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Review

Satellite data of atmospheric pollution for U.S. air quality applications: Examples of applications, summary of data end-user resources, answers to FAQs, and common mistakes to avoid

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HIGHLIGHTS

- Review of the primary uses of satellite data for air quality applications.
- Background information on satellite capabilities for measuring pollutants.
- Summary of the resources available to data end-users.
- Answers provided to common questions in plain language.

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ABSTRACT

Satellite data of atmospheric pollutants are becoming more widely used in the decision-making and environmental management activities of public, private sector and non-profit organizations. They are employed for estimating emissions, tracking pollutant plumes, supporting air quality forecasting activities, providing evidence for "exceptional event" declarations, monitoring regional long-term trends, and evaluating air quality model output. However, many air quality managers are not taking full advantage of the data for these applications nor has the full potential of satellite data for air quality applications been realized. A key barrier is the inherent difficulties associated with accessing, processing, and properly interpreting observational data. A degree of technical skill is required on the part of the data end-user, which is often problematic for air quality agencies with limited resources. Therefore, we 1) review the primary uses of satellite data for air quality applications, 2) provide some background information on

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End-user resources
Remote sensing

satellite capabilities for measuring pollutants, 3) discuss the many resources available to the end-user for accessing, processing, and visualizing the data, and 4) provide answers to common questions in plain language.

1. Introduction

There is now a wealth of atmospheric composition satellite data for air quality (AQ) applications that has proven valuable to environmental professionals: nitrogen dioxide (NO_2), sulfur dioxide (SO_2), ammonia (NH_3), carbon monoxide (CO), some volatile organic compounds (VOCs), and aerosol optical depth (AOD), from which surface particulate matter ($PM_{2.5}$) may be inferred. The data are primarily collected by instruments on satellites operated by the National Aeronautics and Space Administration (NASA) and National Oceanic and Atmospheric Administration (NOAA). A barrier to using these data is the inherent difficulties associated with accessing, processing, and properly interpreting them. A degree of technical skill is required on the part of the data end-user, which is often problematic for organizations with limited resources. Therefore, the purpose of this review article is to inform data end-users of 1) how data are being used by the environmental community for U.S. AQ applications (Sections 2 and 3), 2) what free resources are available for accessing and processing the data (Section 4), and 3) straight answers in plain language to frequently-asked questions, including common mistakes to avoid when working with data (Section 5). Our intended audience is AQ managers and other environmental professionals, particularly those who do not currently use satellite data for their AQ applications, but wish to, or do so sparingly.

There are other informative review articles on various aspects of the use of satellite data for AQ applications that will provide additional information to the uninitiated end-user. Examples are Fishman et al. (2008) on the current capabilities of satellite instruments to measure pollutants and Streets et al. (2013) on the use of satellite data for estimating surface emissions of pollutants. The National Science and Technology Council (NSTC) provides an overview of satellite observations relevant to AQ applications (NSTC, 2013). The instructive review articles of Martin (2008) and Hoff and Christopher (2009) are more technical in their discussions and, therefore, more appropriate for the intermediate and advanced satellite data end-user. Ichoku et al. (2012) provide a comprehensive, but technical, overview of using satellite data to characterize various properties of wildfires, such as emission strength and plume rise.

In this review, we focus on satellite data that provide information on the distributions of pollutants and pollutant emissions. We do not discuss the many ways that meteorological satellite data are used in AQ applications. We refer the reader to Table 1 of Streets et al. (2013) and Table 1 of Kahn (2012) for lists of the main satellite gas and aerosol products relevant for AQ applications. The reader should refer to Table 1 for a list of acronyms that are frequently used in this article.

2. Current satellite data applications in the U.S.

The U.S. Environmental Protection Agency (EPA) and many state AQ agencies recognize the utility of satellite data and some of them are actively considering how they can be further used for monitoring and regulatory purposes. We identified four main categories of current applications (i.e., tracking pollutant plumes, support for AQ forecasting, evidence in exceptional event demonstrations, and input to AQ models and data for model evaluation) and two main categories of potential applications (i.e., estimating ozone precursor and aerosols emissions, and monitoring regional long-term trends in ozone precursors and aerosols), all of which take advantage of the primary strength that satellite data have over the conventional ground-based monitoring networks – spatial coverage (e.g., Fig. 1). The four main categories of current applications are discussed in this section and the two main categories of potential applications are discussed in Section 3.

2.1. Tracking pollutant plumes

Over the last decade, satellite data have been used widely to track pollution from agricultural and wild fires. For example, Fig. 2 shows AOD data from the Visible Infrared Imager Radiometer Suite (VIIRS) instrument on the Suomi National Polar-orbiting Partnership (NPP) satellite and illustrates the long-range transport of

Table 1
Frequently used acronyms and terms.

Acronym/name	Phrase/description
AQAST	NASA *Air Quality Applied Sciences Team*; http://acmg.seas.harvard.edu/aqast/
ARSET	NASA *Applied Remote SEnsing Training*; http://arset.gsfc.nasa.gov/
Chemical species	
AOD	*Aerosol Optical Depth*, also referred to as Aerosol Optical Thickness (AOT) – the degree to which aerosols prevent the transmission of light by absorption or scattering of light through the entire vertical column of the atmosphere from the ground to the satellite's sensor
NO_x	*Nitrogen Oxides*, the sum of NO and NO_2
PM, $PM_{2.5}$	*Particulate Matter*, <2.5 μm in aerodynamic diameter
SO_2	*Sulfur Dioxide*
VOCs	*Volatile Organic Compounds*
Agencies	
EPA	*Environmental Protection Agency*
ESA	*European Space Agency*
EUMETSAT	*European Organisation for the Exploitation of Meteorological Satellites*
NASA	*National Aeronautics and Space Administration*
NOAA	*National Oceanic and Atmospheric Administration*
Instruments	
AIRS	NASA Aqua *Atmospheric Infrared Sounder*
GASP	*GOES East Aerosol/Smoke Product* on the NOAA GOES East satellite
GOES	NOAA *Geostationary Operational Environmental Satellite*
GOME-2	*Global Ozone Monitoring Experiment-2* on the EUMETSAT Metop-A satellite
MISR	NASA Terra *Multi-angle Imaging SpectroRadiometer*
MOPITT	NASA Terra *Measurements of Pollution in the Troposphere*
MODIS	*Moderate Resolution Imaging Spectroradiometer* on the NASA Terra and Aqua satellites
OMI	NASA Aura *Ozone Monitoring Instrument*
TEMPO	*Nasa Tropospheric Emissions: Monitoring of Pollution*
VIIRS	*Visible Infrared Imager Radiometer Suite* instrument on the Suomi National Polar-orbiting Partnership (NPP) satellite
Other	
AQ	*Air Quality*
AQS	EPA *Air Quality System* of monitoring stations
NAAQS	EPA *National Ambient Air Quality Standards*
VCD	*Vertical Column Density* – the number of molecules of an atmospheric gas between the satellite instrument and the Earth's surface per area of the Earth's surface

Fig. 1. An early photo taken in 1973 from the NASA Skylab space station. It shows a thick layer of smog in the Los Angeles Basin (circled). The photo illustrates the "bird's eye" view provided by satellites. Photo credit: Image Science & Analysis Laboratory, NASA Johnson Space Center.

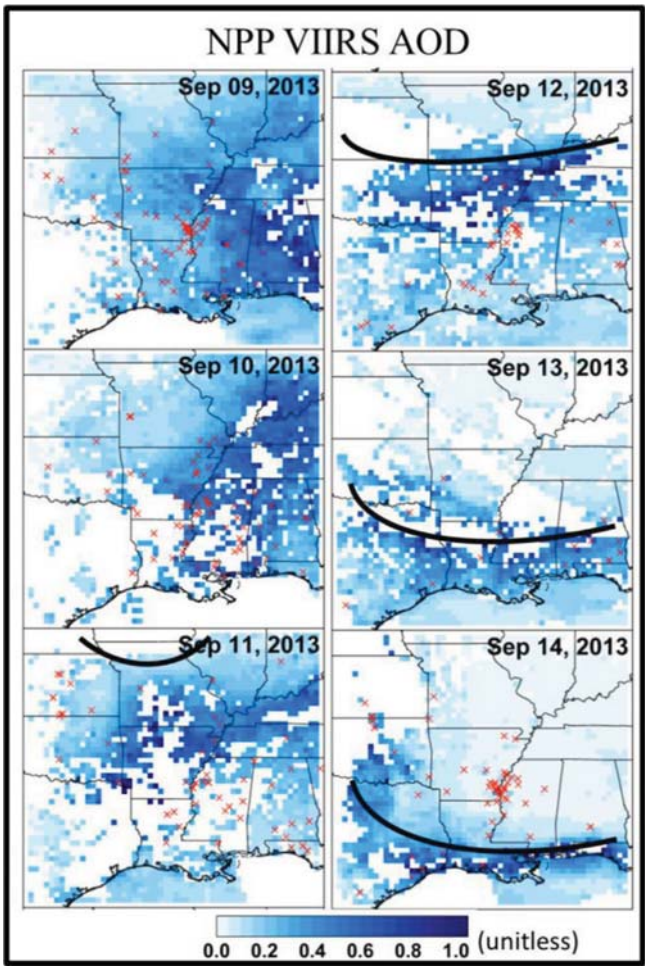

Fig. 2. The aerosol optical depth (AOD) product (unitless) from the Visible Infrared Imager Radiometer Suite (VIIRS) instrument on the Suomi National Polar-orbiting Partnership (NPP) satellite indicates that aerosols, which were associated with agricultural fires in the Mississippi Valley, accumulated in the central US and were transported ahead of a cold front to the Gulf Coast. The location of each fire detected by VIIRS is shown with a red "x". The black lines show the approximate locations of the cold front at 1:00 pm local time each day. White areas indicate missing data, mainly due to the presence of clouds.

