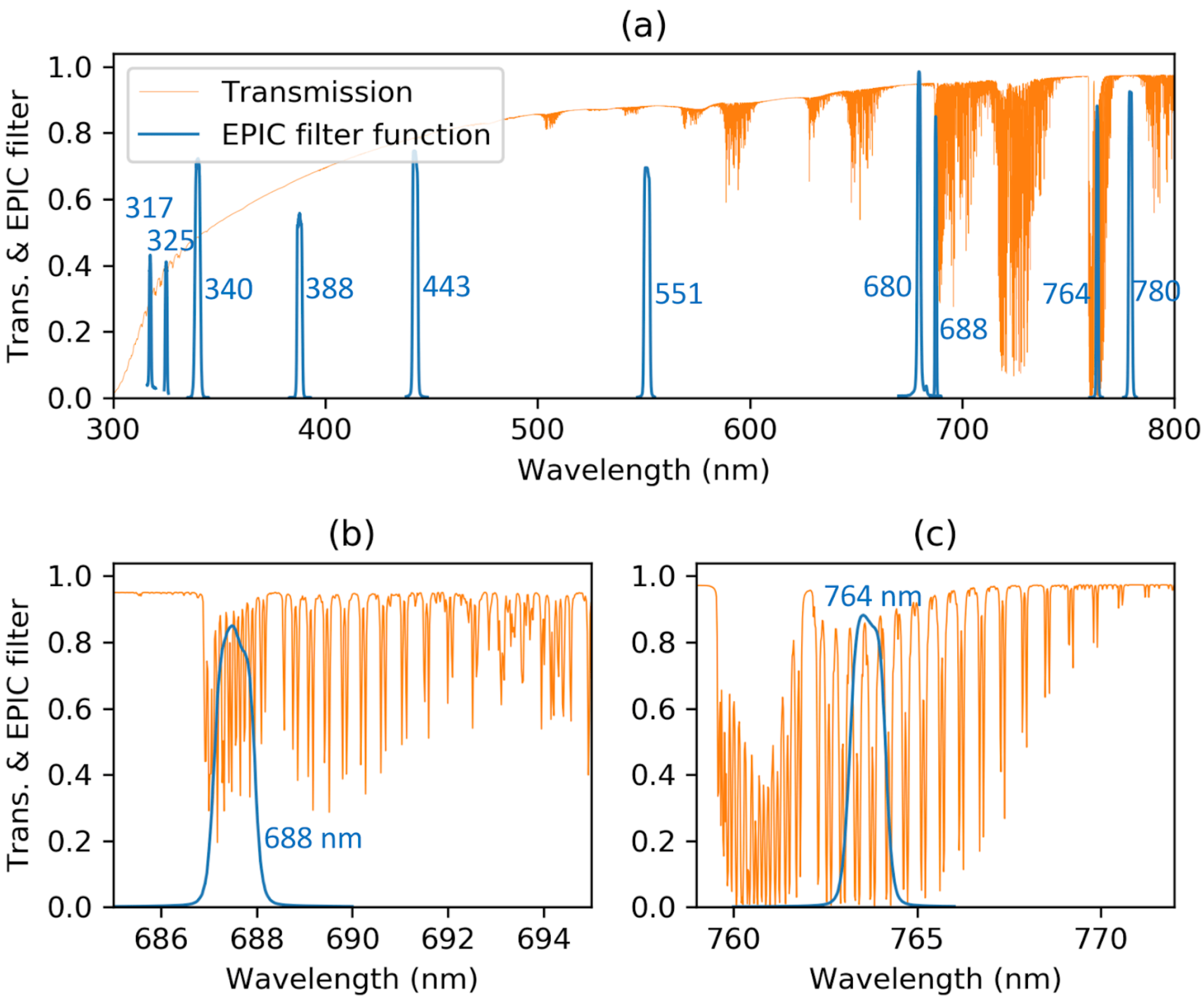


Figure 8. Transmittance function for the EPIC spectral coverage to illustrate the oxygen A-band and B-band spectral coverage needed for aerosol layer height retrieval. EPIC is a 10-channel spectroradiometer operating on NOAA's DSCOVR platform at the Lagrange-1 point.

3. NOAA’s Atmospheric Composition Applications and the Value of GEO-XO Capabilities

AC observations are critical to meet NOAA’s “weather and water” mission. NOAA’s forecasting applications include forecasts for air quality, weather and climate, fire weather, and hazards, while NOAA monitoring activities include stratospheric O_3, GHGs, and air quality. AC monitoring also includes NOAA’s efforts in developing foundational understanding of the Earth System, which in turn feeds into more operational activities. This science application (carried out largely within NOAA’s Office of Oceanic & Atmospheric Research [OAR]) would both benefit from GEO-XO capabilities and would help improve them, via in-situ data validation.

These seven NOAA application areas will benefit from the GEO-XO observables listed in *Table 1*. The following sections describe each application area in detail and highlight the GEO-XO AC observation products that will benefit each application.

3.1. Forecasting Applications

NOAA's forecasts predict changes in a variety of natural systems in response to drivers such as climate variability, extreme weather conditions, anthropogenic activity, natural disasters, and/or hazards. These forecasts can also provide information about how communities and economies may be affected. Local authorities and members of the public rely on these timely warnings to make decisions to protect the health and well-being of a particular area. AC informs forecasting operations at nearly all of NOAA’s line offices, particularly the National Weather Service (NWS), National Marine Fisheries Service (NMFS), National Ocean Service (NOS), and OAR *(as seen in Section 2.1.2)*.

AC predictive capabilities are explicitly called for in Annex 10 of the FY19-21 Strategic Implementation Plan (SIP) for Evolution of Next Generation Global Prediction System (NGGPS) to the UFS, (NWS, 2020a) as part of the suite of physical parameterizations, including the interaction of AC with other physical parameterizations through radiative impacts and wet and dry deposition processes. Data assimilation for atmospheric composition is also explicitly called for in the SIP. It is recognized that an “atmospheric composition data assimilation system is critical for constraining not only atmospheric composition species and aerosol size and number concentrations (chemical data assimilation or CDA), but also the emission (emission data assimilation or EDA).”

3.1.1. Air Quality Forecasting

Although weather-related fatalities in the US amount to around 500 each year (NWS, 2020b), over 100,000 premature deaths occur annually due to exposure to elevated concentrations of O_3 and PM2.5 (Fann et al., 2012) *(Figure 9)*. The components of air pollution, such as O_3 and fine aerosol particles (e.g., PM2.5), have myriad impacts on respiratory and cardiovascular health. Poor visibility, particularly from dust or wildfires, impacts air and ground transportation. Further, air quality in many parts of the US is predicted to degrade under most climate change scenarios if more stringent emissions reductions are not instituted. Indeed, wildfires and dust storms have increased in past decades and this trend is expected to continue as temperatures increase and precipitation shifts. Poor air quality is also detrimental to agriculture, both from direct impacts of O_3 on vegetation as well as the decrease in visible solar radiation needed for photosynthesis. Solar energy production will be hampered by smoggy conditions where aerosols scatter incoming solar radiation away from the surface. Air quality forecasts are used to understand the impacts of air quality regulations and the long-range transport of pollutants, along with their resulting health and environmental outcomes.

Mandated by Congress under provisions of the Energy Policy Act of 2002, NWS has provided forecast guidance for surface air quality over the US through NAQFC since 2004. NAQFC was developed through a collaborative effort between the NOAA Air Resources Laboratory, the NWS National Centers for Environmental Protection (NCEP) and the US EPA and began, in 2004, providing next-day forecasts of surface O_3 concentrations over the northeastern US. Currently, as a result of close collaboration between the OAR laboratories, NCEP and the National Environmental Satellite, Data, and Information Service (NESDIS), NAQFC provides 48-hr operational air quality forecast guidance for surface concentrations of O_3 and PM2.5 across the entire US, including Alaska and Hawaii, as well as standalone forecasts for smoke and dust, as both surface concentrations and vertically integrated column values. Current dust and smoke forecasting operations are provided by three models -- HYSPLIT (CONUS, Alaska, Hawaii), CMAQ (CONUS, Alaska, Hawaii), and GEFS-Aerosols (Global Ensemble Forecast System with Aerosols)—all of which can benefit from GEO observations, such as dust detection, fire detection and characterization, aerosol optical depth, and surface conditions.

These forecast guidance products are used by numerous state, local and tribal governments to provide official air quality forecasts, public advisories and air quality alerts in communities all across the country that are collected by the US EPA in the form of the Air Quality Index (AQI) national maps (AirNow, 2020). Other stakeholders for NAQFC products include the National Park Service (NPS), Federal Aviation Administration (FAA), the Department of Transportation's Federal Highway Administration (DOT/FHWA), and the Centers for Disease Control (CDC).

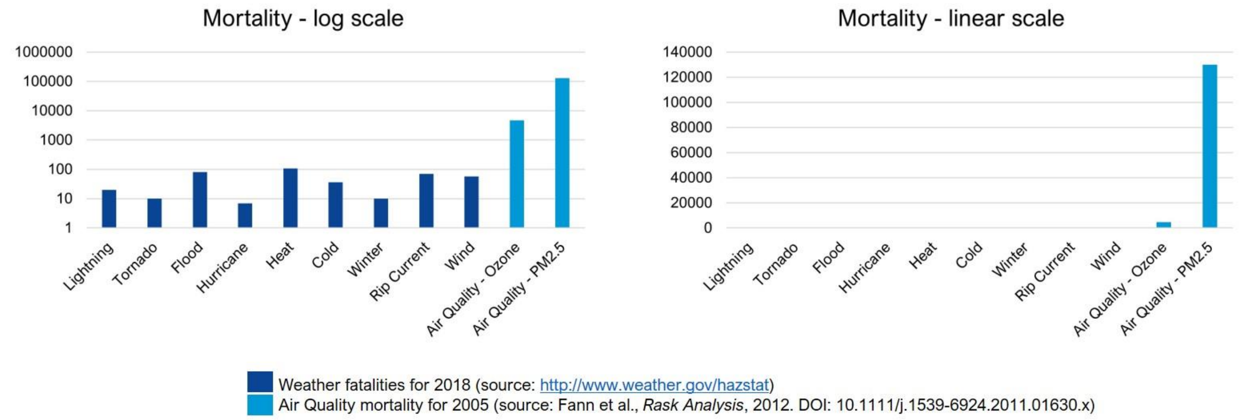


Figure 9. Annual mortality in the US due to poor air quality and all weather phenomena. Data gathered from NWS (2020b) and Fann et al. (2012).

Data from GEO-XO satellites hold the potential for significantly enhancing the capabilities of both NAQFC air quality and UFS composition forecast guidance. Additional AC data, including both trace gas species and aerosols, would benefit the forecasting efforts by allowing more comprehensive evaluations of the forecast models, thereby helping to improve their scientific basis. GEO-XO observations of AC could also be utilized in global and regional chemical data assimilation systems. Assimilation of GEO-XO trace gases and aerosols within regional NAQFC will allow for improved initialization. Assimilation of GEO-XO trace gases and aerosols within the UFS, as part of a global observing system, will help constrain lateral boundary conditions for regional NAQFC models during an individual forecast cycle, leading to more accurate forecasts. An example of CMAQ model aerosol assimilation study using GOES hourly AOD vs. MODIS once-a-day AOD is shown in *Figure 10*. Time series of predicted surface PM2.5 by CMAQ model compared to observations for base case, simulation with GOES AOD assimilation, and simulation with MODIS AOD assimilation shows that model predictions are close to observations when mini cycles updating model initial conditions using GOES AODs are performed.

