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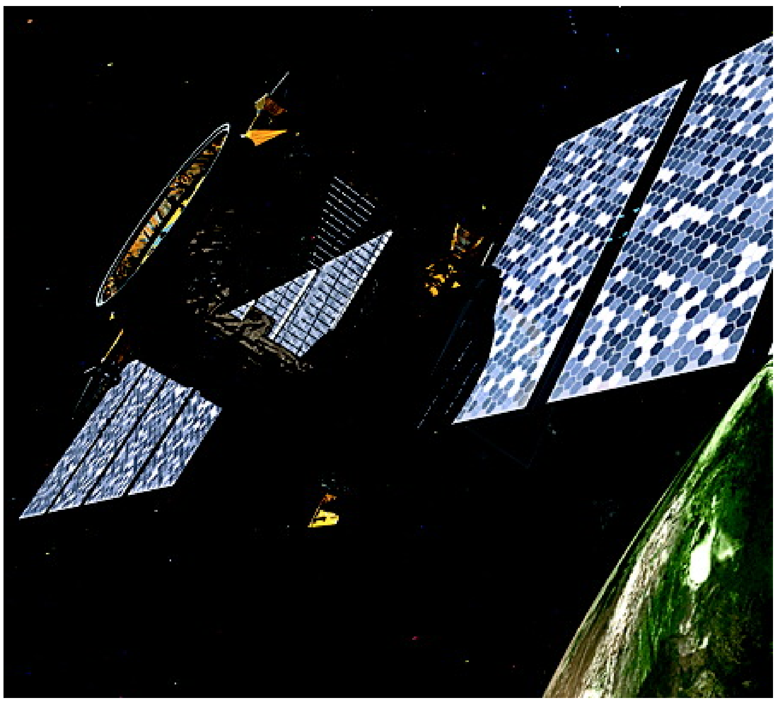

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Practical Aspects of Using Satellite Data in Air Quality Modeling

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To use satellite data to improve air quality models, it is vital to understand the data-handling procedures.

NASA

The evaluation of regional air quality models is typically conducted using ground-level measurements, and in some instances, airborne in situ data. Satellite remote-sensing data provide two important sources of information compared with surface and aircraft monitoring data: more complete spatial coverage and a vertically integrated measure of atmospheric components (*1, 2*). An increasing number of studies have recently focused on air quality applications of satellite remote sensing, including identifying specific air quality events such as forest fires (*3*), characterizing the long-range transport of some pollutants in combination with global-scale modeling (*4*), and evaluating regional air quality model simulations (*5*–*7*). There is clearly an enormous potential for using satellite data to improve air quality modeling. Therefore it is of particular interest to investigate and understand how satellite measurements can be used to improve our characterization of the atmosphere.

We describe here the practical aspects of using satellite data to evaluate regional tropospheric air quality models and improve their performance via data assimilation. We first present an overview of satellite remote-sensing data relevant to air quality studies, then outline the steps involved in the acquisition and processing of satellite data for air quality applications, and finally discuss the major air quality applications for satellite data. We focus on satellite data of chemical species, particularly those from U.S. missions. We do not discuss data on other parameters that affect air quality, such as meteorology and land use.

Overview of satellites and remote sensing of air quality

Each constituent of the Earth's atmosphere, such as ozone, water vapor, and so forth, has its own unique spectral characteristics for the emission and absorption of electromagnetic radiation. Sensors aboard satellites are designed to detect the scattering, absorption, or emission of electromagnetic radiation from these constituents. Geophysical quantities of interest are extracted from the measured radiances through a process known as the "retrieval".

The satellites commonly used for the remote sensing of air quality are polar-orbiting sun-synchronous low earth orbit (LEO) satellites. Polar-orbiting satellites can be used to view only the poles or to view the same place on Earth at the same time each 24 hour (h) day; these are usually at an altitude of about 800 km. A sun-synchronous orbit is a special case of a polar orbit that crosses the equator at the same time each orbit. Polar-orbiting satellites have a poor temporal resolution: at best, a 12 h measurement repeat cycle for a given geographic location. However, such satellites tend to offer higher vertical and horizontal resolution than geostationary (GEO) satellites because of the greater proximity of the LEOs to the Earth's surface.

The primary agencies/organizations in North America and Europe that launch and operate satellites used in the remote sensing of air quality include NASA, the National Oceanic and Atmospheric Administration (NOAA), the Canadian Space Agency (CSA), the European Space Agency (ESA), the Centre National d'Études Spatiales (CNES), and the Swedish Space Corporation (SSC). Table 1 lists the key satellites and their sensors currently used for remote sensing of chemical constituents of the Earth's atmosphere (see the Supporting Information for an expansion of the acronyms used in this article).