pollution from agricultural fires in the Mississippi Valley to Houston, Texas. (AOD is the degree to which aerosols prevent the transmission of light by absorption or scattering of light through the entire vertical column of the atmosphere from the ground to the satellite's sensor. The terms "aerosol" and "particulate matter" are often used interchangeably and refer to suspensions of solid or liquid particles in air, though particulate matter is usually associated with a specific particle size range, such as < 2.5 μm for $PM_{2.5}$ and <10 μm for PM_{10}.) As detailed in Case Example #1 (Section S.1), the agricultural fire pollution did not elevate $PM_{2.5}$ levels at the surface in Houston, but it did several kilometers above the city and at the surface in the Mississippi Valley. This event illustrates 1) the complementary nature of the satellite observations to data collected by surface AQ monitors, 2) the power of satellite data to provide an overview of the regional buildup and the long-range transport of pollution, which can degrade AQ far downwind, 3) the limitations of the satellite data (e.g., the lack of information on the vertical distribution and chemical composition of the aerosols, and gaps in spatial coverage due to clouds), and 4) the complicated relationship between AOD, relative humidity, and $PM_{2.5}$, showing that high AOD values do not necessarily translate to high surface $PM_{2.5}$ levels (e.g., Ziemba et al., 2013) – a common mistake to avoid.

2.2. Support for AQ forecasting

One of the most frequent applications of satellite data is for AQ forecasting support. Satellite imagery is often accessed on a daily basis by state AQ agencies, such as the Virginia Department of Environmental Quality (DEQ), the Idaho DEQ, and the California Air Resources Board (CARB). The use of satellite data for AQ forecast support is generally qualitative, such as imagery which has a natural color rendition similar to a photograph (e.g., Fig. 3), and AOD, CO and smoke extent maps. For instance, the Idaho DEQ used imagery to support their AQ forecasts during the summer wildfire season of 2012. Each day, staff at the DEQ combined satellite data with surface monitor information to produce a daily report that was forwarded to the forecasters. The information in the report included NASA Moderate Resolution Imaging Spectroradiometer (MODIS) smoke imagery, NASA Aqua Atmospheric Infrared Sounder (AIRS) CO, and fire detection maps downloaded from web tools and then imported into geographic information systems (GIS). (For other examples, the reader is referred to Case Example #2 (Section S.2)). Two of the most popular web tools among AQ forecasters are the NOAA Infusing Satellite Data into Environmental Applications (IDEA) and the NOAA Hazard Mapping System Fire and Smoke Product (HMS) web tools. Section 4 and Table 2 provide more details on these web tools.

2.3. Evidence for exceptional event demonstrations

Section 319 of the Clean Air Act defines an event as exceptional "if the event affects air quality; is an event that is not reasonably controllable or preventable; is an event caused by human activity that is unlikely to recur at a particular location or a natural event; and is determined by EPA to be an exceptional event". It also "requires a State air quality agency to demonstrate through reliable, accurate data that is promptly produced that an exceptional event occurred" and that "a clear relationship be established between a measured exceedance of a NAAQS and the exceptional event …" (Federal Register, 2007). These "exceptional events" may be

Fig. 3. (top) NASA Terra MODIS true color image from June 12, 2008, showing widespread smoke from the Great Dismal Swamp and Evans Road wildfires in Virginia and North Carolina. (bottom) NASA Aqua MODIS true color image from July 11, 2008, showing extensive smoke from wildfires over northern California.

exempted by EPA from counting towards regulatory decisions, such as non-attainment determinations. The "weight of evidence" presented in an exceptional event demonstration may include data from surface monitors and satellites alongside model simulations that clearly demonstrate that the exceedances of the National Ambient Air Quality Standard (NAAQS) threshold would not have occurred "but for" the exceptional event. Exceptional events include dust storms, wild fires and fireworks.

For exceptional event demonstrations, state AQ agencies use satellite data to illustrate the long-range transport of dust and aerosols from wildfires, and the impact of stratospheric intrusions of ozone-rich air on surface ozone (e.g., Lin et al., 2012; Fiore et al., 2014). Until recently, NASA Terra and Aqua MODIS true color imagery (e.g., Fig. 3) and AOD data from NOAA's Geostationary Operational Environmental Satellite (GOES) Aerosol/Smoke Product (GASP; Knapp et al., 2005; Prados et al., 2007) have been the main image types used. In addition to aerosols, satellite instruments are able to detect the number of molecules of some gases between the instrument and the Earth's surface; this quantity is typically referred to as a "vertical column density" (VCD) in units of molecules per unit area of the Earth's surface. Ozone VCD data have been included in exceptional event demonstrations as discussed in Case Example #3 (Section S.3); however, they were not used to demonstrate high surface ozone levels since surface ozone cannot be discriminated from these data (Section 5.2.1). In Sections S.2 and S.3, we provide Case Examples #2 and #3 to illustrate how NASA data are used in exceptional event demonstrations.

2.4. Evaluating output of models and providing input to models

Satellite data can be applied in a variety of ways to improve AQ models used to develop State Implementation Plans (SIP). Specifically, they can be used to evaluate the quality of the model-predicted pollutant concentrations (e.g., Kondragunta et al., 2008) and to constrain model input, such as pollutant emissions (e.g., wildfires with fire-counts and fire radiative power data), biogenic emissions of VOCs (e.g., with photosynthetically active radiation and leaf area index data), and photolysis rates (e.g., ozone VCD data). As a specific example, the NASA Aura Ozone Monitoring Instrument (OMI) NO_2 VCD data could be used to evaluate the simulation of NO_x (=NO + NO_2), an important ozone precursor, in the EPA Community Air Quality Model (CMAQ). Such an evaluation may reveal inaccuracies of emissions as well as deficiencies in the chemical mechanism. For instance, a long-standing problem for simulating NO_x is the uncertainties associated with the lifetime and chemical fate of alkyl nitrates (e.g., Kasibhatla et al., 1997).

3. Potential satellite data applications in the U.S.

There are two applications, estimating pollutant emissions (Section 3.1) and monitoring long-term trends (Section 3.2), that are actively used by the research community, but are under-used by the applied community. A third potential application is to help guide surface monitor siting by regulatory agencies around point sources, particularly large NO_x sources.

3.1. Estimating anthropogenic pollutant emissions

As discussed in Section 2.3, satellite instruments are able to detect the number of molecules of a particular gas between the instrument and the Earth's surface – a "vertical column density" (VCD) in units of molecules per unit area of the Earth's surface. If pollution transport, deposition, and chemical conversion are minimal or can be appropriately taken into account, then the observation can reflect the emission rate of the chemical species. The main areas of application and opportunity are NO_x and SO_2 emissions from point sources and NO_x, CO, methane, ammonia, and VOC emissions from area sources. Derivation of surface $PM_{2.5}$ from satellite AOD has been the subject of extensive research (Hoff and Christopher, 2009, Section 5.2.6), but AOD data alone do not provide information on chemical composition or source emission strength. In the next few paragraphs we highlight a number of recent studies from the scientific literature that have focused specifically on the application of satellite techniques to gas emissions estimation; Streets et al. (2013) provide an in-depth discussion on this topic.

Point sources are natural targets for application of satellite data as entities who own facilities that emit criteria pollutants are subject to emissions verification and compliance. When it comes to SO_2 emissions from coal-fired power plants (e.g., Fig. 4), considerable ingenuity and statistical data enhancement techniques are needed to draw out the weak signals (Section 5.8). Fioletov et al. (2011) reported that the detection limit for SO_2 emissions is

Table 2
Data discovery, visualization, and analysis resources for the end-user.