Regional OSSEs have been conducted to assess the impact of geostationary hyperspectral IR, UV, and VIS O_3 retrievals on O_3 analyses as part of the NASA GEO-CAPE pre-mission formulation studies (GEO-CAPE 2018). These studies demonstrated that multi-spectral (IR-UV-VIS) retrievals provided the best constraints on regional O_3 analyses compared to either UV-VIS or UV-only retrievals. These studies demonstrated that the largest impacts on day-time surface O_3 analyses were obtained from assimilation of hyperspectral IR O_3 retrievals during the previous evening. This is because daytime O_3 concentrations are mostly driven by in-situ O_3 production, which is determined by the abundance of O_3 precursors.

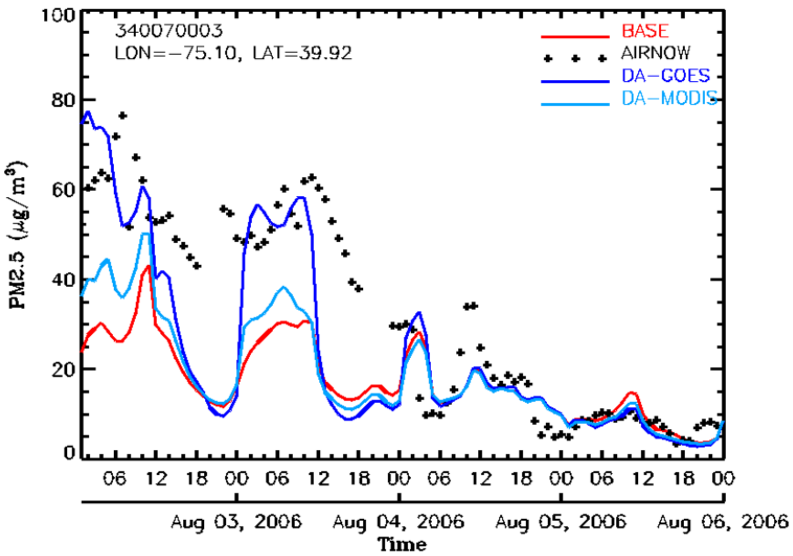
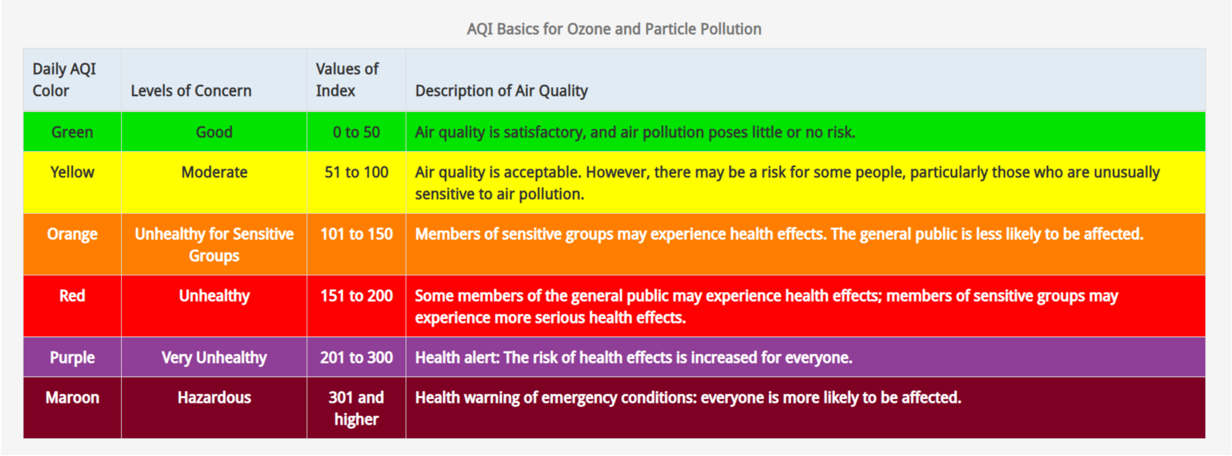


Figure 10. Time series of predicted and observed PM2.5 concentrations for base case (red), GOES AOD assimilation (blue), and MODIS AOD assimilation runs (cyan blue) show that hourly assimilation of AOD improves forecast over once-a-day assimilation of MODIS (Kondragunta, unpublished).

Regional Observation System Experiments (OSEs) have been conducted to assess the impact of TROPOMI UV-VIS NO_2 retrievals, which serve as a proxy for future geostationary TEMPO or GEO-XO UV-VIS NO_2 retrievals, on O_3 predictions using the NAQFC. These studies showed that monthly averaged analysis increments from TROPOMI NO_2 assimilation could be used to provide timely updates of NAQFC anthropogenic NO_x emission inventories, which lead to improved O_3 forecasts in a number of metropolitan areas including Los Angeles and New York City. Hourly measurements of tropospheric NO_2 abundances would provide additional constraints on mobile source emissions, including improved representation of daily traffic flow patterns. Higher sampling rates in general would also lead to less data loss due to cloud contamination.

Moreover, other data products from GEO-XO may provide improved inputs to the forecast models (e.g., better detection of wildfires and their intensities helping to improve smoke emissions estimates). More accurate air quality forecasts over the US facilitated by new GEO-XO capabilities will have the direct societal impact of helping to save lives as a result of reduced exposure to unexpected severe air pollution events. For example, hospital admission rates associated with poor air quality could be reduced when predictions are available by avoiding outdoor activities.

The US EPA issues a daily AQI for five criteria pollutants. Of these five, the most critical ones are for O_3 and PM2.5. While AQI is provided based on observations and/or numerical model guidance, it is up to each jurisdiction (typically regions with a population greater than 350,000) to develop and provide the AQI to its public *(Figure 11)*. Satellite data play a critical role in this process. For example, air quality models use satellite detected fire emissions as input to predict smoke. Forecasters also use satellite products (imagery) provided through NOAA websites in conjunction with observations and model guidance to provide their daily AQI warnings and watches. AC capabilities in the GEO-XO era will advance the reliance on satellite data from "yesterday's observations" to "today's observations."



AQI Basics for Ozone and Particle Pollution

Daily AQI Color	Levels of Concern	Values of Index	Description of Air Quality
Green	Good	0 to 50	Air quality is satisfactory, and air pollution poses little or no risk.
Yellow	Moderate	51 to 100	Air quality is acceptable. However, there may be a risk for some people, particularly those who are unusually sensitive to air pollution.
Orange	Unhealthy for Sensitive Groups	101 to 150	Members of sensitive groups may experience health effects. The general public is less likely to be affected.
Red	Unhealthy	151 to 200	Some members of the general public may experience health effects; members of sensitive groups may experience more serious health effects.
Purple	Very Unhealthy	201 to 300	Health alert: The risk of health effects is increased for everyone.
Maroon	Hazardous	301 and higher	Health warning of emergency conditions: everyone is more likely to be affected.

Figure 11. The US EPA guidelines for daily AQI alerts.

A GEO-XO mission would therefore improve NOAA's air quality forecasting and the products provided to its stakeholders by incorporating the following instruments and products:

- A VIS-IR imager providing information on fires and aerosol type and optical depth, which is especially important for NAQFC fine particulate matter guidance.
- Multi-spectral (IR-UV-VIS) O_3 retrievals for better constraints on regional O_3 analyses.
- UV-VIS NO_2, CH2O, and $C_2H_2O_2$ retrievals for timely updates and better constraints on anthropogenic NO_x VOC emission inventories, along with aerosol index and aerosol layer/mixing height, for improved NAQFC O_3 and fine particulate matter forecast guidance.

Additional details of these capabilities are discussed in *Section 3.2.3*.

3.1.2. Weather and Climate Forecasting

The composition of the atmosphere leading to the greenhouse effect is what makes life as we know it possible on Earth. Aerosols directly impact Earth's energy budget by absorbing or scattering incoming shortwave or outgoing longwave radiation, depending on the size of the particles and the specific mix of chemical components in the aerosol. Aerosols also can indirectly affect the energy budget through changes in snow albedo (i.e., through the deposition of dark soot on snow and ice surfaces). Aerosols also impact cloud microphysics by changing the formation and droplet composition of clouds, and therefore indirectly control cloud lifetimes and radiative properties. Additionally, many trace gases (including but not limited to CO_2, CH_4, O_3 and water vapor) absorb and reemit longwave radiation. The net radiative effects from these compounding factors drive a number of processes relevant on both weather and climate timescales. These include land-atmosphere interactions with impacts on the water cycle, boundary layer dynamics, cloud and precipitation development, and subsequent feedbacks from these processes.

Weather and climate forecasting are mission-critical activities of NOAA that broadly inform the nation's social and economic welfare. Currently the operational weather and climate forecast systems at NWS NCEP use climatological parameterizations for aerosols and most trace gases (O_3 and water vapor are prognostic variables). As part of NOAA's effort to move towards a UFS, medium-range weather (MRW) and subseasonal-to-seasonal (S2S) modeling applications are incorporating fully-coupled Earth systems (atmosphere + land + ocean + sea ice + waves + atmospheric composition). NOAA has already invested heavily in these improvements, with current support from the UFS Research-to-Operations (R2O) project, and a variety of OAR funding streams. OAR, NWS and NESDIS spent the past five years developing the GEFS-Aerosols model, coupling the Goddard Chemistry Aerosol Radiation and Transport (GOCART) aerosol model to the Global Forecast System FV3-based atmospheric model to provide prognostic aerosol species. GEFS-Aerosols was implemented in operations in September of 2020, with aerosol forecasts to 5 days and plans to extend to S2S ranges through UFS R2O funding. In recent NCEP testing, GEFS-Aerosols demonstrated a big advancement in skill over prior NOAA global aerosol forecasts and comparable to multi-model ensembles that use aerosol data assimilation.

The operational UFS global model relies heavily on satellite products, including aerosol optical depth and inputs to emissions calculations for trace gases and aerosols, for initialization and verification. In the future, greenhouse gases will also ultimately be included in the UFS, in order to provide forecasts out to even longer timescales. Such advancements must be pursued if the US intends to match global modeling capabilities at peer institutions such as the Copernicus Atmosphere Monitoring Service (CAMS) at the European Centre for Medium-Range Weather Forecasts (ECMWF).

Through 2019 Disaster Supplemental appropriations, Limited Area Model (LAM) 3-km resolution Short Range Weather (SRW) forecasts of the FV3-based UFS are now underway. The FV3-LAM model incorporates a much more sophisticated description of gas phase and aerosol chemistry than GEFS-Aerosols, with the aim of providing air quality forecast guidance for the CONUS within the next-generation NAQFC. A key feature of the FV3-LAM SRW forecasts is that they will allow for two-way coupling of the chemistry and meteorology, so that the chemical composition affects radiative transfer and cloud microphysics. Current development of the FV3-LAM SRW focuses on capturing the aerosol radiative and microphysical impacts of the aerosols produced by wildfire smoke. Once this infrastructure is in place, future FV3-LAM improvements may extend these algorithms to the full range of anthropogenic and natural sources and their subsequent chemical complexity.

