BAMS
Meeting Summary

Global Atmospheric Composition Needs from Future Ultraviolet–Visible–Near-Infrared (UV–Vis–NIR) NOAA Satellite Instruments

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2022 NOAA UV–Vis–NIR Workshop

What: Stakeholders and end users with diverse backgrounds in atmospheric science gathered to provide the state of the science and user needs for operational atmospheric composition measurements to inform future NOAA low-Earth-orbit satellite missions.

When: 14–15 June 2022

Where: Online

KEYWORDS: Greenhouse gases; Satellite observations; Aerosols/particulates; Air quality; Atmospheric composition; Trace gases

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The U.S. National Oceanic and Atmospheric Administration (NOAA) has a long history of satellite observations, including for atmospheric composition. Stratospheric ozone measurements have been made by NOAA since the 1980s, and over the years, NOAA's weather satellites have added other atmospheric composition capabilities, particularly volcanic ash, dust, smoke aerosols, and limited tropospheric trace gas measurements (e.g., Zhang et al. 2022; Nalli et al. 2020; Shephard et al. 2020; Wells et al. 2022; Li et al. 2015). These products already support a number of applications, especially timely information about aerosols and wildfire smoke observations provided through AerosolWatch.

Expanding its spaceborne atmospheric composition focus, NOAA has made plans for a dedicated ultraviolet–visible (UV–Vis) instrument aboard its next-generation geostationary constellation, GeoXO, expected to launch in the 2030s. As NOAA begins planning for the next generation of low-Earth-orbit (LEO) satellites, it is users' input on the needs for LEO satellite data in the 2040s and beyond, when NOAA's current operational Joint Polar Satellite System (JPSS) series of satellites will reach end of life. The (virtual) workshop that took place on 14–15 June 2022 discussed applications that require atmospheric composition products from space-based UV, Vis, and near-infrared (NIR) measurements.

Workshop structure and atmospheric composition applications overview

The workshop consisted of two half days of virtual presentations and discussion. Presentations spanned a range of applications: the public health impacts of poor air quality and environmental justice; greenhouse gas measuring, monitoring, reporting, and verification (GHG MMRV); stratospheric ozone monitoring; and various applications of satellite observations to improve models, including data assimilation in global Earth system models. Presentations ranged in scope from large-scale, long-term improvements to NOAA's capabilities in Earth system modeling to tracking and forecasting specific events, such as the impact of western wildfires on air quality in Connecticut and the effects of COVID-19 restrictions on air quality.

The NOAA JPSS program opened the workshop and provided the charge for gathering user requirements, with encouragement to consider NOAA's international partnerships with the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT) and Japan Aerospace Exploration Agency (JAXA) to deliver LEO measurements for NOAA applications. In this collaborative context, future NOAA LEO satellite data users can expect a more disaggregated architecture, wherein the approach of flying multiple sensors on a single spacecraft would be replaced by individual spacecraft dedicated to individual instruments for greater flexibility and agility within a constellation of satellites. The workshop also encouraged discussion on GEO–LEO synergies, consideration of commercial data, and other opportunities that might emerge in the future.

The first session started with a historical overview of UV–Vis–NIR atmospheric composition measurements, including the Ozone Monitoring Instrument (OMI), the Tropospheric Monitoring Instrument (TROPOMI), *Orbiting Carbon Observatory* (*OCO*)*-2* and *OCO-3*, GOME, SCIAMACHY, and the *Greenhouse Gases Observing Satellite* (*GOSAT*). Examples of available products included ozone, sulfur dioxide (SO_2), formaldehyde, nitrogen dioxide (NO_2), and GHGs, and their applications in recent years, such as the use of OMI NO_2 data for air quality monitoring.

The second keynote presentation highlighted NOAA's National Air Quality Forecasting Capability (NAQFC), which currently provides 72-h forecast guidance for ozone, fine particulate matter ($PM_{2.5}$), smoke, and dust. The NAQFC is being enhanced to ingest satellite NO_2 and aerosol optical depth (AOD) data for improved emissions inventories and better forecast accuracy. Timely delivery of consistent data were highlighted as critical for operational forecasting applications.

The third keynote presentation focused on the needs for GHG monitoring as part of an integrated urban monitoring system to complement current ground-based and aircraft measurements. The other two keynote presentations by public health experts highlighted the capabilities of satellite data to both improve the understanding of pollution exposure on human health and address environmental injustice. Existing satellite data (particularly NO_2 from TROPOMI) demonstrate the unequal distribution of air pollution in U.S. cities. For example, satellite data show that disparities in NO_2-attributable pediatric asthma are widening. Future operational satellite measurements could provide detailed, timely, high-resolution information about air pollution at the census tract scale, potentially supporting future science-based decisions to lower air pollution exposure.