Name	Description	Website
ARSET	NASA *Applied Remote SEnsing Training.*	http://arset.gsfc.nasa.gov/
AQAST	NASA *Air Quality Applied Sciences Team.*	http://acmg.seas.harvard.edu/aqast/
Multi-purpose[a]		
EOSDIS	*Earth Observing System Data and Information System.* Useful web tools are available to search data files by instrument and pollutant type.	http://earthdata.nasa.gov
EOSDIS/LANCE	*Land Atmosphere Near-real-time Capability for EOS* is NASA's main tool for visualization and download of near-real-time data and imagery.	https://earthdata.nasa.gov/data/near-real-time-data/
EOSDIS/Reverb	Search, access and download data files, with spatial and temporal sub-setting.	http://reverb.echo.nasa.gov/reverb
GES DISC	*Goddard Earth Sciences Data and Information Services Center.* A NASA data center where pollution and aerosol files may be found.	http://disc.sci.gsfc.nasa.gov
GES DISC/Giovanni	An interactive visualization and analysis web tool.	http://disc.sci.gsfc.nasa.gov/giovanni/
GES DISC/Mirador	Search on time, space, and keywords for datasets and data files.	http://mirador.gsfc.nasa.gov
LaRC ASDC	*Langley Research Center Atmospheric Science Data Center.* A NASA data center where pollution and aerosol files may be found.	http://eosweb.larc.nasa.gov
LAADS Web	*Level 1 and Atmosphere Archive and Distribution System.* Access MODIS L1, Atmosphere and Land products, and VIIRS L1 and Land products.	http://ladsweb.nascom.nasa.gov
True color imagery and smoke		
Worldview	An interactive visualization and analysis web tool.	https://earthdata.nasa.gov/labs/worldview/
HMS	NOAA *Hazard Mapping System* Fire and Smoke Product. Access near-real-time data.	http://www.ospo.noaa.gov/Products/land/hms.html
EOSDIS/ FIRMS	*Fire Information for Resource Management System.* Access near-real-time data.	http://earthdata.nasa.gov/data/near-real-time-data/firms
Application specific		
IDEA	NOAA *Infusing Satellite Data into Environmental Applications.* Near-real-time access to MODIS and GOES aerosol products and meteorological information.	http://www.star.nesdis.noaa.gov/smcd/spb/aq/
IMAPP	NOAA IDEA-I *International MODIS/AIRS Processing Package.* A software package that uses either Terra or Aqua MODIS AOD to identify areas of high aerosol loading from which 48-h forward trajectories are initialized.	http://cimss.ssec.wisc.edu/imapp/ideai_v1.0.shtml
RSIG	EPA *Remote Sensing Information Gateway.* Facilitates comparisons between NASA imagery and CMAQ model output.	http://ofmpub.epa.gov/rsig/rsigserver?index.html
EE DSS	*Exceptional Event Decision Support System.* Facilitates the analysis of both surface and satellite data for exceptional event demonstrations.	http://www.datafed.net
The Smog Blog	A discussion of current air quality in the U.S. and around the world.	http://alg.umbc.edu/usaq/

[a] There are web tools that provide access to multiple parameters relevant to AQ (e.g., aerosols and gases), data files, and visualizations, and in some cases other features, such as temporal and spatial sub-setting of the data, and limited data analysis.

~70 Gg per year for North American power plants. The instrumental NO_2 sensitivity is much stronger than for SO_2 (Sections 5.7 and 5.8), and therefore it is possible to detect emissions from a much wider range of source types. Kim et al. (2006, 2009) and Russell et al. (2012) examine NO_x emissions from U.S. power plants. Duncan et al. (2013) showed that known changes of emissions reported by the Continuous Emissions Monitoring Systems (CEMS) from large power plants are generally consistent with observed changes in OMI NO_2 VCD data over individual facilities. While time trends are believed to be credible, further research is still needed to develop reliable emission estimates for individual plants.

When sources are many, small, and widespread (i.e., "area sources"), it presents a challenge for traditional emission inventory approaches and an opportunity for the use of satellite data for estimating emissions. With the ability to estimate emissions over a wide area, satellite observations can be used to validate or improve existing inventory approaches. NO_x emissions have received the most attention, with a wide variety of studies using NO_2 VCD data to derive emissions from vehicles (Russell et al., 2012), tar sands operations (McLinden et al., 2012), shipping (de Ruyter de Wildt et al., 2012), and cities as a whole (Beirle et al., 2011), as well as natural sources like lightning (Martin et al., 2007; Bucsela et al., 2010) and soils (Hudman et al., 2012). However, to our knowledge, the studies have not been extended to monitoring or regulation of point source emission trends.

At even larger scales, regional, national, and continental CO emissions from small-scale combustion operations, agricultural burning, forest fires, etc., have been estimated in many studies since the launch of the NASA Terra Measurements of Pollution in the Troposphere (MOPITT) instrument in 1999 (e.g., Hooghiemstra et al., 2012). Two pollutants that are emitted from dispersed sources over wide areas, methane (Bloom et al., 2010) and ammonia (Clarisse et al., 2009), are being studied because emission inventories are unreliable in their characterization of emissions from rice cultivation, fertilizer application, small-scale oil and gas operations, coal production, etc. The most useful of the VOC species that can be observed from space are formaldehyde and glyoxal because they are chemical products of the oxidation of isoprene, a VOC emitted by vegetation, and therefore indicators of the amount of secondary organic aerosol production (e.g., Palmer et al., 2006).

The ability to construct time trends of inferred emissions at scales from days to years has enabled a number of key indicators of human activity to be observed from space, particularly in relation to area-wide NO_x emissions. Weekly cycles of emissions (Kaynak et al., 2009), the effectiveness of temporary emission controls of about monthly duration (Witte et al., 2009), and the impact of economic recessions on emissions of about yearly duration (Castellanos and Boersma, 2012; Russell et al., 2012) have all been reported in the scientific literature. But these applications are under-used by

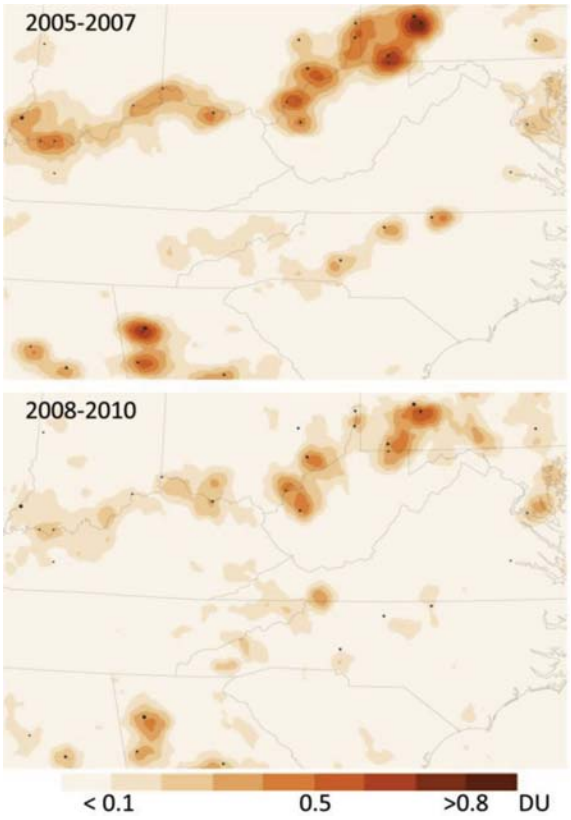

Fig. 4. OMI SO_2 VCD data (DU; 1 DU = 2.69 × 10^{16} molecules/cm^2) illustrate the success of emission control efforts between 2005 and 2010 at power plants, indicated by dots, in the eastern U.S. (adapted from Fioletov et al., 2011). The averages in both the top and bottom panels are averages of three years each, 2005–2007 and 2008–2010, respectively.

environmental professionals. Lamsal et al. (2011) showed that emissions estimates can be rapidly updated, while the laborious process of gathering new source data to update emission inventories can take years.

3.2. Monitoring long-term trends of ambient pollutant concentrations

As a result of environmental regulations (e.g., the 1998 NO_x SIP Call, the Clean Air Interstate Rule (CAIR), and the Tier 1 and 2 standards of the Clean Air Act Amendments) on point and mobile source emissions, most pollutants that can be measured from space show a significant decrease over the U.S. during the satellite data record (1996-present). These changes are generally consistent with decreases in surface observations reported by EPA (EPA, 2012). For instance, Fig. 5 illustrates OMI NO_2 VCD data which shows that NO_2 over the U.S. declined significantly (~30–40%) during both the ozone season (i.e., May–September; Fig. 5a) and annually (Fig. 5b) from 2005 to 2012. Russell et al. (2012) used their version of OMI NO_2 VCD data to infer that NO_x emissions changes from large power plants were variable because of regionally-specific regulations, decreasing by 26 ± 12% from 2005 to 2011. They also estimated an average total reduction of 32 ± 7% in NO_2 for U.S. cities from 2005 to 2011 with a 34% decrease in NO_2 from mobile sources. They attributed part of the observed decline in the data to the turnover in the mobile source fleet and part to the global economic recession that began in 2008. OMI data also show that emissions of SO_2 and NO_x have decreased dramatically from coal power plants in the U.S. with the implementation of scrubber technology and emission control devices. Fioletov et al. (2011) found a 40% decline in SO_2 over the largest power plants between 2005 and 2010 (Fig. 4), which is consistent with the 46% decrease in emissions as reported by CEMS. Duncan et al. (2013) concluded that it is practical to use OMI NO_2 VCD data to assess changes of emissions from power plants that are associated with the implementation of emission control devices. The cumulative data records from four similar sensors (i.e., European Remote Sensing (ERS-2) Global Ozone Monitoring Experiment (GOME); Envisat SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY); Aura OMI; and European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT) Metop-A GOME-2) make it possible to estimate long-term trends of NO_2 and SO_2 from 1996 to present (e.g., Lu and Streets, 2012; Fioletov et al., 2013).