GEO-XO observations would be used to both verify and better initialize forecasts of aerosols and trace gases as part of the UFS coupled global weather and climate prediction systems. These improved global model fields would then provide better boundary conditions for regional air quality applications. Observations of aerosols and trace gases from geostationary platforms could also be used to improve the quality of retrievals from satellite radiance observations from NESDIS by incorporating additional information on the spectral absorption in each atmospheric profile. In particular, accurate soundings of atmospheric state variables such as temperature or water vapor require co-retrieval of trace gases, such as CO_2 and CH_4, which absorb in the same parts of the IR spectrum as water vapor. Similarly, information on the spatial distribution of O_3, NO_2, and aerosols is needed to accurately simulate incoming shortwave solar radiation, a critical variable needed in forecasts generally as well as a key input used by the solar energy industry. GEO observations of trace gases and aerosols are therefore integral to improvement of key meteorological inputs controlling weather and climate forecasting systems. The ability to resolve radiative effects in the UFS through more accurate depictions of aerosol and trace gas species will ultimately lead to improved forecast skill, benefiting stakeholders at all levels of government and the general public.

In summary, GEO-XO instruments and products that would benefit NOAA's weather and climate forecasts include:

- A VIS-IR imager to capture fire behavior and emissions, AOD and aerosol type.
- TIR and SWIR soundings of greenhouse gases.
- O_3 retrievals in the UV/VIS/IR.

- Aerosol index and layer height retrievals in the UV-VIS.
- UV/VIS products for O_3 and aerosol precursors (e.g., NO_2, CH_2O, $C_2H_2O_2$).

3.1.3. Fire Weather Forecasting

While fire weather forecasting combines both air quality and weather forecasting, it is important to acknowledge separately because of its unique niche at NOAA and the wide group of stakeholders for NOAA's fire products. Using a combination of its LEO and GEO satellite observations, NOAA makes operational predictions of fire location, behavior, emissions, duration, strength, interactions with meteorology, and air quality impacts. Current operational model systems treating fires and their impacts include NAQFC-CMAQ, HRRR-Smoke, GEFS-Aerosols, and others. Fires are an increasing cause of poor air quality in many parts of the US. Fire smoke has direct impacts on radiative forcing, influencing weather and climate. Interactions of smoke aerosols affect cloud formation, and inclusion of these interactions may help to improve precipitation forecast by numerical weather prediction models. Satellite monitoring of the vegetation state is used to determine the conditions of biomass fuel and to help forecast wildfire risk. Satellite AOD and trace gas measurements can be used in inversion/data assimilation studies to estimate fire emissions. NOAA has contributed extensively to research investigating the linkages between climate change, fire activity, and air quality. NOAA's visibility forecasts rely on fire products to accurately predict conditions for ground and air transportation. NOAA must capture the impacts of fire plumes in its forecasts of surface radiance for solar energy production. As in air quality and weather/climate forecasting, there is a growing number of activities at NESDIS, NWS, and OAR and collaborations between these line offices to develop and generate fire satellite products and to build improved descriptions of fires in NOAA's operational modeling systems. Stakeholders for NOAA's fire weather products include a wide variety of federal agencies (US EPA, USFS, NASA, CDC, etc.) and many state and local partners (first responders, incident meteorologists, environmental regulators, and decisionmakers), as well as the private sector and the general public.

Wildland fire emissions vary dramatically in space and time due to fuel and weather conditions, human activities, and fire suppression. It is paramount that the location and intensity of the fires are monitored continuously and that these data are ingested into fire weather and air quality models (e.g. HRRR-Smoke, NAQFC-CMAQ) in real time with minimum latency. Assimilating high-frequency fire radiative power (FRP), AOD and trace gas measurements from the same geostationary satellite will likely greatly improve the accuracy of fire weather and air quality forecast models in the future. Additionally, assimilating the state of vegetation, weather conditions and lightning rates into future fire weather and air quality models will help to improve forecasts of wildfire danger risk, fire spread and fire emissions.

An inverse modeling system, the HYSPLIT-based Emissions Inverse Modeling System for wildfires (or HEIMS-fire), has been developed at NOAA/OAR/Air Resources Laboratory (ARL) in collaboration with NOAA/NESDIS (Kim et al, 2020). The system estimates wildfire emissions using the transport and dispersion of smoke plumes at hourly or higher temporal resolutions captured by GOES aerosol products. A quasi-operational smoke forecasting system is being developed at ARL to test smoke emissions estimates based on the VIIRS and GOES-16/17 ABI aerosol and smoke products. The wildfire smoke emissions estimated by assimilating aerosol and smoke products from multiple satellites are expected to benefit other forecast systems such as HRRR-Smoke and NAQFC-CMAQ systems, which are much more expensive to run and cannot easily assimilate the satellite observations directly at this time. It should be noted that current satellite smoke products provide only surface or column information. Adding smoke layer height retrievals or providing vertical profiles through additional sensors would enable more constraints on model forecasts. A demonstration of such an inverse system by Chai et al. (2017) used volcanic ash cloud top height observations to improve volcanic ash predictions.

Fire detections, quantitative estimates of FRP, and fire size information for the GEO-XO AC mission will come from the meteorological imager in the 3.9 µm band at 1 km or better spatial resolution, compared to a longwave window band. A combination of imager and UV-VIS-IR spectrometer measurements will be needed to synergistically interpret the observations of smoke and trace gases emitted from fires. There are many methods to derive emissions to be ingested into models, and research is ongoing on how to model fire behavior in the forecast time period. By the time that GEO-XO spacecraft are in orbit, research will likely have advanced to assimilate current observations of fire characteristics in order to forecast fire behavior for the next 24 or 48 hours, depending on the model configuration.

3.1.4. Hazards Forecasting

This section focuses on response to episodic high-risk events in which a hazardous substance is released into the atmosphere with the potential to cause immediate, severe harm. Prediction responsibilities for volcanic ash, smoke, dust, radioactive and hazardous material are assigned to NOAA. NOAA is the primary Department of Commerce (DOC) agency to assist Federal, state, & local organizations responding to a radiological emergency. Dust dispersion forecasts are covered in *Section 3.1.1*, while fire/smoke dispersion forecasts are discussed in *Section 3.1.3*.

Satellite products play an important role in detecting, monitoring, and informing forecasts for these events. Observations with high temporal resolution are critical as these events occur unpredictably and often exhibit large variations over the course of minutes to hours. Observations and dispersion forecasts are used to aid in the development of evacuation and no-fly zones. Uncertainties in the forecasts are usually high due to uncertainties in the source term (initial position and quantity of substance), meteorological fields used to drive the dispersion model, and the dispersion model parameterizations. Even modest improvements to the forecasts could save lives and produce significant economic savings. For these applications, improvements to weather forecasting, particularly wind speed and direction and planetary boundary layer height, will lead to corresponding improvements to dispersion forecasts. Satellite products may be used to significantly improve the estimation of the source term for some hazard forecasting applications.

3.1.4.1. Volcanic ash

Volcanic ash is a major aviation hazard. The transfer of ARL transport and dispersion capabilities to the NWS was prompted by the 1989-1990 eruptions of Redoubt Volcano in Alaska, during which a jet unknowingly flew into the ash cloud on approach to Anchorage, temporarily losing all engines.

NOAA operates two of the nine Volcanic Ash Advisory Centers (VAACs) in the world. The VAACs issue VAAs to the aviation community (i.e., FAA and airline companies) in accordance with International Civil Aviation Organization (ICAO) International Airways Volcano Watch (IAVW) standards, which are defined in Annex 3 to the Convention on International Civil Aviation (ICAO, 2007) and further detailed in the Handbook on the IAVW. Currently, VAAs consist of polygons denoting where ash is thought to be present at the time of VAA issuance, as well as 6, 12, and 18 hours in the future. In addition to the VAACs, meteorologists at the NOAA Meteorological Watch Offices issue Significant Meteorological Information warning messages (SIGMETs) for volcanic ash which impacts the US.

Aviation stakeholders, through the appropriate ICAO and World Meteorological Organization (WMO) bodies, have emphasized the need for more quantitative VAAs that can support quantitative risk management systems, as the risk to aircraft is now known largely to be a function of the ash concentration and cumulative exposure time. As a result, ICAO Annex 3 updates in 2023, 2026, and 2029 are scheduled to include modifications to the IAVW that results in more quantitative VAAs, including the provision of ash concentration charts and a quantitative volcanic SO_2 information product (CGMS-48). Future VAAs will also include information on uncertainty. The provision of high quality quantitative VAAs is an enormous challenge that requires sophisticated observational and modeling capabilities.

Although volcano observatories operated by the USGS and other entities monitor some volcanoes using instruments such as seismographs and webcams, satellite observations still provide the primary means of detecting and monitoring eruptions. The high temporal resolution of GEO-XO products is highly beneficial because ash can reach cruising altitudes within tens of minutes of an eruption and prompt detection and issuance of advisories is a priority. Because of the large amount of satellite data and number of volcanoes that need to be monitored, automatic alerts generated from satellite data are an increasingly important tool for analysts. Such alerts need to maintain a very low false alarm rate (Pavolonis et al., 2015).

The VAA polygons at 6, 12, and 18 hours are derived from atmospheric transport and dispersion model forecasts, usually heavily curated by analysts. Several modeling techniques which rely on the availability of high-quality satellite products that estimate column mass loading and ash height have been developed, and their implementation is critical to providing reliable quantitative forecasts of volcanic emissions (Crawford et al., 2016; Chai et al., 2017). Reliable quantitative nowcasts of ash concentrations will require estimates of column mass loading and top height obtained from satellite retrievals, as well an estimate of cloud thickness, which may be obtained from model output or some simpler algorithm. In most cases, without satellite products to help constrain the source term, simulated ash concentrations will have uncertainties of several orders of magnitude.

Pavolonis et al. (2015) describe the algorithm developed to detect volcanic ash and retrieve ash cloud properties. The main instruments are listed in Table 2 of

Pavolonis et al. (2015) and include AVHRR, COMS-MI, GOES-R ABI, Himawari, MODIS, MTSAT imager, MSG SEVIRI, MTG FCI, and VIIRS. The combinations of spectral channels utilized for each imager are shown in Table 1 of Pavolonis et al. (2015). In general channels centered near 0.65, 3.9, 7.3, 8.5, 11 and 12 µm are employed. A GEO-XO imager with similar channels will be fundamental to future improvements to VAAs. A GEO-XO UV-VIS spectrometer would add quantitative constraints on the intensity and temporal variability of emitted SO_2.

3.1.4.2. Chemical Releases

Weather Forecast Offices (WFOs) are a critical part of the response to the release of a hazardous material into the atmosphere. Examples of such cases include refinery fires and train derailments. In addition to providing more frequent local weather forecasts and helping to disseminate information to the public, the WFOs may provide dispersion model output to emergency managers. WFOs often run the dispersion model multiple times utilizing different source terms and meteorological data and assess the output by comparing with any available observations. Surface measurement stations can often be quite helpful in providing observations of many hazardous or toxic compounds (including NO_2/NO_x, benzene, toluene, xylene, SO_2, and hydrogen sulfide) that can monitor the plumes from these chemical release events and validate dispersion modeling of the plumes. Some events are large enough that the plume can be observed from space in the visible and near infrared. The combination of a GEO-XO imager and UV-VIS spectrometer could provide validation of dispersion model predictions of pollutants and provide guidance on where to place mobile ground monitoring stations which are sometimes used.