Current measurement capabilities

Subsequent sessions of the workshop, summarized below, focused on particular products and applications, including the need for expanding the set of retrieved species, particularly ammonia and volatile organic compounds (VOCs).

Air quality impacts of trace gases. Currently, tropospheric column retrievals of trace gases that are criteria pollutants impacting air quality are available from a number of LEO instruments, e.g., OMI, TROPOMI, and the Ozone Mapping and Profiler Suite (OMPS). Applications of these data include air quality forecasting, tracking power plant and wildfire smoke plumes, addressing urban air quality challenges, and identifying and quantifying emissions. Operational air quality forecasting at global and regional scales using these satellite products is taking place at the Copernicus Atmosphere Monitoring Service (CAMS), and similar capabilities are emerging at the National Weather Service.

NOAA and the U.S. Environmental Protection Agency (EPA) use similar satellite data for air quality model evaluation. The combination of methane (CH_4), carbon dioxide (CO_2), carbon monoxide (CO), and NO_2 retrievals can improve confidence in emissions inventories and model performance, and together these data products would be of use in future air quality management tools. EPA is moving toward an integrated observing system of trace gases observed in the UV/Vis (i.e., NO_2 and formaldehyde) combining surface and satellite measurements of these species. A similar integrated observing system could be envisioned for gases detectable in the NIR spectrum such as CO, CO_2, and CH_4. The combined suite of longer- and shorter-lived trace gas retrievals and measurement scales would enhance capacity to assess air quality models and emission inventories.

The ability to retrieve additional trace gases (e.g., ethane, isoprene, and ammonia) in the thermal IR along with those measured in the UV–Vis–NIR region would be extremely useful for air quality applications, including source apportionment analysis (e.g., for oil/natural gas extraction, biogenic, and agricultural sources). High-resolution near- and thermal IR observations on LEO platforms would greatly complement the UV–Vis instruments on current and planned GEO platforms.

COVID-19 related lockdowns and the associated reduction in human activity showed the need for near-real-time emission estimates, especially for use in air quality forecasts. The emissions discussed were those from the transportation sector, oil and natural gas production and distribution, and the use of volatile chemical products in personal care, cleaning, construction, and manufacturing. NO_2, CO_2, CH_4, and VOCs (e.g., formaldehyde and glyoxal) satellite products would be of most value for quantifying those emission changes.

Another specific example highlighting the need for timely satellite products is air pollution exposure inequalities, such as urban NO_2. Typically, this type of work relies on the time averaging of LEO datasets to produce higher-spatial-resolution products. However, coarser products at daily resolution can still provide useful assessments of the inequalities and temporal variations in pollution distributions. Daily satellite observations capture the degree of intraurban pollution inequalities, provided at least 30%–60% of the city is covered to ensure sufficient sampling of population groups (Dressel et al. 2022).

Even more serious air pollution problems are seen globally, in cities without the network of ground-based measurements available in U.S. cities. LEO observations provide the ability to study and intercompare air pollution in the world's urban areas, especially the growing megacities on the African continent that are not covered by the current plans for GEO constellations.

Although neither measured routinely nor required operationally so far, VOCs are important species for identifying chemical processes that lead to the formation of ozone and aerosols, and VOCs can help in identifying the sources of air pollution (e.g., anthropogenic versus biogenic). One such example is tracking emissions from oil and gas production. Satellite NO_2 products, such as from OMI or TROPOMI, can track changes in activity in oil and gas producing basins on time scales of days, seasons, and years (Dix et al. 2020). Satellite CH_4 retrievals, measured most recently by TROPOMI, can help identify methane leaks and hot spots of drilling and oil and gas production activity (de Gouw et al. 2020). Meanwhile, VOCs such as formaldehyde, observable from OMPS and TROPOMI, are a potentially useful proxy for other hydrocarbons coemitted during the oil and gas production process and that produce formaldehyde in the atmosphere. Ideally, formaldehyde retrievals would continue on NOAA's post-JPSS LEO platforms.