Relating satellite-derived VCD data trends for a relatively long-lived gas (e.g., CO) to trends in surface pollutant concentrations is

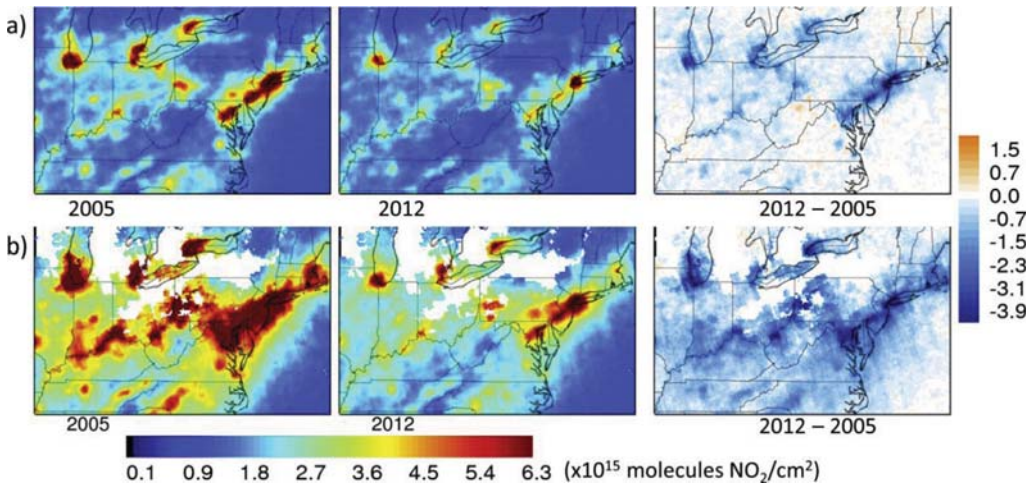

Fig. 5. a) OMI tropospheric NO_2 VCD data (×10^{15} molecules/cm^2) as an average for the ozone season (May–September) in 2005 (left) and 2012 (middle) over the eastern U.S. The difference (×10^{15} molecules/cm^2) between the two years is also shown (right). b) The same as a), but as an annual average (January–December). In the left and middle panels, the white areas indicate regions where at least one month has three or less days of data with which to create the monthly averages, such as in winter with persistent snow and/or cloud cover.

more difficult than for a short-lived gas (e.g., SO_2, NO_2). Most of the VCD for a short-lived gas is found near its surface emission sources because its chemical lifetime is short (i.e., hours to about a day depending on meteorological conditions) and its background level is low relative to the level in industrialized areas. On the other hand, a long-lived gas can have a high background concentration relative to that in industrialized areas. MOPITT data show that CO decreased by ~1.4%/yr from 2000 to 2012 over the eastern U.S. (Worden et al., 2013), while surface observations show a much stronger response (~5%/yr) over this same period (EPA, 2012). However, He et al. (2013) compared the near-surface MOPITT CO product (Section 5.2.4; Deeter et al., 2012) to EPA Air Quality System (AQS) observations and found that the estimated decreases were similar (~40%) from 2000 to 2011 in the Baltimore–Washington, DC metropolitan area. As with all data, whether from satellite instruments or surface monitors, the confidence associated with an estimated trend is correlated with the magnitude of the trend relative to data uncertainties (Section 5.7).

4. Data basics, including processing and visualization resources

Data access is a common barrier to data use because of the increasingly large number of data types, metadata, and websites for finding data, all of which can be daunting for the first time user. This section provides the basics of using satellite data for AQ applications, including direction for finding imagery, data maps, and data files, and a list of some of the most popular and free web-based analysis tools (Table 2). The datasets available from the websites in Table 2 are free and available to everyone.

4.1. ARSET and AQAST

The NASA Applied Sciences Program, within NASA's Earth Science Division, initiated two programs to promote and facilitate the use of satellite data in the decision-making and environmental management activities of public, private sector and non-profit organizations, such as EPA, state AQ agencies, the American Heart Association, public utilities and other for profit entities, and Non-Governmental Organizations (NGOs). In 2008, the Applied Remote SEnsing Training (ARSET) program (http://arset.gsfc.nasa.gov/; Prados, 2012) began providing in-person and on-line AQ courses, workshops and other capacity building activities for end-users. Since then, the program has expanded to include water resources, disaster management and ecological forecasting. The ARSET website contains free training materials, and information on instructional webinars and in-person courses. Organizations interested in in-person trainings may submit an application through the ARSET webpage. ARSET personnel provide general guidance to end-users on data for specific AQ applications, but they do not provide data analysis upon request. Instead, end-users are encouraged to contact members of the Air Quality Applied Sciences Team (AQAST; http://acmg.seas.harvard.edu/aqast/), which directly engage the management of end-user organizations, serving their applied research needs with a combination of satellite data, sub-orbital measurements, and computer models.

4.2. Levels of data and spatial resolution

Satellite data come in various 'Levels' which indicate the degree of processing. Level 0 (L0) data are the raw data obtained from the instrument and are processed to Level 1 (L1). L1 data are produced by applying the instrument pre and post-launch calibrations to produce radiances and then geolocating these data. Level 2 (L2) and Level 3 (L3) data are processed from L1 to a geophysical parameter, such as AOD or NO_2 VCD. The relevant Levels for AQ applications are L2 and L3. The key difference between L2 and L3 is that L2 data are the original geolocated observations and not spatially gridded while the L3 data are mapped to a regular spatial grid (e.g., 0.25° latitude × 0.25° longitude), and averaged over time, such as a day or month. Fig. 6 shows an example of a Terra MODIS L2 image of AOD. The spatial resolutions of L2 data vary widely between instruments. L3 data generally have lower spatial and temporal resolutions than L2 data, but they have the advantage of being easier to read, visualize, and analyze. L3 data may be adequate for most regional AQ applications, but the majority of end-users find that L2 data are better suited for examining point sources or urban pollution.

4.3. Temporal resolution and latency

The temporal resolution of satellite data is determined by many factors, including the satellite type (e.g., polar-orbiting vs. geostationary; Section 5.5), the orbital swath width of the instrument (i.e., the width of the "stripe" of the Earth's surface observed as a satellite overpasses), and the degree of snow cover and cloud cover (e.g., Fig. 5b). Most data are from instruments on polar-orbiting satellites (e.g., Terra, Aqua, and Aura) that have 90-min sequential orbits, thus achieving global coverage in a day or two. That is, the data are collected daily at approximately the same local time (±45 min) at every location of the globe. For instance, the Aura satellite overpasses any given location once in early afternoon local time while the Terra satellite overpasses a location once in mid-morning. L2 data have a time stamp in the data files associated with each ground pixel. L3 data, which are processed to a specific horizontal grid and are an aggregate of the L2 data over time, do not have a time stamp associated with each observation.

Latency refers to the time after an observation is made until the data become publicly available through a web portal. An increasingly large number of "near-real-time" products become available via websites (Table 2) within a few hours of the instrument's data collection. The data are processed quickly to obtain L2 and L3 products that are intended for operational use, such as AQ forecasting or disaster management. While near-real-time products are

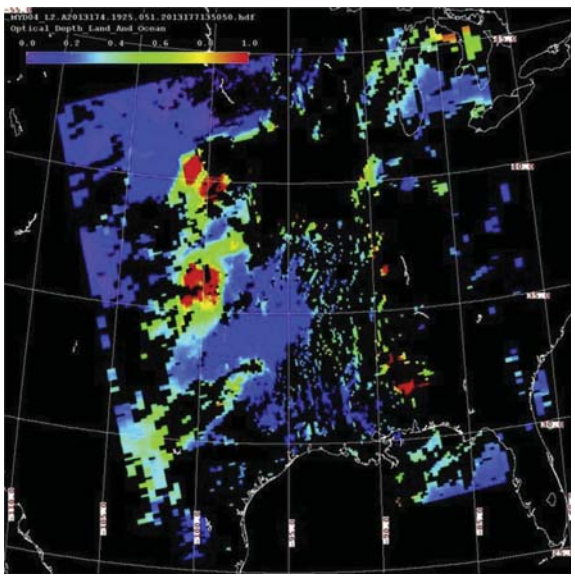

Fig. 6. MODIS Level 2 image from the Level 1 and Atmosphere Archive and Distribution System (LAADS) web tool (Table 2) showing enhanced AOD levels due to fire activity in the central U.S.

often high quality, the L3 data are carefully reprocessed later, so that the near-real-time and final products may not be identical.

4.4. Access to data files

Official NASA products are managed by NASA's Earth Observing System Data and Information System (EOSDIS) and its twelve data centers, which archive data from the beginning of each mission, thus enabling retrospective studies and analysis. EOSDIS has several search engine tools, such as Reverb, which allows end-users to search available data files by instrument, sensor, and pollutant type. Files can also be temporally and spatially sub-setted so that it is not necessary to download entire global files, which can be large. Gas and aerosol products can be found at the Goddard Earth Sciences Data and Information Services Center (GES DISC) and at the Langley Research Center Atmospheric Science Data Center (LaRC ASDC). Near-real-time products can be accessed via NASA's Land Atmosphere Near real-time Capability for EOS (LANCE) (Fig. 7).

4.5. Visualization and analysis tools

The most commonly used tools for the visualization and analysis of satellite data are described in this section and Table 2. Most websites provide imagery in commonly-used file formats, including gif, png, kml or kmz (for Google Earth visualization), web map service (wms), and GIS. For a comprehensive list of web tools please visit the ARSET website, which provides tables of available web tools for accessing satellite data for 1) specific pollutants, such as NO_2, CO or aerosols, 2) fire and smoke products, and 3) true color imagery. Many products are available from multiple web tools. To help end-users find the most suitable tool for their needs, the ARSET tables also contain information on the characteristics of the satellite data in each web tool, such as spatial and temporal resolution, data file formats and level of processing (e.g., L2, L3).