Oil spills from offshore platforms and tankers are another form of hazardous chemical releases closely monitored by NOAA. The 2010 Deepwater Horizon oil spill is regarded as the largest marine oil spill in the history of the petroleum industry. When the accident occurred, NOAA was able to quickly redirect its WP-3D Orion aircraft to assess the incident. Remarkably, the aircraft happened to be conveniently outfitted with chemical instruments for an extensive field campaign that was taking place in California at the same time. As part of a multi-agency effort, scientists from NOAA's Chemical Sciences Division (CSD) were able to utilize a suite of complementary instruments in order to provide a much-needed preliminary analyses which showed health risks to workers were not as great as originally feared. They were able to characterize individual black carbon particles using the chemical instruments aboard (e.g. NOAA's single-particle soot photometer, for more information, see CSL 2011a and CSL 2011b).

Time-sensitive situations like this one could have benefited from a geostationary satellite whose AC products had the necessary temporal frequencies to assess the dire situation without relying on the good fortune of a well-timed field campaign. Given the unpredictable chemical nature of such chemical releases, the most comprehensive suite of GEO-XO AC instruments would be ideal. If the event is large enough, the combination of a GEO-XO imager and spectrometer could be used to detect plumes and provide quantitative information on concentrations of a variety of pollutants. These data would be important inputs and constraints to hazard dispersion models.

3.1.4.3. Radiological Releases

Regional Specialized Meteorological Center (RSMC) Washington, along with RSMC Montreal (operated by the Canadian Meteorological Centre), provide meteorological guidance and dispersion predictions using their respective models in the event of an atmospheric release of radioactive or hazardous materials crossing international boundaries in North, Central, and South America. OAR Air Resources Laboratory, together with NOAA's NWS/ NCEP, comprise the Washington RSMC for transport and dispersion products through WMO. Details on model products are given in WMO Technical Document No. 778 and include air mass trajectories and dispersion forecasts of 24-hour average exposure and deposition for 3 days (WMO, 2014).

The Department of State and NOAA entered into a Memorandum of Agreement for projects to make in-kind contributions to the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO) on September 20, 2012 in accordance with the NOAA Backtracking Support to CTBTO Statement of Work of July 11, 2012. Through this project, an operational on-demand backtracking capability was implemented at NOAA to provide potential source locations to CTBTO.

Accurate global weather forecasts are key for the dispersion forecasting and backtracking capability. These applications will benefit enormously from the improvements in the forecasting of boundary layer dynamics and precipitation fields described in *Section 3.1.2*. Thus, the improvements to weather forecasts resulting from a combination of GEO-XO imager and UV-VIS-NIR spectrometer would benefit dispersion forecasts of releases of radiological and other hazardous materials.

3.2. Monitoring Applications

Monitoring and observations constitute a large portion of NOAA's service to the Nation and the international community. In the context of AC, NOAA monitors and reports on the recovery of stratospheric O_3, tracks global levels of greenhouse gases, and monitors air quality for both currently identified and potentially emerging pollutants. Monitoring not only upholds legislation and international mandates, but also informs and supplements observation systems managed by national and global partners.

AC monitoring within NOAA OAR includes an extensive effort of in-situ and remote (ground and aircraft based) observations that are both routine and ad hoc, such as focused field campaigns involving the NOAA WP-3 and Twin Otter aircrafts. For all applications described below, corresponding field campaigns can and do benefit from current NOAA satellite systems (e.g., fire detections and radiative power that helped guide deployment of research aircraft during the Fire Influence on Regional to Global Environments and Air Quality [FIREX-AQ] field campaign), and would benefit even more from high frequency observations from a geostationary platform. In turn, focused OAR field campaigns with detailed measurements of AC offer a great opportunity for validation of satellite products.

3.2.1 Stratospheric Ozone Monitoring

Stratospheric O_3 is a naturally-occurring gas that filters most of the sun's UV radiation from reaching the surface. Reductions in stratospheric O_3 allow more damaging UV-B radiation to reach the Earth's surface, potentially harming plants and animals and impacting human health and agriculture.

Increases in transport of O_3 from the stratosphere, as may occur with global climate change, can degrade tropospheric air quality. The distribution of stratospheric O_3 also has been shown to affect tropospheric weather conditions on seasonal to sub-seasonal time scales, as well as impacting large scale circulation patterns. Continual monitoring of stratospheric O_3 with good global coverage on weekly to monthly time scales will feed into improved understanding of radiative and dynamical processes and feed into improved seasonal to sub seasonal forecasts. Furthermore, one future concern regarding stratospheric O_3 is how it may be impacted by climate intervention methods that introduce excess aerosols into the stratosphere. For this reason, maintaining vertically and spatially resolved satellite measurements of both O_3 and aerosol is critical, as are measurements of other chemically and radiatively active species in the stratosphere. High temporal resolution is not essential for long-term albedo modification monitoring, but fairly high vertical resolution can help to establish causes for observed changes.

The US Clean Air Act mandates that NOAA and NASA regularly report on the state of the stratospheric O_3 layer to Congress. The Montreal Protocol also requires periodic updates on new scientific findings related to the O_3 layer to guide policymakers making decisions about changes to strengthen the agreement. NOAA has played a major role in preparing these assessments, which require satellite data in addition to ground-based and balloon-borne observations to monitor the health of the stratospheric O_3 layer. Stakeholders of NOAA's stratospheric O_3 monitoring include numerous Federal agencies (NOAA, NASA, EPA, USDA), the private sector (agricultural interests), and a variety of international bodies (parties to the Montreal Protocol, UNEP, WMO, and the World Climate Research Programme [WCRP]).

NOAA Solar Backscatter Ultraviolet (SBUV) O_3 profile and total column observations detected the beginning of the O_3 hole development in the Antarctic, provided quantification of the global stratospheric O_3 decline, and captured the start of the O_3 layer's recovery. With the addition of the Ozone Mapping and Profiler Suite (OMPS) instrument to Suomi-NPP (since 2011) and then NOAA-20 (since 2017) observing platforms, this satellite record of stratospheric O_3 extends for 40 years through the present time. In addition to stratospheric O_3 records, the SBUV/OMPS time series has been providing information about SO_2 observations that are associated with volcanic aerosols uplifted to the stratosphere and transported globally. Tracking the enhancements in stratospheric aerosol loads has become of great importance in recent years to identify unsanctioned attempts in anthropogenic modification of the atmospheric albedo. NOAA has the historic precedent and continuous capacity for verification of satellite products with ground-based remote and in-situ observations, along with assimilation and chemical modeling to interpret satellite observations.

Stratospheric O_3 monitoring by SBUV and OMPS is from LEO. GEO sampling geometry is essentially nadir viewing, so its vertical resolution will not match that of limb occultation, emission, or scattering instruments. However, higher temporal measurements of the total O_3 column could aid in understanding the contribution to degradation of tropospheric air quality in conjunction with complementary measurements of tropopause height and transport fields. Methods to combine estimates of stratospheric O_3 fields with total column O_3 fields to derive tropospheric O_3 residual estimates (see Ziemke et al., 2019) will benefit from increased temporal and spatial resolution that reduces interference from the cloud contamination. The combination of a GEO-XO backscatter UV spectrometer with a high-spectral resolution IR sounder would add an improved understanding of the impacts of stratospheric O_3 on the troposphere. Collocated O_3 and aerosol measurements from GEO could also aid in identifying potential perturbations to the O_3 layer if climate intervention methods are deployed.

3.2.2. Greenhouse Gas Monitoring

Long-term global monitoring of GHGs is needed for climate forecasting and tracking expected carbon-climate feedback mechanisms, such as the competition between the release of carbon from thawing permafrost, changing vegetation patterns, and increased plant uptake of carbon associated with CO_2 fertilization. Accurate representation of carbon-climate feedbacks in climate models is critically needed to inform policies aimed at limiting future warming.

Sustained observations of CO_2, CH_4, and other GHGs are needed to test climate model simulations and to monitor the efficacy of anticipated GHG emissions mitigation efforts. Comprehensive monitoring is particularly important for assessing progress towards achieving the goals of the Paris Agreement, including the global stocktake, as well as for understanding impacts of potential future geoengineering testing and implementation.

NOAA has a long-standing and foundational role in global GHG monitoring. NOAA's Global Greenhouse Gas Reference Network (GGGRN) includes more than 50 cooperative whole-air sampling locations around the world, along with continuous in-situ measurements from NOAA's atmospheric baseline observatories and tall broadcast towers, complemented by routine vertical profile sampling from light aircraft. Some records extend 50 years or more. NOAA partners with institutions across the US and around the world to produce a well-calibrated global dataset that provides the basis for current understanding of emissions and removals.

Satellite measurements of CO_2 and CH_4 are extremely challenging but can potentially provide new information about GHG budgets for crucial regions where in-situ measurements are impractical, such as tropical ecosystems in Africa and South America. High-resolution mapping sensors can identify unexpected large point sources such as CH_4 leaks from oil and gas facilities. Measurement requirements for satellite GHG sensors are extremely challenging, and retrievals are subject to systematic biases associated with thin clouds and aerosols. If satellite retrievals are to be useful for tracking sources and sinks of GHGs from regional to continental scales, then it is essential that the measurements are anchored by a comprehensive network of in-situ surface and vertical profile measurements. NOAA is the only agency capable of rigorously and comprehensively coordinating measurements across platforms to advance climate research and decision support.

Satellite measurement approaches including multispectral SWIR, TIR, and lidar have already been prototyped and flown, but the US currently lacks a coherent strategy for long-term multi-platform monitoring. NOAA scientists serve on the science team for NASA's SWIR Orbiting

Carbon Observatory (OCO)-2 mission (Crisp et al., 2017; Eldering et al., 2017) and are working to develop strategies for joint assimilation of in-situ data from the NOAA GGGRN with OCO-2 retrievals along with retrievals from TIR sensors such as NOAA's CrIS.

The Decadal Strategy for Earth Observation from Space (2018) identified space-based measurement approaches for GHGs including:

- Global observations of CO_2 and CH_4 at horizontal resolution of a few km and daily revisit with sufficiently high precision to constrain regional budgets of surface fluxes on a weekly time scale. This might be achieved with SWIR spectrometers that observe the atmospheric column with sensitivity down to the surface, complemented by TIR spectrometers that provide additional information on vertical distribution as well as data over the oceans and at night. Lidars may provide complementary information with sensitivity down to the surface over the oceans and at night.
- GEO continental-scale observations with sub-km horizontal resolution and revisit of at most a few hours. This could involve SWIR spectrometers with high precision, possibly complemented by TIR spectrometers. The capability to observe over selected regions with large surface fluxes may provide unique insights into daily variations of these fluxes and sporadic high emissions.
- LEO observation of plumes from point sources using SWIR spectrometers with very high spatial resolution (less than 50 m) over limited viewing domains. Precision should be sufficient to quantify source magnitudes on the basis of a single pass of the satellite.

Current LEO observations are severely limited by cloud and aerosol contamination. GEO orbits are uniquely useful for obtaining CO_2 and CH_4 total column retrievals in persistently cloudy regions such as the tropics since sensors can dwell on a location while clouds pass underneath. Passive satellite observations from existing LEO platforms, such as from OCO-2, Japan's Greenhouse gases Observing Satellite (GOSAT) and GOSAT-2, TROPOMI, lack spatial coverage over some critical GHG source regions, such as cloudy or low-light environments (e.g., Arctic, tropics).The planned NASA GeoCARB mission will demonstrate SWIR CO_2, CH_4, and CO observations from GEO and the utility of increased temporal coverage over CONUS and the Amazon.