Ozone is produced in the atmosphere through reactions of many of the emitted species discussed above. Ground-level ozone is one of six criteria pollutants for which the EPA sets National Ambient Air Quality Standards (NAAQS) to protect against human health and welfare effects. While monitoring networks generally measure surface-level ozone, these networks are spatially sparse. Retrieving near-surface ozone from Vis LEO observations would be extremely valuable for improving model performance and assessing the impacts of potential emissions control strategies, as well as for monitoring in regions with inaccurate emission inventories and noticeable lack of measurements (i.e., the tropics).

The retrieved species discussed in this section would ideally feed into an integrated data assimilation system, although significant challenges to multispecies chemical data assimilation remain.

Stratospheric ozone. Stratospheric ozone monitoring using satellites has been a long-term, reliable, and accurate way to assess the status of the ozone hole recovery. Globally, stratospheric ozone and climate change are coupled in complex ways, requiring continuous monitoring to detect long-term trends. For these reasons, data from multiple LEO satellite missions are needed, since no single instrument will cover the period of stratospheric ozone depletion and recovery, while anthropogenically driven climate change trends extend over decades.

One of the desired future improvements over current satellite capabilities includes an ozone profiling capability in both the troposphere and stratosphere. This could be accomplished with increased vertical resolution, particularly by including both nadir and limb measurement capabilities. Additionally, a constellation of small satellite instruments could allow for increased sampling coverage and/or a look at diurnal capabilities.

Aerosols. Satellite aerosol products are some of the many operational atmospheric composition products provided by NOAA. As noted by keynote speakers, these products have proven to be very useful for the prediction of air quality, especially smoke emitted from wildfires. NOAA has a mandate to provide forecast guidance for concentrations of $PM_{2.5}$ near Earth's surface across the United States. Because of the detrimental impacts of $PM_{2.5}$ on human health, the EPA has established NAAQS for $PM_{2.5}$ which includes a daily standard set at a 24-h average concentration of 35 $\mu g\ m^{-3}$. NOAA provides hourly forecast guidance of surface $PM_{2.5}$ over a 72-h time period. The forecast guidance is, in turn, used by state and local air quality forecasters to issue air quality index forecasts and issue air quality alerts.

Speakers in the aerosol session identified emissions of aerosols and their precursors, both anthropogenic and natural, as critical inputs to the global and regional air quality forecast models. This input can be provided to the models in near–real time. Additionally, satellite derived AOD or UV–Vis–NIR reflectances are assimilated into models to adjust aerosol concentrations and provide initial conditions for air quality forecasts.

While current NOAA operational satellites produce near-real-time information on biomass burning emissions sources and AOD, the adjustment of aerosol species in current data assimilation schemes can be challenging due to limited information content of Vis–NIR passive sensors and the lack of well-calibrated, vertically resolved extinction profiles from elastic backscatter lidars. Though techniques to derive aerosol layer height using oxygen absorption bands in the visible are emerging, the full vertical profile is not well resolved (Xu et al. 2017). Having a UV–Vis–NIR sensor on operational satellites allows for the expansion of the current capabilities, allowing for better constraints on aerosol speciation, vertical structure, and absorbing/scattering properties. These improvements, in turn, will advance aerosol data assimilation in atmospheric composition models, leading to better predictions of surface $PM_{2.5}$ and more accurate characterization of aerosol impacts on radiation, clouds, and precipitation. Speakers showed case studies where the knowledge of aerosol composition and height could advance AOD data assimilation in air quality models to improve $PM_{2.5}$ predictions.

Greenhouse gases (CO_2 and CH_4). NOAA's global surface network measuring GHGs is relatively sparse and could be complemented by routine and reliable satellite observations with high spatial and temporal coverage, such as from future NOAA operational satellites. To track changes in GHG emissions and distinguish very small biosphere and fossil fuel signals requires high accuracy and precision over time scales of decades. For surface carbon flux estimates, the key instrument feature is spectral coverage in the NIR regions between

0.75 and 3 μm, which is dominated by reflected sunlight. Measurements of GHGs at wavelengths longer than 3 μm, where Earth's thermal emissions dominate, have little sensitivity near the surface. For CH_4, the 1.65 μm band may yield more accurate retrievals as compared to its 2.3 μm band, by references to CO_2 absorption that occurs at close wavelengths, thereby limiting interferences from aerosols, clouds, and surface reflectance.