4.5.1. Gas and aerosol products

Maps and basic customized analysis of satellite and ground-based geophysical parameters, such as pollutant VCDs or aerosol extinction profiles, can be obtained from a variety of NASA websites. These web-based tools enable end-users to easily make images online by searching and selecting the needed parameters and specifying the dates and geographical area of interest. Three of the most popular tools are Worldview, Giovanni, and LAADS Web (e.g., Fig. 6). The LANCE interface (Fig. 7) provides access to Worldview and is NASA's main tool for visualization and download of near-real-time data and imagery, including for gases, aerosols, fire locations and true color imagery. Giovanni allows the user to perform simple analysis, such as time series and multi-day area-averaged image maps, without the need to download software (Prados et al., 2010). Data files and images of aerosol and gas observations are available under the "Air Quality" or "Atmospheric Portals" sections. LAADS Web provides easy access to L1 data from MODIS and VIIRS.

There are also multiple stand-alone image visualization packages for download, many at no cost. They range from simple visualization tools, such as *Panoply* from the NASA Goddard Institute of Space Studies, to more sophisticated packages, such as *HDF Look*, that provide both data visualization and analysis capabilities. ARSET trainings provide guidance on the use of all these tools, and training modules can be found on the ARSET website under the "tools" section.

Other federal agencies provide visualization and analysis capabilities of NASA satellite products. The Infusing Satellite Data into Environmental Applications (IDEA) web tool is supported by the NOAA National Environmental Satellite, Data, and Information Service (NESDIS) and provides near-real-time access to MODIS and GOES aerosol products and meteorological information. IDEA also provides maps and time series of both $PM_{2.5}$ measured by surface monitors and $PM_{2.5}$ derived from satellite AOD data to facilitate comparisons between satellite and surface observations. The $PM_{2.5}$

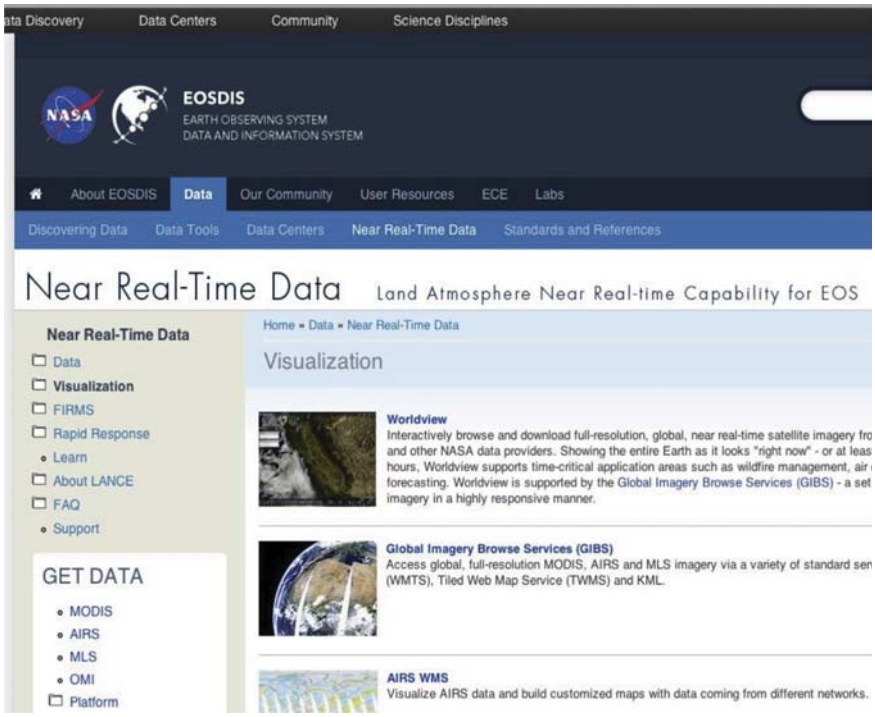

Fig. 7. Interface of the EOSDIS LANCE web tool. As seen in the menu to the left, LANCE provides near-real-time data, including the capability of downloading data files and images, and number of visualization options relevant to AQ applications. Worldview, which can be accessed by clicking on the Visualization tab to the left, is a mapping interface where one or more images can be overlaid on a map, such as a MODIS true color image and an OMI NO_2 VCD plot. The web tools allow the end-user to customize the images (Table 2).

maps also include forward trajectories at multiple pressure levels initialized in regions of enhanced AOD. The EPA Remote Sensing Information Gateway (RSIG) tool is designed to facilitate comparisons between CMAQ model output and NASA and NOAA satellite data.

4.5.2. Near-real-time true color imagery and fire products

True color imagery provides qualitative information that can be very valuable in representing the "big picture" of what is occurring regionally, such as for determining the location of forest fire smoke plumes and smoke plume extent (e.g., Fig. 3). This type of imagery closely resembles what the naked eye sees. Current fire locations and burned area products from the MODIS instrument are available from the LANCE FIRMS website. The NOAA Hazard Mapping System Fire and Smoke Product (HMS) provides fire locations from MODIS and smoke plume extent from GOES and MODIS, and is used frequently by first responders, forecasters, and in exceptional event demonstrations. For a comprehensive list of websites that provide true color imagery, including near-real-time imagery, visit the ARSET website under the "Satellite Imagery" section.

4.5.3. Exceptional Event Decision Support System (EE DSS)

The Washington University in St. Louis has developed an Exceptional Event Decision Support System (EE DSS) that facilitates the analysis of both surface and satellite data for exceptional event submissions. EE DSS is hosted by DataFed, which provides a wealth of satellite and surface AQ data from NOAA, NASA, EPA, and other entities. EE DSS features distinct data analysis portals for the various criteria required by EPA to justify data exclusions due to an exceptional event. Time series of ozone, PM_{10} and $PM_{2.5}$ from surface monitors can be easily plotted along with the relevant NAAQS to help determine whether the measured concentration is above the NAAQS threshold and whether it is beyond typical levels. There is also a console that provides MODIS true color imagery, AOD and NO_2 data, and meteorological data hosted by DataFed, to help regulators seeking to analyze a causal relationship between the measurement under consideration and the exceptional event.

5. Straight answers to frequently-asked questions (FAQs)

Here are answers to some of the most frequently-asked questions concerning the use of satellite data for AQ applications.

5.1. How does a satellite instrument measure gases and aerosols?

Most satellite instruments that collect data relevant for AQ applications are "passive". ("Active" instruments, such as lidars or radars, send a signal and detect the portion of the signal that returns.) Passive instruments detect electromagnetic radiation from the Sun that is absorbed and reemitted, reflected, and scattered by the Earth and atmosphere. The incoming radiation passes through a spectrometer, a device that measures energy intensity as a function of wavelength, to create a spectrum of wavelengths that are then detected. When individual photons strike the instrument's detector, the energy is converted into electrons as a way of measuring the amount of incoming energy at various wavelengths. The infrared (IR), visible, and ultraviolet (UV) regions of the electromagnetic spectrum contain the most useful wavelengths for observing pollutants relevant for AQ applications as these gases and aerosols absorb IR wavelengths (e.g., water vapor) or scatter visible and UV wavelengths (e.g., dust, NO_2).

5.2. Can satellites measure "nose-level" concentrations?

The short answer is "no" because the majority of satellite instruments that measure pollutants of interest to the AQ community are downward-looking, providing limited information on the vertical structure of the pollutant in the atmosphere. Satellite instruments that measure ozone, NO_2, formaldehyde, and SO_2 detect the number of molecules between the instrument and the Earth's surface (i.e., a VCD). Nevertheless, these data are highly useful in many AQ applications, including for inferring "nose-level" concentrations as discussed in this section. For aerosols, satellite instruments observe AOD, which is a measure of the integrated extinction by aerosols of light passing through the entire atmospheric column from the surface of the Earth to the satellite instrument. Surface $PM_{2.5}$ may be inferred from AOD data in many instances (Section 5.2.6). For more in-depth discussions of issues associated with detecting surface concentrations from space, beyond what is presented in this section, the reader is referred to Fishman et al. (2008), Martin (2008), and Hoff and Christopher (2009).

5.2.1. Are there satellite data for surface ozone?

The development of a surface ozone product is fraught with many obstacles, so that such a product is not currently feasible. First, the portion of the ozone VCD that is in the troposphere is about 10 times less than the amount in the stratosphere (e.g., "ozone layer"), making it very difficult for satellite instruments to discriminate the stratospheric and tropospheric amounts. There are several methods to separate the portion of ozone found in the stratosphere from that found below the stratosphere (e.g., Fishman et al., 2003). However, the relation is complicated for the tropospheric, including lower tropospheric, ozone VCDs and near-surface ozone (e.g., de Laat et al., 2005; Chatfield and Esswein, 2012). A model is required to properly interpret the tropospheric ozone VCD data. Nevertheless, the tropospheric ozone VCD data sometimes correlates well with surface data, including in urban areas (Kar et al., 2010). Flynn et al. (2014) suggest that ozone partial column densities from future satellite instruments with sufficient sensitivity to the lower troposphere can be meaningful for surface AQ analysis. Second, ultraviolet (UV) wavelengths of light, which are used for detecting and measuring ozone, are strongly obscured by atmospheric scattering, which limits their ability to reach the Earth's surface. Infrared (IR) wavelengths can also be used for inferring ozone in the troposphere, but the products are sensitive to the input parameters used to create them (Section 5.3). Research is ongoing that could enable measurements of boundary layer ozone, which is based on using the combination of UV and IR wavelengths (e.g., Worden et al., 2007; Zoogman et al., 2011; Bowman, 2013).