A GEO-XO AC mission would combine GHG measurements with a suite of air quality tracers and, in coordination with international partners, play a critical role in the future Global Climate Observing System. Recommended GEO-XO instruments and products for this application include:

- GEO continental-scale SWIR observations of total column CO_2, CH_4, nitrous oxide (N_2O), and CO with at least 1-km, and preferably sub-km, horizontal resolution and revisit of at most a few hours, possibly complemented by a TIR spectrometer to provide information about vertical distribution. A GEO SWIR instrument could observe selected regions with large emission and uptake fluxes to measure day-to-day and diurnal variations of these fluxes and detect sporadic high emissions. This capability will be especially valuable for detecting and quantifying large CH_4 emissions associated with fossil fuel extraction operations and agriculture as well as natural seeps.

- Simultaneous measurements of a suite of air quality tracers such as SO_2, NO_2, CH_2O, $C_2H_2O_2$, O_3 and aerosols measured with a UV-VIS spectrometer and a VIS-IR imager would provide powerful constraints for source attribution, so that biospheric influences can be reliably distinguished from anthropogenic and fire sources.

3.2.3. Air Quality Monitoring

Air quality monitoring tracks the efficacy of various environmental public laws, including the Clean Air Act (1970), the subsequent 1990 Clean Air Act Amendments, the Clear Air Interstate Rule (2006), and the Cross State Pollution Rule (2011). The Clean Air Act resulted in the establishment of National Ambient Air Quality Standards (NAAQS) for near-surface criteria pollutants including O_3, particulate matter, CO, SO_2, and NO_2. Responsibility for air quality monitoring lies within the purview of the US EPA, which monitors air quality using a variety of ground-based sensors. However, the US EPA relies on space agencies such as NASA and NOAA to provide satellite data in regions where there is sparse coverage from ground monitors. Space-based air quality monitoring provides routine tracking of contributions to poor air quality from natural events like wildfires and dust storms and from anthropogenic activities including electricity generation, transportation, manufacturing, and oil and gas exploration.

Air quality monitoring data are essential for evaluation of NOAA's air quality forecasts *(see Section 3.1.1)*. The US EPA's network of surface monitors is the standard dataset used to evaluate NOAA's NAQFC. However, satellite air quality monitoring provides comprehensive spatial coverage that is very useful for validating NAQFC, particularly in large swaths of the US that lack surface monitoring, including agricultural areas and fossil fuel production basins. Future development of NAQFC will require chemical data assimilation to provide realistic constraints on the model's complex chemical schemes. Because of their extensive spatial and temporal coverage, space-based air quality monitoring data are ideal for chemical data assimilation.

While air pollution across the US has improved over the past decades, (US EPA, 2019) millions of people in the US are still exposed to days of unhealthy air pollution which exceed one or more of the NAAQS. Air quality monitoring is critical for understanding human exposure to poor air quality, so that regulatory authorities can issue air quality alerts and individuals can avoid breathing air with harmful levels of pollutants. High levels of pollutants such as tropospheric O_3 are harmful to crops, while visibility impacts from high aerosol loading hinder transportation systems. In addition to the US EPA, NOAA and NASA, stakeholders for air quality monitoring data include a variety of other Federal agencies (e.g., National Institutes of Health [NIH], CDC, USDA, FAA, US Department of the Interior [DOI]), environmental regulators in every state, tribal and local jurisdiction, and the public. National and international assessments of the longer term impacts of air quality on human health have largely relied on surface-based air quality monitoring data, while more recent efforts have demonstrated that remote-sensing data can also be of use in understanding pollutant exposure. For example, the Tropospheric Ozone Assessment Report (TOAR) brings together a wide variety of surface-based, balloon-borne, aircraft, and satellite retrievals of O_3 (Gaudel et al., 2018). TOAR metrics for human exposure to O_3 have recently been used by the Global Burden of Disease (GBD) in their latest estimates of human mortality due to O_3. These results, a part of the larger GBD 2020 publication published in *The Lancet*, rely on a merge of TOAR data and global model output (GBD, 2020; Chang et al., 2019).

3.2.3.1. Tropospheric Column NO2

NO_x (including nitric oxide [NO] and NO_2) are respiratory irritants, and highly reactive gases that play an important role in the formation of ground level O_3, PM2.5, and contribute to acid rain and dry deposition impacting critical loads of nitrogen in ecologically sensitive areas and aquatic environments. NO_x is primarily emitted by fossil fuel combustion, soil microbial processes, biomass burning, and lightning. Anthropogenic sources of NO_x include automobiles, trucks, and various non-road vehicles (e.g., construction equipment, boats, etc.) as well as industrial sources such as power plants, industrial boilers, cement kilns, and turbines. The effective and efficient implementation of pollution control strategies as required by the CAA requires an informed understanding on the spatial and temporal distribution of NO_x emissions across the various source sectors. High temporal and spatial resolution of NO_2 satellite column densities are needed to inform and quality assure improvements in the US National Emissions Inventory (NEI) for NO_x emissions. The NEI is a decision support system used by EPA, tribal, state, and local air quality agencies to help inform national-to-local control strategies to reduce air pollution and attain the NAAQS. The NEI is also used to inform NOAA NWS air quality forecast models, and used by hundreds of researchers at federal agencies, state agencies, and academic institutions to support their research. The NEI has broad impacts for air pollution management and research across the US.

LEO retrievals of NO_2 spanning multiple decades (including Global Ozone Monitoring Experiment [GOME], SCIAMACHY, OMI, GOME-2, OMPS, TROPOMI) have significantly advanced and matured, most demonstrably with respect to spatial resolution between GOME (40 km x 320 km) launched in 1995 and present-day TROPOMI (5.6 km x 3.5 km). The advancement in spatial resolution has allowed for real-time monitoring of anthropogenic sources of NO_x at both regional and global scales, arising due to environmental regulations, growth in industrial and energy extraction activities, and impacts of global recessions, civil unrest, and the global COVID-19 pandemic (Duncan et al., 2016; Tong et al., 2015; Russell et al., 2012; Laughner et al., 2019; Bauwens et al., 2020). In particular, the COVID-19 pandemic has tested the potential of satellite-based air quality monitoring to detect sudden changes in AC from human and economic activity. *Figure 12* illustrates an example of reduced tropospheric NO_2 columns from S5P TROPOMI at the onset of the COVID-19 pandemic. Though meteorology and chemistry can influence changes in AC year-to-year, reduced NO_x emissions are anticipated due to lower levels of traffic and industrial activity, both domestically and abroad (Forster et al., 2020). In turn, dynamically accounting for changes in precursor NO_x emissions is important for improving air quality forecasting capabilities of O_3 and secondary fine particulate matter *(Section 3.1.1)*, which can be impacted in non-linear ways. Often emission inventories are provided with two to three years of lag, which is problematic when emission sources change quickly due to environmental regulations, such as those implemented on transportation (McDonald et al., 2012) and power plants (Frost et al., 2006), or from changes in economic conditions (Tong et al., 2015; Bauwens et al., 2020). In short, retrievals of satellite NO_2 have matured significantly over the past two decades from multiple campaigns that have cross-validated satellite retrievals with airborne and ground-based spectrometers (Judd et al., 2020). Satellite-based inversions of NO_x emissions have been demonstrated (Jiang et al., 2018), and data assimilation techniques can be employed to improve air quality forecasting of a critical precursor to air pollution (Tong et al., 2015)

Compared to LEO, a GEO capability provides retrievals of NO_2 at spatial and temporal scales relevant to air quality planning. The horizontal resolution of the geostationary TEMPO satellite, currently anticipated to be launched in 2022, is approximately 2 km x 4 km (Zoogman et al., 2017), which is sufficient to capture urban core-suburban-rural gradients in NO_2. While LEO satellites have been successful in tracking trends in NO_x emissions over urban and power plant plumes, attribution to specific emission source sectors has proven more challenging (e.g., transportation, industry, airports, etc.). Understanding the source locations and source strength is not always possible using emission inventory tools and measurements. NO_2 tropospheric column measurements from instruments such as OMI and TROPOMI have played an increasingly important role in understanding the distribution of NO_x emission sources. However, LEO's limited once-a-day look from space cannot adequately capture or characterize the temporal and spatial variations in NO_2 from different NO_x emission source sectors through the day.

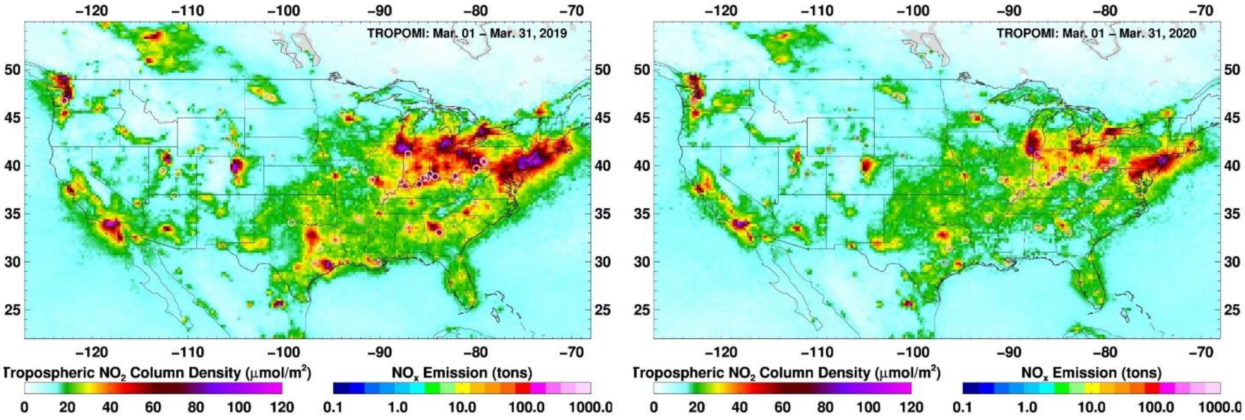


Figure 12. Tropospheric NO_2 vertical column density (VCD) from S5P TROPOMI for (left) March 2019 in the year preceding COVID-19 and (right) March 2020 at the onset of shelter-in-place measures during COVID-19.

To monitor and assess the temporal and spatial variations in different NO_x emission source(s), there is a measurement need for high temporal and spatial frequency of NO_2 column data from GEO-XO. This would allow for a more effective assessment of data gaps in EPA National Emission Inventories for NO_x emissions, improved quality assurance, and focusing resources on improving bottom-up methods for poorly characterized source sectors. Such improvements would greatly assist in the national and local decisions on emission control strategies, via more robust air quality modeling scenarios, which can result in large cost savings while achieving national air quality standards *(see Section 4 and EPA 2011)*.

Examples of poorly-characterized emission sources that would benefit from GEO-XO observations are agriculture and lightning (Silvern et al., 2019). As combustion sources of NO_x decrease due to environmental regulations, the role of agriculture and the use of fertilizer is expected to grow as a source of NO_x emissions, even in populated regions such as the Central Valley of California (Almaraz et al., 2018). While LEO satellites have been able to observe the influence of agricultural emissions, a complication is that soil NO_x emissions are highly variable and dependent on temperature and precipitation (Hudman et al., 2010). Similar complications arise with lightning, a known source of NO_2 to the upper troposphere. While numerous studies have attempted to utilize space-based observations to quantify lightning NO_x emissions, the production rates of lightning NO_x remain highly uncertain (Lapierre et al., 2020). By observing over the entire day at high spatial resolution, GEO observations may be able to better capture sporadic emission sources like agricultural soils and lightning, and improve characterization of regional and background sources of NO_x that impact air quality forecast models of O_3 and fine particulate matter *(Section 3.1.1)*.