NOAA has looked to existing satellite measurements provided by other agencies, such as those from the NASA *OCO-2* to evaluate its CarbonTracker data assimilation system. NOAA provides validation of those satellite datasets through its various in situ measurements made routinely (e.g., biweekly aircraft observations, AirCore) and in targeted field campaigns. NOAA's AirCore in particular has been useful in validating existing CO_2 products from the JPSS Cross-track Infrared Sounder (CrIS) instrument (Nalli et al. 2020). NOAA also cooperates with other institutions carrying out ground-based remote sensing measurements of GHGs (e.g., the Total Carbon Column Observing Network) that can provide a link between the in situ observations and satellite retrievals. NOAA's plans for returnable gliders and commercial aircraft measurements offer the promise of expanded validation opportunities for its future space-based GHG capabilities.

In addition to existing instruments deployed by NASA, NOAA, and their European and Asian partners, several NGO and private sector entities have focused on delivering spaceborne GHG measurements, particularly of methane (e.g., *GHGSat*, MethaneSAT). Carbon Mapper was the primary example discussed at the workshop, which delivers CH_4 and CO_2 point-source data that can both inform GHG emission inventories for stock takes and trend analyses and provide direct GHG mitigation guidance. While informing large-scale inventories is an important use of GHG monitoring data, a large fraction of anthropogenic methane emissions come from a relatively small number of sources. Thus, high-resolution and low-latency data are critical in enabling rapid targeted mitigation of CH_4 emissions.

Greater availability of satellite GHG data could enable current and future global data assimilation efforts (e.g., with *OCO-2*, *GHGSat*, TROPOMI), with the goal of improving the understanding of human emissions and the natural exchange of CO_2 between the land, ocean, and atmosphere. Data assimilation also provides the ability to track global and regional changes in GHG concentrations as well as to quantify radiative forcing and temperature impacts. As data availability increases, merging multiple satellites should provide a more complete picture of global and regional carbon fluxes. NASA plans to include CO_2 and CH_4 state estimation in its upcoming reanalysis of the twenty-first century (R21C), and its evaluations of assimilations of TROPOMI and CrIS retrievals for CH_4 are ongoing. NOAA, whose CarbonTracker data assimilation system currently delivers CO_2 and CH_4 global and regional fluxes, plans to connect these capabilities with its operational Unified Forecast System. As demand for carbon fluxes and concentrations grow, especially for MMRV purposes, it will be important to expand cyberinfrastructure and data services to support easier access and greater interoperability of CO_2 flux and concentration products.

Future instrument recommendations

Each of the above applications comes with a specific set of observational requirements, some of which are being addressed with current capabilities that should be continued in post-JPSS LEO constellations. New capabilities should be added as well. Of particular importance for improving NOAA's operational capabilities are greater spectral coverage that includes the entire Vis–NIR region, higher spectral resolution, and higher spatial resolution.

Recent NOAA plans for GeoXO, GOES-R's future replacement, have already demonstrated the need for and value of space-based atmospheric composition products. While NOAA's GEO measurements will add tremendous value with their high temporal resolution over much of North America, global coverage of atmospheric composition will still need to be delivered from LEO. LEO observations, especially in the afternoon orbit, will complement morning-orbit instruments deployed by European and Asian partners and those planned by the private sector, especially for GHGs (e.g., MethaneSAT).

NOAA is uniquely positioned within the U.S. government to deliver continuous and reliable operational data. Future NOAA LEO observations should provide information on global air quality, near-real-time estimates of GHG fluxes, surface gas and aerosol pollutants, and monitoring of stratospheric ozone. To that end, it will be important to enhance NOAA's current LEO capabilities with an instrument similar to TROPOMI that is capable of measuring at high spatial and spectral resolution across the UV–Vis–NIR spectral ranges.

The workshop highlighted the many challenges of combining satellite and in situ datasets and the ongoing needs for robust satellite validation. NOAA's ground and aircraft-based measurements are well positioned to provide all manner of validation for future space-based observations (e.g., Nalli et al. 2020; Ciren and Kondragunta 2022). Presenters and participants agreed that U.S.-based measurement assets for validation continue to improve and that an integrated approach across the agencies involved in air quality would aid in improving validation resources (CEOS 2019).

Final remarks

NOAA's LEO satellites have been and will continue to be a reliable source of operational data for decades, especially for weather forecasting, monitoring of the stratospheric ozone hole recovery, and critical global hazards like the Pinatubo eruption or the 2020 Australian fires. As technology for measuring atmospheric composition from space matures and the demand for such information grows, NOAA should be expected to continue and expand the delivery of atmospheric composition information with the next generation of its LEO satellites. This workshop is a first step in NOAA's planning process by engaging the broader community in refining the requirements for future LEO atmospheric composition capabilities and working with users to maximally exploit these products when they become available.

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