There are satellite data that give information near the surface on ozone's chemical precursors (i.e., NO_x (Section 5.2.2) and VOCs (Section 5.2.3)). Together, NO_2 and formaldehyde VCD data can be used to infer the chemical sensitivity (i.e., "VOC-limited" versus "NO_x-limited" regimes) of ozone production near the surface. Sillman (1995) used correlations between surface observations of various pollutants (e.g., formaldehyde and total reactive nitrogen (NO_y)) to determine this chemical sensitivity. Martin et al. (2004) applied the technique of Sillman (1995) to satellite observations, using the ratio of the VCDs for formaldehyde and NO_2 from GOME. Duncan et al. (2010) expanded on the work of Martin et al. (2004) with OMI data, finding that the majority of the U.S. is now in the NO_x-limited regime due to recent NO_x emissions reductions (Fig. 5).

5.2.2. Are there satellite data for surface NO_2?

While it is not feasible to measure surface NO with current instruments (e.g., Bovensmann et al., 1999), surface NO_2 is readily

detected. The NO_2 VCD serves as an effective proxy for NO_x and correlates well with surface levels of NO_2 in industrialized regions (e.g., Leue et al., 2001; Velders et al., 2001). Most of the NO_2 VCD is found near its surface emission sources because its chemical lifetime is short (i.e., hours to about a day depending on meteorological conditions) and its background level is low relative to the level in industrialized areas. Like ozone, there is a significant contribution to the NO_2 VCD from the stratosphere, but it can be subtracted (e.g., Bucsela et al. (2013) and references therein). Even if the stratospheric portion is not removed, the local gradients in the VCD are associated with gradients near the surface in polluted regions as the distributions of NO_2 in the stratosphere are rather uniform. This subtraction is already done in the L2 and L3 OMI NO_2 products (Section 4.2). Airborne measurements over polluted areas suggest that the portion of the NO_2 VCD in the boundary layer could be over 75% of the tropospheric VCD over land (Martin et al., 2004; Bucsela et al., 2008). Ordóñez et al. (2006) demonstrated a strong correlation between the tropospheric NO_2 VCD and surface NO_2 observations. Lamsal et al. (2008, 2010) developed a method for estimating surface NO_2 from OMI NO_2 VCD data, finding that their OMI-derived surface NO_2 concentrations were well correlated with surface AQS measurements, both temporally ($r = 0.3–0.8$) and spatially ($r = 0.76$). Knepp et al. (2013) found that VCD data from a ground-based suntracking spectrometer system, which is similar to OMI, compared well to "nose-level" NO_2 data collected nearby when the daily cycle of boundary layer mixing was taken into account.

5.2.3. Are there satellite data for surface VOCs?

There is a myriad of VOC compounds that contribute to ozone formation, but only a few can be detected from space (e.g., methanol, formaldehyde, glyoxal, and peroxyacetyl nitrate (PAN)). Formaldehyde can serve as a proxy for total VOC chemical reactivity with the hydroxyl radical (OH; e.g., Chameides et al., 1992) as most VOCs react with OH and are, subsequently, oxidized to formaldehyde. It has been shown that the variability in the distribution of formaldehyde is highly correlated with isoprene (Palmer et al., 2003, 2006; Millet et al., 2008), a VOC emitted by trees that is known to play an important part in the formation of ozone in the eastern U.S. (Chameides et al., 1988). The strong temperature-dependence of isoprene emissions has been inferred from satellite data (Abbot et al., 2003; Palmer et al., 2006). Like NO_2, most of the horizontal gradient in formaldehyde VCD data is correlated with the distribution of surface sources as its chemical lifetime is relatively short. Formaldehyde VCD data have a large uncertainty associated with them, so care should be taken when using them (Section 5.7).

5.2.4. Are there data for surface CO?

There are several instruments that measure infrared (IR) wavelengths of light to infer CO concentrations. Instruments that observe thermal-infrared (TIR) wavelengths can measure CO in the free troposphere, though the vertical resolution is rather poor (e.g., only one or two levels). Data from these instruments have been shown to be useful, for instance, in tracking the long-range transport of pollution, such as from wildfires, but they do not provide information on "nose-level" CO. Instruments that observe near-infrared (NIR) wavelengths give information on the CO VCD, which can be used to infer surface emissions and where high levels of CO occur. Currently, Terra MOPITT measures near-surface CO (surface – 900 mb). It observes both TIR and NIR wavelengths and the recent algorithms are making use of this complementary information to infer CO near the surface (Deeter et al., 2012). There are several limitations of this product: only land surfaces during daytime have information in the NIR and the measurement sensitivity to near surface CO has large variability over different surface types.

5.2.5. Are there data for surface SO_2?

SO_2 data have proven quite useful for some AQ applications, such as observing changes in pollutant levels near large point sources (e.g., Fig. 4; Fioletov et al., 2011), but it is not currently useful for analyzing day-to-day variations, such as during an AQ event; SO_2 data need to be carefully processed and interpreted (Section 5.8). Research is ongoing to improve the data and there have been recent important advances (e.g., Li et al., 2013).

5.2.6. Are there data for surface $PM_{2.5}$?

Satellite instruments do not measure $PM_{2.5}$, but do observe AOD. If $PM_{2.5}$ is well mixed in the boundary layer and skies are free of clouds, the AOD-$PM_{2.5}$ relationship can be expressed as:

$$\mathrm{AOD} = \mathrm{PM}_{2.5} \times H \times f(\mathrm{RH}) \times \frac{3Q_{\mathrm{ext,dry}}}{4\rho r_{\mathrm{eff}}} \quad (1)$$

where H is the boundary layer height, f(RH) is the ratio of ambient and dry extinction coefficients, ρ is the aerosol mass density, $Q_{\mathrm{ext,dry}}$ is the Mie extinction efficiency, and r_{eff} is the particle effective radius (Hoff and Christopher, 2009). The conversion of AOD data to surface $PM_{2.5}$ data is complicated as it requires knowledge of various factors that influence AOD, such as relative humidity (e.g., Case Example #1 in Section S.1), aerosol composition (e.g., soot, dust), and the altitude of the aerosol layer (e.g., Wang and Christopher, 2003; Engel-Cox et al., 2004; Zhang et al., 2009; Crumeyrolle et al., 2013). Section S.4 contains a discussion of satellite prediction of surface $PM_{2.5}$ levels.

5.2.7. Are there data for surface ammonia?

Ammonia is of interest to the AQ community as it can lead to PM formation. Data products with near-surface information on ammonia levels are under development (e.g., Zhu et al., 2013; Van Damme et al., 2014) and have the potential to be used to identify sources (e.g., intensive livestock production and agriculture), including small ones.

5.3. Why are there multiple products for the same species?

Satellite instruments measure the scattering or emission of electromagnetic radiation by the atmosphere, not atmospheric quantities of pollutants (Section 5.6). The conversion of electromagnetic radiation to an atmospheric quantity, which is referred to as a "retrieval algorithm", is a complicated and multi-step process (e.g., Sections 5.6 and 5.7). Often there are a number of ways posed and tested by research groups to derive this atmospheric quantity. Consequently, multiple products can exist for the same pollutant from the same instrument. In addition, the refinement of a specific retrieval algorithm may occur over many years, leading to multiple versions (presumably with incremental improvements) of a given product from the same research group. For example, NO_2 VCD data have proven highly valuable for AQ applications as discussed in Section 3. There are two main products that are available for OMI. The early releases of the products, one from NASA and the other from the Royal Netherlands Research Institute (KNMI), often disagreed by up to a factor of two for some regions (e.g., Lamsal et al., 2010). However, the current, refined retrieval algorithms of both research groups, though different in their approaches, now produce very similar atmospheric quantities (e.g., Bucsela et al., 2013). The refinement of these algorithms will likely continue for some time as researchers strive to improve their products.

Some atmospheric quantities are measured by several satellite instruments. This occurs for a variety of reasons. First, individual countries, including the U.S., the European Space Agency (ESA), and Japan, support their own satellite programs. Second, some instruments provide data for a particular area (e.g., North America) or a particular time of day. As an example, the GOES satellite observes AOD levels over North America in a geostationary orbit, while the MODIS instruments on the Terra and Aqua satellites provide global coverage at approximately 10 am and 2 pm local times, respectively. Third, replacement instruments are generally launched before the end of life of aging instruments so that there is a period of overlap when both instruments are collecting data. This is important for the creation of long-term data records from multiple instruments (e.g., Lu and Streets, 2012; Fioletov et al., 2013). Finally, in some cases, instruments designed to measure a particular pollutant or set of pollutants will have sufficient capability to observe other pollutants that the instrument was not originally designed to measure.

Ultimately, the onus is on the end-user to understand the strengths and limitations of a particular product so as to decide which one is most appropriate for the particular AQ application and to properly interpret the data. There are now a number of helpful resources at the disposal of the end-user to simplify this task (Section 4).