NASA has been conducting field campaigns to fly a TEMPO/GEMS like instrument on an aircraft to demonstrate why a GEO capability is needed to monitor NO_2 and CH_2O. An example of diurnal changes of NO_2 and CH_2O over Seoul Metropolitan Area during the Korea-US Air Quality Study by airborne Geostationary Trace Gas and Aerosol Sensor Optimization (GeoTASO) instrument is shown in *Figure 13*. The NO_2 measurements shown in *Figure 13* were made on June 9, 2016 to demonstrate the capabilities of GEMS. This flight captured the buildup of NO_2 from transportation and industrial emissions sectors during a stagnation event. Observations over time show localized NO_2 and CH_2O in the early hours expanding and covering the whole domain due to deepening boundary layer and lateral dispersion of NO_2 in the later hours of the day (Judd et al., 2018). As discussed in *Section 3.2.3.2*, while contributions of NO_2 and CH_2O towards O_3 production vary and depend on several other factors, observations made during this stagnation event showed how rapid increase in O_3 due to these local emissions sources can occur (Peterson et al., 2019). Hourly revisit times of GEO satellites provide more observations and a stronger constraint for inversion-based models to constrain NO_x emission inventories and rates of photochemistry, which can lead to improved air quality forecast models through data assimilation techniques *(see Section 3.1.1)*.

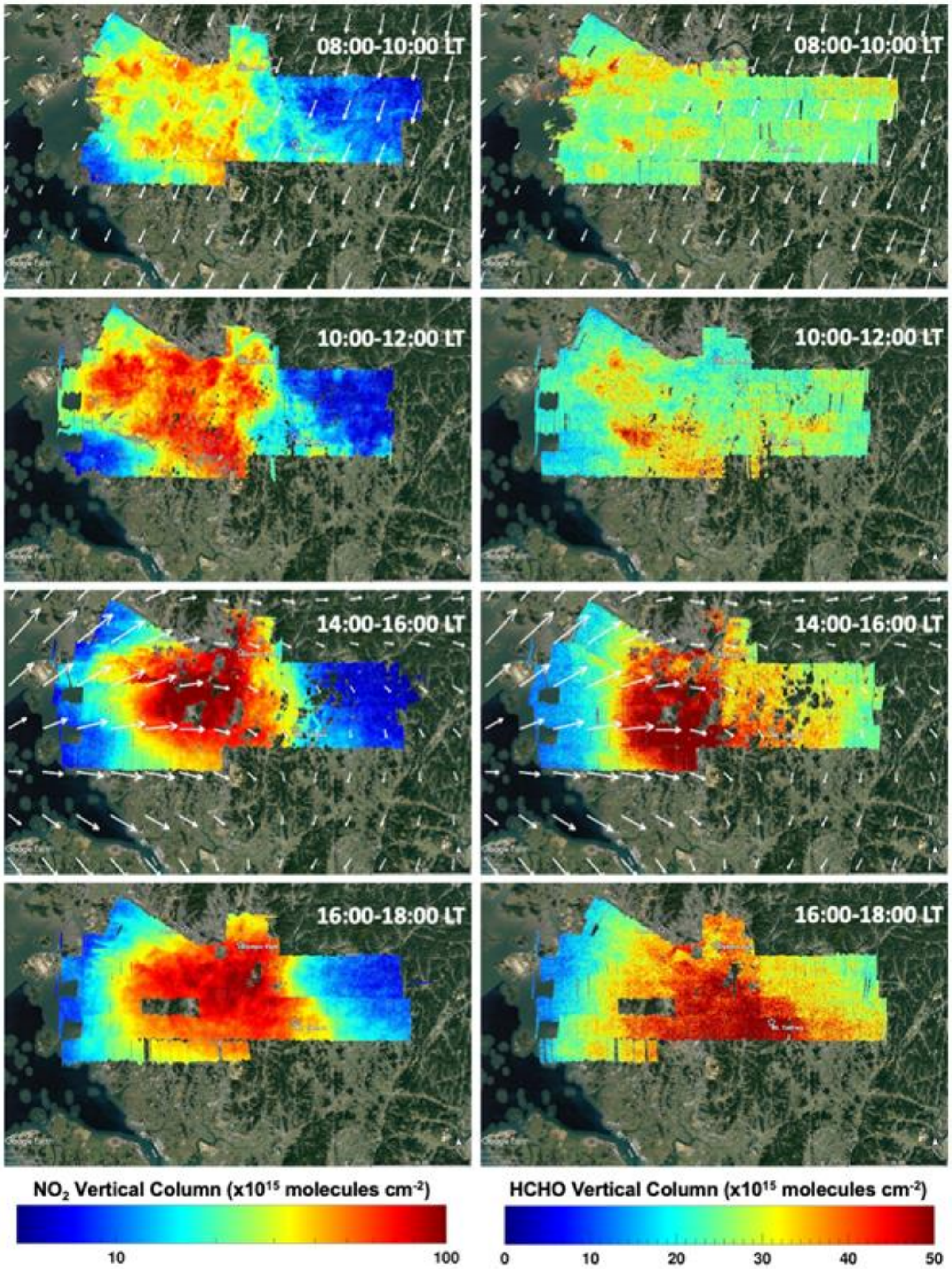


Figure 13. GeoTASO observations of tropospheric vertical column NO_2 (left) and CH_2O (right) on June 9, 2016, acquired at four times of day progressing from early morning (top) through late afternoon (bottom). Figure adapted from Judd et al., 2018.

3.2.3.2. Tropospheric Column Formaldehyde (CH_2O), Glyoxal ($C_2H_2O_2$), and Isoprene

CH_2O is a non-methane VOC that is both directly emitted as a combustion byproduct and secondarily formed in the atmosphere. Like NO_2, CH_2O is simultaneously retrieved from space-based UV-VIS spectrometers (including GOME, SCIAMACHY, OMI, GOME-2, OMPS, TROPOMI). CH_2O is chemically formed in the atmosphere from natural vegetation, biomass burning, and anthropogenic sources. Similar to NO_2, due to its relatively short atmospheric lifetime (~few hours), CH_2O provides an additional diagnostic on emission source regions of highly reactive VOCs and secondary air pollution. CH_2O has been used to evaluate biogenic inventories and chemistry (Wolfe et al., 2016; Zhu et al., 2016). Several studies have explored the utility of the CH_2O /NO_2 ratio in inferring the sensitivity of tropospheric O_3 to NO_x and VOC emissions (Duncan et al., 2010; Jin et al., 2017; Jin et al., 2020;). However, it should be noted that the variability in the vertical structure overlying complicates the use of the CH_2O /NO_2 ratio as a metric (Schroeder et al., 2017). Historically the detection limit of CH_2O is noisier than for NO_2. For example, the uncertainty of TROPOMI CH_2O is estimated at ~50% for the total column versus ~10% for the tropospheric column of NO_2 (Veefkind et al., 2012). Urban source regions are typically distinguishable from regional background only under heavily-polluted conditions (Streets et al., 2013). Case study examples include Houston (Zhu et al., 2014), Los Angeles (Kim et al., 2018), and Seoul (Souri et al., 2020a; Souri et al., 2020b). Given the uncertainty and lower detection limit of space-based observations of VOCs, a GEO capability would provide more observations spatially and temporally across the day, and potentially help improve signal-to-noise through spatial averaging. By improving the retrieval of CH_2O /NO_2, higher quality information can be provided to air quality managers in identifying the most cost-effective control strategy paths to lowering tropospheric O_3 and fine particulate matter formation.

$C_2H_2O_2$ is also another non-methane VOC that is also retrieved along with NO_2 and CH_2O in the UV-VIS. Since $C_2H_2O_2$ forms at different rates and from different VOC precursors than CH_2O, the $C_2H_2O_2/CH_2O$ ratio has been proposed as a diagnostic to distinguish anthropogenic and biogenic source regions of reactive VOCs (Vrekoussis et al., 2010). Though the ratio is potentially useful at the global scale, challenges exist in interpreting $C_2H_2O_2/CH_2O$ in regions dominated by biogenic sources such as the southeastern US (Kaiser et al., 2015). However, signatures of $C_2H_2O_2$ present in smoke plumes from fires are being reported by S5P TROPOM science team *(Figure 14)*. This warrants further research to determine the information content and usefulness for air quality models.

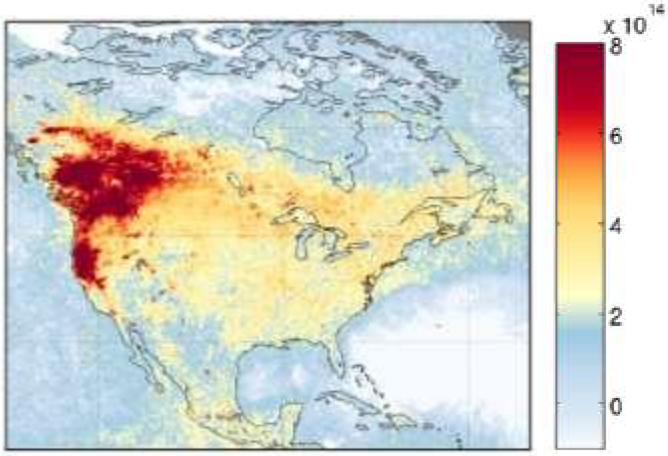


Figure 14. S5P TROPOMI $C_2H_2O_2$ for August 2018 during extreme fires in the Pacific Northwest (units are molecules per square centimeters). Figure obtained from Diego Loyola, German Aerospace Center (personal communication).

A recent study combining CrIS isoprene measurements with other satellite data (Wells et al., 2020) demonstrated that CrIS can directly detect a primary emission from the biosphere and improve biogenic VOC emission inventories. Isoprene is the single largest reactive VOC globally (Goldstein & Galbally, 2007), which controls global atmospheric chemistry with subsequent implications for modeling O_3 and fine particulate matter. Similar capabilities on a GEO-XO AC mission would ensure that biogenic VOC emissions are improved for air quality forecast models *(Section 3.1.1)*, which will help improve predictions of O_3 and fine particulate matter. Biogenic VOC emissions exhibit a strong temperature dependence across the day that would benefit from hourly GEO observations. Biogenic VOC emissions are also impacted by weather and climate *(Section 3.1.2)*, including drought-related stress resulting in higher O_3 levels (Lin et al., 2020). Changes in biogenic VOC emissions under a changing climate is relevant to air quality managers in determining cost-effective emission control strategies to improve air quality (Trainer et al., 1987; Chameides et al., 1988).

3.2.3.3. Tropospheric Column, Profile and Boundary Layer Ozone

Current satellite products of O_3 are usually columns, especially the tropospheric O_3 column from the surface to the thermal tropopause such as those produced by Tropospheric Residual Methods (Total Column O_3 estimates minus Stratospheric O_3 estimates). In order to better address air quality and climate questions related to O_3, we need products with higher vertical resolution.

The TROPOMI team is about to release a profile product of O_3 with 5-7 independent levels throughout the entire atmosphere with one layer for the troposphere. The GEO-XO O_3 retrievals could provide such profiles with three independent levels in the troposphere (lower troposphere, mid-troposphere, upper troposphere or an independent UTLS layer).

Combined UV/IR retrievals (CrIS+OMPS and AIRS+OMI) have been developed to optimize the vertical information content.

TEMPO is expected to have an hourly boundary layer O_3 product (0-2 km) based on UV and visible radiances, with horizontal resolution of approximately 8.4×4.4 km^2 (Zoogman et al., 2014, Zoogman et al., 2017). This is a big improvement over OMI/MLS and IASI (Infrared Atmospheric Sounding Interferometer) which only provide infrequent LEO retrievals of the full tropospheric column (Gaudel et al., 2018). Likewise, a new product uses IASI and GOME-2 retrievals to provide a 0-3 km column O_3 product over land, but it is very limited in temporal resolution because the instruments are in LEO (Cuesta et al., 2013; Gaudel et al., 2018).

TEMPO provides a template for the minimum capabilities of GEO-XO O_3 retrievals. While TEMPO will only monitor O_3 across the USA, plus southern Canada and northern Mexico, the combination of JPSS and GEO-XO could provide boundary layer O_3 monitoring across both the northern and southern hemispheres. This is important because current O_3 increases observed at mid-latitudes are being driven by O_3 production in the tropics, with subsequent O_3 export to mid-latitudes (Gaudel et al., 2020; Zhang et al., 2016).

A variety of measurements, including Pandora (special algorithm), Brewer, Umkehr, lidar, ozonesonde, commercial aircraft (In-Service Aircraft for a Global Observing System [IAGOS]) tall towers are available for verification of satellite O_3 products.

3.2.3.4. AOD and Surface PM2.5

In the last two decades, satellite observations of aerosols, specifically AOD, have advanced to the extent that operational agencies around the world have begun to rely on them for their air quality and public health related decision support systems. Satellite derived AOD can be used as a proxy to monitor surface particulate matter, PM2.5, and to fill in the gaps in coverage by ground monitors (e.g., Engel-Cox, 2004; Liu et al., 2009; Hoff & Christopher, 2009; Zhang et al., 2009). A primary limitation in using AOD as a proxy for surface PM2.5, however, is the lack of knowledge of the vertical location of the aerosol and aerosol type when AOD is retrieved using satellite observations. An accurate PM2.5 estimation based on satellite observations also requires the availability of meteorological information such as relative humidity and temperature (Gupta & Christopher, 2009). In essence, the best use of AOD comes when the altitude of the aerosol layer and aerosol composition (type, single scattering albedo) are known. When aloft, aerosols do not impact near-surface air quality, while different types of aerosols have different health impacts.

Thus far, the use of AOD as a proxy for surface PM2.5 has involved polar-orbiting satellite sensors such as Moderate Resolution Imaging Spectroradiometer (MODIS) on Aqua and Terra satellites, with the algorithms transitioning to VIIRS on Suomi NPP and NOAA-20 satellites (Zhang et al., 2009; Hoff & Christopher, 2009). This method has worked well to estimate daily average surface PM2.5 using a singular AOD observation from polar-orbiting satellites (e.g., van Donkelaar et al., 2012; van Donkelaar et al., 2016). However, Zhang and Kondragunta (2020) have shown that while AOD observed at 1:30 PM from polar-orbiting satellites is often a good proxy for daily average surface PM2.5, it is not when there is a substantial diurnal variation in surface PM2.5 either due to boundary layer variation, wind speed and direction changes, or vertical stratification of aerosols

(Figure 15). In fact, the relationship between AOD (an optical measurement) and PM2.5 (a chemical measurement) involves aerosol layer height and type (knowledge of aerosol mass extinction efficiency) information (Hoff & Christopher, 2009). This can be achieved with a synergistic retrieval approach using a set of GEO satellite imagers/spectrometers (GEO-XO Imager and UV-VIS spectrometer), we can derive AOD, aerosol layer height, aerosol composition (type/single scattering albedo) and apply them to derive surface PM2.5 in near real time.

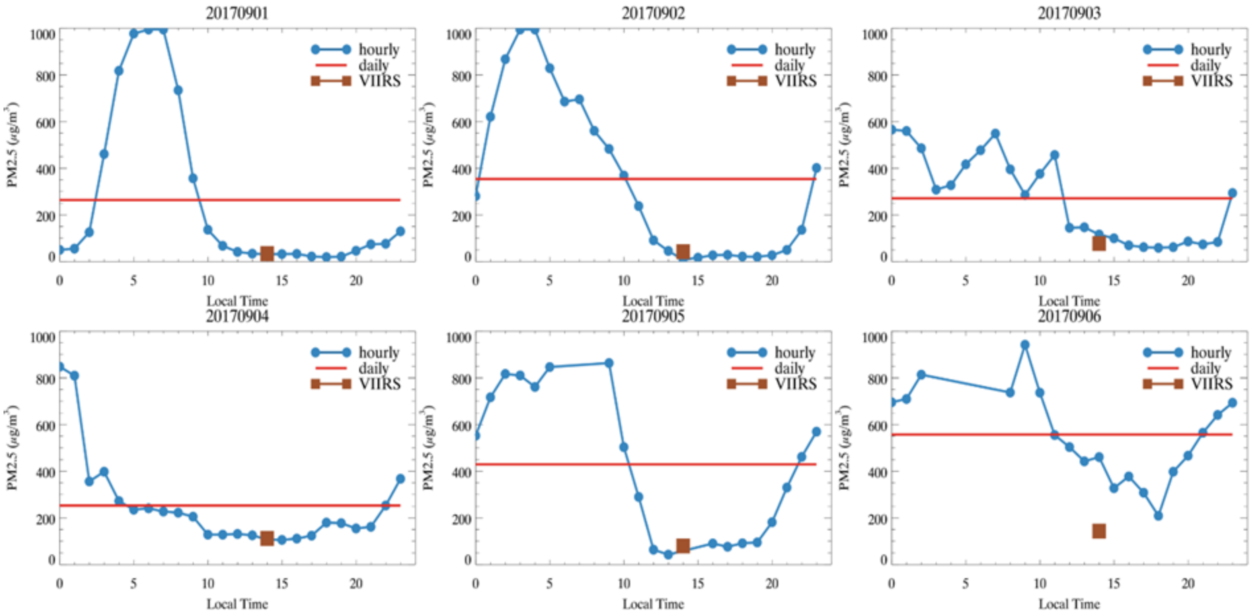


Figure 15. Diurnal variation of surface PM2.5 at Seeley Lake, Montana for September 1-6, 2017 during a smoke event. Daily average PM2.5 shown in solid red line. Surface PM2.5 estimated from once daily VIIRS aerosol optical depth observation is shown by brown square. Results show that when substantial diurnal variability in surface PM2.5 occurs, satellite observations are also needed at sub-daily time scales.

3.2.3.5. Ammonia (NH_3)

Ammonia (NH_3) is a major precursor of PM2.5, and contributes nitrogen dry deposition impacting ecologically sensitive areas and aquatic environments. NH_3 is primarily emitted by agriculture practices (e.g., fertilizer application, manure management), with smaller contributions from biomass burning and fossil fuel combustion. As the primary atmospheric base, NH_3 influences cloud pH and associated aqueous oxidation reactions and particle pH which influences acid-catalyzed reactions and other processes. In particular, NH_3 influences the response of PM2.5 nitrate to NO_x emission controls. The effective and efficient implementation of pollution control strategies of PM2.5 requires an informed understanding on the spatial and temporal distribution of NH_3 fluxes. These effects are relevant to EPA's work on secondary NAAQS.

High temporal and spatial resolution of NH_3 satellite column densities are needed to inform and quality assure improvements in the US NEI for NH_3 emissions. They are also essential in improving the comprehensiveness of Earth System Models (ESMs), such as GFDL's ESM, which impacts NOAA's global prediction capabilities. The high spatial and temporal variability of NH_3 concentrations combined with the currently limited surface monitoring make characterizing NH_3 challenging.

LEO retrievals of NH_3 are relatively new, but they have already proven to be important to NOAA global model development and could inform EPA monitoring and regulatory activities. So far, NH_3 profiles have been retrieved from the Tropospheric Emission Spectrometer (TES, aboard Aura), AIRS, IASI (Van Damme et al., 2018) and CrIS instruments, all in TIR. A particular advantage of NH_3 measurements from space is overcoming the difficulty of in-situ measurement, due to the nature of the compound itself. Thus, the potential improvement in both data availability and quality from GEO-XO measurements would be revolutionary.

4. Outline of Potential Valuation Use Cases for GEO-XO Atmospheric Composition Products

4.1. Initial Considerations

The Weather Research and Forecasting Innovation Act of 2017 requires value assessments for any next generation observing systems with potential costs over $500 million. This paper states the motivation and necessity for GEO-XO AC capabilities in seven NOAA application areas, representing an initial assessment of the value of these capabilities. Future efforts will build on this work to develop valuation use cases that demonstrate the enormous benefit to cost ratio of GEO-XO for these various AC applications. These quantitative valuation cases should consider both the economic benefits (e.g., how do GEO-XO's AC capabilities contribute to the global satellite-based Earth observation market) and societal benefits (in terms of lives saved, health improvements, property protected, etc.). These valuation efforts would ideally consider up to four complete sets of AC instrumentation, each including an imager and spectrometers covering the TIR to the UV of the spectrum, designed to last 20 years. Such calculations should consider not only the annual value of current instrument capabilities for AC, but also the increased value as new technology and products are developed.

Future GEO-XO AC valuation efforts can build on similar assessments that have already been done to quantify the value of AC observations from space. For example, a decade of work by the GEO-CAPE science team, including numerous OSSEs to test the efficacy of GEO AC concepts, provides very useful information on potential spacecraft constellations, instrument payloads, and specific measurement capabilities (GEO-CAPE, 2018). The GEO-XO AC valuation process can also examine the usefulness of GEO instruments that are either now in orbit or will be launched in the next few years. South Korea's GEMS UV-VIS spectrometer has been in orbit since February 18, 2020 and is about to release its first observations of the distributions and diurnal variations of pollutants such as NO_2 over all of East Asia. NASA's TEMPO instrument, with capabilities similar to GEMS, will be launched by 2022. Since NASA announced the choice of TEMPO as the US's first GEO air pollution instrument, the TEMPO science team has engaged in extensive outreach to a variety of stakeholders to determine their needs for products to inform Earth system research, operational air quality and weather forecasts, environmental planning and rule-making, emergency first response, and public health applications. GEO-XO's value assessment effort could be expedited by leveraging the work of the science and applications teams for GEMS, TEMPO, GeoCARB, and EU's Sentinel-4 UVN instruments to establish the value of GEO AC applications.

GEO-XO already has its own robust user engagement efforts, beginning with the 2020 topical workshops and user surveys led by Vanessa Escobar and her team. These GEO-XO user engagement activities have highlighted the NOAA space-based products relied on by the weather, fire, human health, oceans, and agricultural communities. GEO-XO's technical teams are now in the process of identifying which of these products could be provided or improved by GEO-XO instruments. A comprehensive GEO-XO AC valuation estimate should incorporate the insights gained from these user engagement efforts.

Technical experts on GEO-XO's AC observation capabilities and the applications of GEO-XO AC products will likely work with the staff of NOAA's chief economist's office to derive valuation estimates. While the current report assessed the value of GEO-XO AC capabilities for seven broad NOAA application areas, work on quantitative valuation using comprehensive economic analysis will likely focus on a few specific use cases. Economic analysis is time-consuming; related GEO-XO valuation efforts, such as the benefit of an IR sounder to NOAA's Weather Enterprise, lasted two years or more. This report therefore lays out a few examples of use cases for GEO-XO AC capabilities that could be explored by a future collaboration between NOAA's technical and economic experts.