5.4. Are there data with finer spatial resolution?

As discussed in Section 4.2, the spatial resolutions of products vary widely, depending on the instrument and the level of data processing. Ultimately, the data with highest spatial resolution for a specific product is a tradeoff between the sensitivity and pixel size of the instrument. As with a photo from a common digital camera, the image produced from a satellite instrument is composed of many pixels. The spatial area of the Earth's surface observed by a pixel is often referred to as a pixel's "footprint". The footprints of individual pixels on the same instrument can vary, particularly if the instrument scans the atmosphere from either side of the orbital track where the pixel size increases as the viewing angle increases. The pixel that views the atmosphere directly below it (i.e., perpendicular to the Earth's surface) is referred to as the "nadir" pixel and has a footprint of, for instance, 13×24 km^2 in the case of OMI and 10×10 km^2 or 3×3 km^2 for MODIS. For OMI, the largest footprint is ~$13 \times$ ~150 km^2 (Levelt et al., 2006). All the pixels together observe an area 2600 km wide, which is referred to as the "field of regard", with each overpass.

The advantage of a wide field of regard is that it allows for daily global coverage of the entire Earth's surface. The disadvantage is that the footprints of many pixels are too large for AQ applications. Advanced versions of OMI are under development which will have smaller pixel sizes (Section 5.11.1). Statistical methods can be used to decrease pixel size, such as the technique of "oversampling" the data (e.g., de Foy et al., 2009; Fioletov et al., 2011; Streets et al., 2013), but this requires averaging data over time and losing some temporal resolution to achieve statistical significance (Section 5.8) of the data on the finer horizontal grid.

5.5. Are there data that span the entire day?

For AQ applications, an instrument on a satellite in geostationary (or geosynchronous) orbit is ideal as this allows for continuous observations of the same region (e.g., the U.S.); the satellite's orbital period matches the Earth's rotational period, so the satellite appears to be motionless to an observer on the Earth's surface. The NOAA GOES series is an example of geostationary satellites and the current GASP product from the GOES-West and GOES-East instruments provides AOD at 30 min intervals throughout the day. NASA is actively planning an instrument, called Tropospheric Emissions: Monitoring of Pollution (TEMPO), on a geostationary satellite that will measure pollutants relevant for AQ applications and NOAA will launch the GOES-R series beginning in 2016, which will also provide aerosol products (Section 5.11).

Currently, almost all instruments that provide information on pollutants, such as AOD, NO_2, SO_2, and formaldehyde, are onboard polar-orbiting satellites, which overpass a given location in the U.S. approximately once a day during daylight hours. Because polar-orbiting satellites have different overpass times, for certain pollutants it is possible to obtain a limited amount of information on their daily variability. For instance, data are collected from OMI on the Aura satellite, which has an early afternoon overpass, and from GOME-2 on the EUMETSAT Metop satellite, which has a morning overpass. In addition, Terra MODIS and Aqua MODIS overpass at approximately 10 am and 2 pm local times, respectively. In multi-instrument analysis, it is important to account for differences in the capabilities, biases and other characteristics of the individual instruments (e.g., Boersma et al., 2008; Fioletov et al., 2013).

5.6. How does one quantify the amount of a pollutant in the atmosphere from satellite data?

Each pollutant absorbs and/or reflects specific wavelengths throughout the electromagnetic spectrum. This "spectral signature" is unique to that pollutant, like a fingerprint is unique to each human. (The reader is directed to Fig. 1 of Martin (2008) for an illustration of a spectral signature.) For some pollutants, the unique signature is readily apparent, but for others, the signature overlaps with the signatures of other gases, such as water vapor and ozone in the IR wavelength range (Section 5.7). The magnitude of the quantity of a pollutant in the atmosphere can be inferred by comparing the spectral signature recorded by the satellite instrument to a reference signature measured in a lab using a known quantity of the pollutant. In practice, this requires a complicated model of radiative transfer (i.e., the propagation of electromagnetic energy through the Earth's atmosphere) to interpret what is measured by the satellite instrument. The model accounts for the absorption, emission, and scattering of light by clouds, the Earth's surface, aerosols, and all gases, including the pollutant of interest, as it passes through the Earth's atmosphere to the satellite. Hoff and Christopher (2009) give more details on the equations used in radiative transfer models.

5.7. Why do some products have higher uncertainties than others?

For each satellite product, there is an associated uncertainty which includes bias and precision errors. The overall uncertainty is a combination of uncertainties from a number of sources, such as those associated with the instrument and those introduced during the creation of the product (e.g., Kahn, 2012; Bucsela et al., 2013). For a discussion of the uncertainty, the end-user should consult the documentation that is provided for each product.

5.7.1. Spectral uncertainties

Some pollutants are easier to measure because their spectral signatures are stronger and/or distinct, while others are more difficult, particularly if the spectral signatures overlap with other gases. For example, of the OMI NO_2, SO_2, and formaldehyde VCD data products, the overall uncertainty is lowest for the NO_2 product as NO_2 has strong and distinct spectral structure at wavelengths where it is the dominant absorber. That is, it is relatively easy to remove the effects of other species (e.g., ozone, water vapor, etc.) that absorb in the same spectral region. For formaldehyde and SO_2,

ozone absorption dominates at wavelengths used in their retrievals. The SO_2 absorption is particularly weak as compared to ozone's absorption.

5.7.2. Uncertainties associated with the creation of VCDs

The "slant" column density (SCD) observed by the satellite is converted to a "vertical" column density (VCD) of a pollutant, which is perpendicular to the Earth's surface (e.g., L2 and L3 data; Section 4.2). This conversion process, which is described in Palmer et al. (2001), is required so that the data may be presented in easy to understand geographic maps. There are multiple uncertainties introduced into a product during this multi-step process (e.g., Leue et al., 2001; Bucsela et al., 2013), which may have implications for a specific AQ application. For instance, satellite data for a gas (e.g., CO or NO_2) from wildfires require special treatment to properly estimate the VCDs. During the production of a gas product, it is necessary to 1) account for the presence of aerosols, which absorb and scatter light and can interfere with the detection of a gas, and 2) assume an "initial guess" of the atmospheric vertical profile of the concentration of the gas (Section S.5). Oftentimes, a model is used to estimate the aerosol loading and the vertical profile for typical conditions (i.e., when there is not a wildfire). However, a fire can cause the aerosol loading and the vertical profile of a gas to be dramatically different as compared to typical conditions. While the influence of wildfires is not routinely accounted for, or only partially accounted for, in the generation of many gas products, it should be to properly estimate the VCD of a gas. Otherwise, the gas product is simply qualitative at best for this application.

Research is ongoing to reduce uncertainties, which leads to multiple versions of some gas and aerosol products as incremental improvements are made (Section 5.3). Because of these uncertainties and assumptions made in the retrieval algorithms, we use the term "product" when discussing specific datasets in this article, but use "data" when speaking generically about satellite data.

5.8. How do I know if my data are statistically significant and accurate?

As with all data, including from surface networks, a statistical analysis is required so that the end-user does not draw an erroneous conclusion – a common mistake that should be avoided. Here we discuss briefly random and systematic errors.

5.8.1. Random error

If the error for a given product is random, it will cancel in the average over space and/or time. That is, individual observations may be imprecise, but their average is precise. Therefore, one must consider the time-averaging interval used in a trend analysis, for instance. The overall confidence that the average is statistically significant increases with the square root of the number of individual overpasses (N) included in the average. However, the N required for statistical significance increases as uncertainty increases (i.e., as the precision decreases), so it can vary significantly from pollutant to pollutant. (As a word of caution, it is important to include data with negative values or the end-user may introduce a bias to the averaged data.) As a general rule of thumb, one should average data on the order of weeks for tropospheric NO_2, six weeks or more for formaldehyde, and a year or more for SO_2, depending on the degree of concomitant spatial averaging and overall concentration of the pollutant. For example, Duncan et al. (2013) used OMI NO_2 VCD data as a proxy for the month-to-month changes in NO_x emissions from power plants in the U.S. For their analysis, they required a fine horizontal resolution (0.1° latitude × 0.1° longitude) to isolate the signal of the power plant. However, they found that N was often too low for statistical significance at these horizontal and temporal resolutions, particularly in winter in regions with persistent snow and/or cloud cover (e.g., Fig. 5b). (As a word of caution, it is necessary to filter satellite data for cloud cover. Please consult the data documentation for recommendations on filtering criteria.)

The treatment of errors in AOD is dependent on the specific application. When converting AOD to $PM_{2.5}$, the random AOD retrieval error is often carried through the statistical model (Section S.4) into the $PM_{2.5}$ estimates. Most advanced models developed in the U.S. can estimate daily $PM_{2.5}$ concentrations. These estimates are then averaged spatially (e.g., from the modeling grid cells to a county in order to be linked to population and disease characteristics) and/or temporally (e.g., from daily to weekly, monthly, or a longer period for trend analysis). At this stage, the random error in individual $PM_{2.5}$ predictions is reduced through averaging. For applications requiring daily $PM_{2.5}$ estimates at the model's highest spatial resolution (e.g., air pollution episode analysis), such errors can be quantified at the level of the dataset or individual estimates with standard metrics such as root mean square error, relative error and techniques such as cross-validation. The end-user then must decide whether the model performance is sufficient before drawing conclusions based on the mean $PM_{2.5}$ estimates.