4.2 GEO-XO Atmospheric Composition Example Use Cases

One possible valuation use case involves the benefit of GEO-XO AC capabilities for NOAA's wildfire forecasting and its use to protect the public and to improve health outcomes. Operational wildfire forecasts are made by a variety of NOAA models, including HYSPLIT (see ARL, 2020), the NAQFC (see NWS OSTI, 2020), and HRRR-Smoke (see AVID, 2020). These models are used to inform first responders and local authorities who need to know where the fire will go and where smoke will be the most intense, in order to effectively fight the fire, protect firefighting crews, and get people out of harm's way. As discussed in *Section 3.1.3*, these models, which already rely on a combination of LEO and GEO observations, will be improved by a GEO-XO imager and a spectrometer. Fire detections, fire radiative power, and fire size detected by an imager in the 3.9 µm band at 1 km or better spatial resolution will be essential to future NOAA fire weather forecasting efforts. Trace gas and aerosol data from a GEO-XO UV-VIS-NIR spectrometer making measurements throughout a diurnal cycle will provide critical constraints on fire emissions and downwind smoke chemistry. Even a minor improvement to an operational NOAA fire weather forecast resulting from the inclusion of a GEO-XO AC instrument could result in better decisions during a wildfire event, leading to lives saved and property damage averted.

HRRR-Smoke incorporates the meteorological feedbacks of smoke aerosols, and this capability will become part of GEFS-Aerosols and NAQFC-CMAQ in coming years. Intense smoke directly impacts the atmosphere's radiative balance and changes forecasted boundary layer temperatures and heights. Because wildfires and their smoke vary so rapidly, accurate predictions of smoke plume transport by these modeling systems should benefit from the high-frequency input data of a GEO-XO imager and spectrometer. While the benefits of GEO-XO informing aerosol-meteorological feedbacks will take several years to conclusively demonstrate, these benefits will not be realized if a GEO-XO AC capability does not exist.

NOAA uses its sophisticated air quality models like the NAQFC-CMAQ to predict the pollutants present in smoke plumes and produce forecast guidance used by the nation's environmental regulators to issue pollution alerts. The issuance of air pollution alerts directly impacts people's behavior, particularly those in sensitive groups, such as the elderly and people suffering from respiratory ailments like asthma. Heavy wildfire smoke will likely cause outdoor activities, such as sporting events and social gatherings, to be curtailed or even canceled. If a false smoke pollution alert is issued, such societal restrictions may be unnecessary. Conversely, failing to issue an alert when heavy smoke may impact a populated area could result in people being hospitalized who wouldn't have otherwise ventured outside. Thus, a GEO-XO AC capability that provides even incremental improvement to air pollution alerts resulting from wildfires could produce a cascade of economic impacts.

Wildfire smoke pollutants have been linked to chronic and acute health outcomes. Exposure to the particulates in wildfire smoke has been shown to result in increased risks of asthma attacks, cardiac arrest, and strokes (e.g., see Liu et al., 2017a; Wettstein et al., 2018). In addition, the epidemiological community has shown that lower-income people and people of color tend to suffer disproportionately from the impacts of fire smoke exposure (Liu et al., 2017b). A quantitative valuation exercise would ideally account for the benefit of GEO-XO AC products towards improving wildfire pollution alerts, their impacts on the use of health care resources, the loss of economic activity from societal choices made based on inaccurate forecasts, and the possibly incalculable loss to the nation from environmental injustice.

Similar quantitative valuation use cases could be investigated for improvements to NOAA's air quality forecasting capabilities resulting from GEO-XO AC instruments and their products. As shown in *Figure 9* in *Section 3.1.1*, for example, the number of lives lost prematurely on an annual basis in the US due to all sources of poor air quality is at least two orders of magnitude larger than the annual national death toll from extreme weather events. There is extensive literature documenting the health impacts of poor air quality (for some representative examples and additional references, see Pope et al., 2009; Fann et al., 2012; Gauderman et al., 2015; and World Health Organization, 2016).

Over the past five decades, the US and Europe have implemented a variety of legislation that mandated substantial investment in air pollution controls. The effects of these measures on air quality have been significant (see for example, Samet et al., 2017), with major reductions in near-surface O_3, particulate matter, and precursors such as NO_2 and SO_2. The consequent health benefits of these improvements to air quality are startling. For example, the US EPA (2011) estimated that the total cost of the 1990 Clean Air Act Amendments (CAAA), a cornerstone of the US's air quality regulation, and the CAAA's related programs and compliance actions to be $65 billion in 2020. The benefits of the CAAA and related measures are estimated to be $2.0 trillion in 2020. The 30:1 benefit-to-cost ratio of the CAAA and related efforts comes primarily from: reducing risk of early death associated with exposure to ambient fine particle pollution; reducing risks of premature mortality associated with O_3 exposure; reducing illnesses such as acute myocardial infarction and chronic bronchitis; and protecting the health of ecosystems and other improvements which enhance quality of life, such as improved agricultural yields and better visibility conditions (EPA, 2011). Similarly, savings in the European Union from complying with World Health Organization guidelines on PM2.5 is about EUR 31.5 billion annually, including savings on health expenditures, employment absenteeism, and intangible costs such as well-being, life expectancy, and quality of life (Lahoz et al., 2012).

An analysis of the quantitative benefits on air quality and its consequent impacts on human health resulting specifically from a GEO capability has not yet been done. However, the outline of such a calculation would follow the paths laid out by the US EPA's CAAA cost-benefit analysis and by similar efforts internationally, such as the EU's atmospheric monitoring program analysis described in the Copernicus Market Report *(see Section 4.3)*. As described in *Section 3.1.1*, a GEO-XO AC capability would improve NOAA's air quality forecasts. Better NOAA air quality forecast guidance in turn improves air quality indices generated by the US EPA for criteria pollutants such as O_3 and PM2.5. As described for wildfires earlier in this section of the paper, pollution alerts generated by state and local agencies based on US EPA air quality indices affect people's decisions about activities. GEO AC observations are particularly important to informing timely air quality forecasts and consequent human decisions and health outcomes. Even a few hours of high pollution exposure can lead to increased health risks such as atrial fibrillation (Link et al., 2013). GEO AC products will allow the calculation of human exposure to near-surface PM2.5, O_3 and NO_2 on hourly timescales for population centers across the continental US. Previous analyses described here demonstrate that there is a straightforward path to estimating the benefits of improvements to these and many other related health outcomes derived from a GEO AC capability.

4.3 Copernicus Market Report

An example of the kind of quantitative analysis that could be carried out in the future is the Copernicus Market Report (CMR, PWC France, 2019). The CMR analyzed the cumulative economic value resulting from the overall investment in Copernicus, the European Union's Earth Observation Program. This analysis looked at a wide range of social, environmental, and strategic impacts of Copernicus assets. From 2008 up to 2020, the total investments in Copernicus were forecasted to reach EUR 8.2 billion. Over the same period, this investment generated economic benefits between EUR 16.2 and 21.3 billion (excluding non-monetary benefits). This economic value was generated through the added value created in the upstream space industry, the sales of Copernicus-based applications by downstream service suppliers and the exploitation of Copernicus-enabled products by end users in various economic sectors.

The CMR examined 10 different value chains. The value chain most relevant to this paper is air quality monitoring and its impacts on air quality forecasting and public health. As noted in the CMR, Europe recently expanded its satellite monitoring of air quality from one satellite, ENVISAT, to several spacecraft, including Sentinel-5 Precursor, which carries the TROPOMI instrument discussed earlier in this paper. The timing of the CMR relative to the fairly recent deployment of these Copernicus products likely leads to an underestimate in the report's benefits of the satellite products. Nonetheless, combined economic impacts for Copernicus air quality monitoring totaled between EUR 269 and 537 million.

The CMR notes the increasing use of satellite data in air quality models, and the complementary role that satellite data have compared to traditional ground-based observations. The CMR shows the growing interest in the use of satellite air quality monitoring by individuals who want to make better decisions about their activities. The CMR also points out growing demand for satellite air quality data by industry, and the economic opportunity that Copernicus air quality monitoring data represent.

The main direct user of Copernicus Earth observations is CAMS, the European Union's service for information on air pollution and health, climate, and solar energy. CAMS makes global and regional air quality model nowcasts and forecasts that increasingly rely on Copernicus EO. CAMS model products are used not only within Europe but also globally, since CAMS provides some of the most advanced air quality forecasts available anywhere. CAMS models provide information used by many end users to make economic decisions, affecting the tourism and entertainment industries. The CAMS model products are also used by individuals to make choices about their activities that lead to improved public health outcomes. Because the sources of poor air quality and climate forcing agents largely overlap, Copernicus Earth observations and CAMS models also help to make decisions about reducing the impacts of climate change. These impacts include not only direct environmental effects, but also strategic ones. As the nations of Europe work to set carbon emissions targets, Copernicus Earth observations allow verification of these emissions when ground-based monitoring is not available and provide an overall constraint on European emissions inventories.

It should be noted that the CMR did not examine the benefit of GEO air quality observations alone. To our knowledge, there is as yet no report that specifically investigates the benefits of GEO AC observations throughout the full value chain for a nation, a region like Europe, or globally. However, the CMR offers a straightforward roadmap for how to carry out a complete quantitative value assessment of a space-based asset like the GEO-XO AC capability.

4.4 Conclusion and Future Steps

This report has shown a way forward for evaluating the full value of AC products and their variety of end uses. A complete and quantitative estimate of the economic and social benefits will take significantly more time and a larger investment of effort than was possible in the four months allotted to this report's writing team.

It is useful to compare the situation for the GEO-XO AC value assessment to that faced by the groups working to demonstrate the value of GEO-XO weather observations. GEO-XO economic and societal valuation efforts for weather applications have had several years to plan their work. The GEO-XO weather valuation analyses are only now beginning to demonstrate their findings, which indeed demonstrate the enormous benefits of GEO-XO to the nation's weather forecasting enterprise and its stakeholders. The GEO-XO weather efforts engaged the technical expertise of NESDIS and NASA scientists and engineers designing GEO-XO's next-generation weather instrumentation, NWS forecasters who will ensure GEO-XO products are used in the UFS to produce more accurate forecasts, representatives for a variety of consumers for these improved weather products, and economists who can calculate the wide reach of GEO-XO's improved weather products on the economy and society. We believe that a concerted effort of equal or greater scope will be needed to assess the full impact of GEO-XO on the wide array of atmospheric composition applications and their consequent impacts on the US economy and society. On the other hand, such an effort will be informed by the decade of studies by the GEO-CAPE mission, which laid the scientific groundwork for the valuation analysis.

A valuation assessment will always be at best a snapshot in time, and the applications of GEO-XO AC products will only grow in the future. New products are being developed from LEO AC instruments that can be translated to GEO applications. Synergistic approaches for combining GEO and LEO AC observations are being developed. NOAA forecast model systems will increasingly rely on satellite AC observations to improve predictive skill. The end users for NOAA forecasts will expand. As economic analyses indicate (see, for example, GLOBE NEWSWIRE, 2020), Earth observations collected by the US, the European Union, and other nations are a growing market opportunity that will increasingly be exploited in the coming decades. Societal challenges such as population growth, climate change, natural disasters, and global pandemics have only strengthened the need for timely Earth observations. There are uses for GEO-XO AC data that have not yet been thought about, and so the assessed value of GEO-XO's AC capability will therefore likely be lower than the true value.

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NOAA Technical Report OAR CPO-8
doi.org/10.25923/1s4s-t405