In polluted regions, pollutant levels for AOD and NO_2 may be high enough that one can use the data to analyze an individual AQ episode, which typically lasts only a few days, but a larger N is necessary in less polluted regions. It is not advised to put much faith in VCD data for formaldehyde and SO_2 on the time scales of an AQ episode, even if they appear to be credible; the VCD data will be semi-quantitative, at best, and not statistically significant.

5.8.2. Systematic error

In addition to random error, a systematic error causes data to be biased relative to other "ground truth" observations, such as those taken by instruments on aircraft or in surface networks. That is, a systematic error reduces the accuracy of the data. A bias may be a function of, for example, region and season. As with a random error, a systematic error may be introduced during the conversion of the observed SCD to a VCD, but it cannot be removed by spatial or temporal averaging. Biases may also be associated with instrument artifacts. As an example, a problem that is unique to OMI is that orbital "stripes" appear in horizontal maps of OMI products (e.g., Bucsela et al., 2013). It is worth noting that even a biased product may be precise. The issue of bias is particularly important for SO_2. For instance, Fioletov et al. (2011) used OMI SO_2 VCD data to estimate the change over time in SO_2 emissions from power plants (Fig. 4). They found that the data had large-scale, spatial patterns over the U.S. They were able to account for the spatial bias by averaging SO_2 data within a 300 km radius of a power plant and then subtracting this regional mean from the SO_2 data in the power plant plume. An example for aerosols is that the Terra Multi-angle Imaging SpectroRadiometer (MISR) tends to overestimate AOD at low levels (Kahn et al., 2010) and underestimate AOD at extremely high levels rarely seen in developed countries (Jiang et al., 2007). As a result, using MISR data to estimate $PM_{2.5}$ would potentially lead to an overestimate in a clean environment and an underestimate in a severe pollution episode. The latest MODIS 3 × 3 km^2 AOD product has been shown to have a positive bias in urban areas (Munchak et al., 2013). More importantly, the systematic error of satellite AOD is often proportional to the AOD value itself and can vary with weather conditions (e.g., proximity to clouds) and surface types (e.g., impervious surfaces or snow cover). In the setting of a quantitative analysis, the user is advised to contact the satellite instrument teams early for appropriate procedures regarding systematic error correction.

5.9. What is the best way to evaluate model output with satellite data?

Section S.5 provides a brief description of the steps required to perform an "apples-to-apples" comparison of model output and satellite VCD data using OMI NO_2 VCD data as an example. Since the steps presented in Section S.5 are not universally applicable to all satellite products, the end-user is encouraged to contact the product developers for guidance.

If variables called "scattering weights" or "averaging kernels" are provided in the satellite data file, the end-user should perform the additional step of applying them to a model's vertical concentration profile for a proper comparison. Scattering weights are associated with column density data and averaging kernels are generally associated with data of vertical profiles. They arise from the fact that satellite instruments are more sensitive to the presence of gases at higher altitudes. They are critical for interpreting the information content in the product, particularly for satellite instruments that measure a pollutant using IR wavelengths, such as MOPITT. As a word of caution, the phrase "averaging kernel" is often defined differently for different products.

In addition, a proper comparison of model output to observational data, whether from satellites or surface monitors, requires the end-user to become familiar with the strengths and limitations of the data for evaluating a model's pollutant distributions. It is important to understand the relationship between, for example, surface NO_2 (ppbv) and NO_2 VCD (molecules/cm^2; Section 5.2.2) and AOD (unitless) and $PM_{2.5}$ ($\mu g/m^3$; Section 5.2.6).

5.10. Is it true that satellite data will replace the need for surface observational networks?

No. There remain fundamental limitations to measuring surface pollution from space as discussed above (e.g., Sections 5.2 and 5.7) so that satellite data will not supplant the need for surface networks. As discussed in Section 2, spatial coverage is the strength of satellite data over surface observational networks. That is, satellite data provide complementary information to measurements collected at the surface by "filling the gaps" between monitors. Scheffe et al. (2012) argue for better integration of the existing surface network of observations with alternative observational platforms, including satellite-based ones.

5.11. What new and improved satellite missions are being built?

There is currently no satellite instrument in orbit that is optimized for AQ applications and the few upcoming instruments discussed in this section, though improved as compared to current instruments for AQ applications, will not supplant the need for surface observations (Section 5.10). For a variety of reasons, including the prohibitive costs of some missions and the risk of a satellite failing to reach orbit, NASA is exploring ways to design smaller and more cost-effective orbital and suborbital missions through its Earth Venture program. Both the TEMPO instrument (Hilsenrath and Chance, 2013, Section 5.11.1) and the Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) suborbital mission (Section S.1) are examples of NASA Earth Venture missions that are relevant for AQ applications.

5.11.1. What new and improved satellite missions are being built for gases?

For gas pollutants (e.g., NO_2, SO_2), two satellites, one from NASA and the other from the European Space Agency (ESA), will have sensors similar to Aura OMI and are currently under construction with tentative launch dates within the next five years. Both missions promise enhanced observational capabilities over those of OMI, which is important given the recent, substantial decreases in SO_2 and NO_2 levels in the U.S. (e.g., Figs. 4 and 5). The TEMPO instrument (Hilsenrath and Chance, 2013) will be in geostationary orbit over North America, collecting hourly data throughout the day as opposed to one overpass per day as with OMI. The hourly observations will improve precision of the measurement and enable a better horizontal resolution (2×4.5 km^2) than OMI's. The planned launch is 2018 or 2019. The ESA Tropospheric Ozone Monitoring Instrument (TROPOMI) is an OMI follow-on instrument with finer horizontal resolution (i.e., 7×7 km^2) than OMI and will fly on the polar-orbiting Sentinel-5 Precursor satellite. The planned launch date is 2015. Currently, there are no planned instruments by NASA to replace the Terra MOPITT instrument, which provides CO VCD data that have proven useful for tracking pollution plumes and estimating source emissions (e.g., Streets et al., 2013). TROPOMI will include instrument capabilities similar to SCIAMACHY, which flew on ESA's now defunct Envisat satellite. Therefore, it will provide CO and methane VCD data, but it will not provide information on CO near the surface as is the case with MOPITT.

5.11.2. What new and improved satellite missions are being built for aerosols?

There are few upcoming missions being built that are relevant for estimating surface aerosols. Several instruments currently provide AOD, such as the two MODIS sensors on the Terra and Aqua satellites, and on GOES satellites. Similar to instruments that measure gases, many now in orbit are past their design lives. The NPP VIIRS instrument (e.g., Fig. 2) also provides AOD, and the Advanced Baseline Imager (ABI) on the GOES-R satellite, with a planned 2016 launch, will likely continue the record of AOD. In addition, the geostationary instrument, TEMPO, should give more accurate information on the short-term evolution of aerosol plumes than the GASP product, which is sometimes used in exceptional event demonstrations for wildfires (Section 2.3).

Additional information on aerosols is desired to enable use of satellite data for decision support. First, the importance of the distribution of aerosol in the vertical is illustrated in Case Example #1 (Section S.1). Information on the vertical distribution is currently collected for near-source aerosol plumes by MISR and downwind by the NASA Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) instrument, but there are no follow-on missions currently being built to provide this information. Second, another important piece of information is aerosol type, which MISR has some capability to distinguish (Kahn et al., 2010; e.g., Patadia et al., 2013). Aerosol type data are also available from CALIPSO (nadir view only) and from the surface-based AErosol RObotic NETwork (AERONET; Holben et al., 1998, 2001). However, limitations of these data include spatial and temporal coverage. Third, particle size distribution is another desired piece of information. It is also available from AERONET, qualitatively from MISR, and over water from MODIS. While not in the "build-phase", a NASA satellite called Aerosol/Cloud/Ecosystems (ACE) has been proposed and it would provide more comprehensive measurements of aerosols to distinguish aerosol types and associated optical properties, such as size distribution. Fourth, the retrieval algorithms used to create aerosol products are not optimized for AQ applications. For instance, information is needed on land surface properties in urban areas, such as reflectivity, at high spatial resolution to capture the gradients in aerosol distributions (e.g., Lyapustin et al., 2011a,b; Chudnovsky et al., 2013a,b).

6. Summary and charge to the applied AQ community

Many AQ managers are not yet taking full advantage of satellite data for their applications because of the challenges associated with accessing, processing, and properly interpreting observational data. That is, a degree of technical skill is required on the part of the data end-user, which is often problematic for organizations with limited resources. The overall goal of this review article is to acquaint the end-user with some background information on satellite capabilities for measuring pollutants, discuss resources available to the end-user, and provide answers to common questions in plain language. Though current satellite products cannot provide "nose-level" concentrations of pollutants, we highlight the value of satellite data for AQ applications, including estimating emissions, tracking pollutant plumes, supporting AQ forecasting activities, providing supporting evidence for "exceptional event" demonstrations, monitoring regional long-term trends, and evaluating AQ models.

Current satellite instruments, observing strategies, and retrievals are not designed or optimized specifically for U.S. AQ applications nor has the full potential of satellite data for AQ applications been realized. Therefore, we strongly encourage regulatory agencies engaged in decision support and other stakeholders involved in AQ management to express their needs to the scientists who develop the products so that they may be improved and tailored for the specific needs of the AQ community. This feedback is particularly important for future satellite instrument development and mission planning.

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Appendix A. Supplementary data

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