Table 2 lists chemical species and related "products" monitored by NASA satellites. These U.S.-based missions currently provide the most widely available data and documentation of their kind. ("Product" is a term used by the satellite remote-sensing community.) We focus our discussion on products relevant to regional tropospheric air quality modeling and list only those stratospheric products that are directly relevant to the troposphere or are used to compute tropospheric columns. The air quality products measured by the sensors on the Canadian and European satellites are provided in the Supporting Information for this article. Satellite air quality data are subject to limitations such as coarse temporal, horizontal, and vertical resolutions and the obscuring effect of clouds and ground albedo. These uncertainties are typically minimized or resolved by the retrieval team before releasing the data. A discussion of these uncertainties is presented in the Supporting Information.

Acquisition and processing of satellite data for air quality applications

In the past few years a plethora of data has become readily available, from both current and "historical" satellite sensors.

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TABLE 1. Satellites currently used for the remote sensing of air quality[a,b]

Satellite	Primary organization(s)	Launch date	Sensors used for remote sensing of air quality
ERS-2	ESA	April 21, 1995	GOME
TOMS-EP	NASA	July 2, 1996	TOMS
Terra	NASA	Dec 18, 1999	MISR, MODIS, MOPITT
ODIN	SSC/CSA/CNES/TEKES	Feb 23, 2001	OSIRIS, SMR
ENVISAT	ESA	March 1, 2002	MIPAS, SCIAMACHY
Aqua	NASA	May 8, 2002	AIRS, MODIS
ACE/SCISAT	CSA/NASA	Aug 12, 2003	ACE-FTS, MAESTRO
Aura	NASA	July 15, 2004	HIRDLS, MLS, OMI, TES
PARASOL	CNES/NASA	Dec 18, 2004	POLDER
NOAA-N POES	NOAA/NASA	May 20, 2005	SBUV/2
CALIPSO	NASA	April 28, 2006	CALIOP
GOES-N	NOAA/NASA	May 24, 2006	SEM
MetOp-A	ESA	Oct 19, 2006	IASI, GOME-2

[a] This list includes satellites from North America and Europe with widely disseminated data as of July 2007 and is not comprehensive. [b] See Supporting Information for an expansion of the acronyms used here.

TABLE 2. Chemical species and related products from sensors on the NASA satellites relevant to regional tropospheric air quality modeling

Product[a]	Sensor(s)
Aerosol properties such as aerosol optical depth (AOD)	CALIOP, HIRDLS, MISR, MODIS, OMI
Bromine oxide (BrO)	OMI
Carbon monoxide (CO)	AIRS, MLS, MOPITT, TES
Dinitrogen pentoxide (N_2O_5)	HIRDLS
Formaldehyde (HCHO)	OMI
Glyoxal (OCHCHO)	OMI
Nitric acid (HNO_3)	MLS
Nitrogen dioxide (NO_2)	HIRDLS, OMI
Ozone (O_3)	AIRS, HIRDLS, MLS, MODIS, OMI, SBUV/2, TES, TOMS
Sulfur dioxide (SO_2)	AIRS, MLS, OMI

[a] This list is not comprehensive because additional products continue to be validated and released.

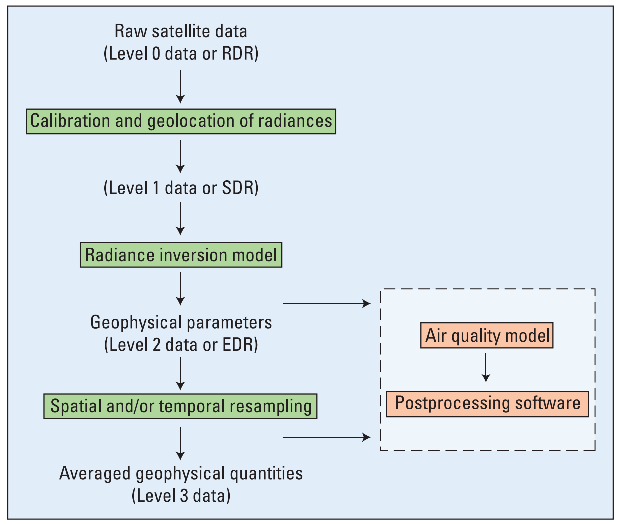

FIGURE 1. Flowchart of the top-level processes that occur when comparing satellite measurements with model outputs. See Table 3 for explanation of the level nomenclature.

The primary location for data from NASA sensors and satellites is the NASA EOS Data Gateway at http://redhook.gsfc.nasa.gov/%7Eimswww/pub/imswelcome. This site contains links to relevant validated data sets and also lists other locations for obtaining data (such as those for European sensors). NOAA data may be obtained from www.class.noaa.gov. Satellite data may also be available directly from organizations or science teams responsible for the data processing. The data are generally provided in a recognized format, such as hdf and are available at different levels, or stages, of data processing.

The steps involved in the processing of satellite data are summarized in Figure 1, although the data nomenclature can vary slightly depending upon the organization responsible for the data. (The two primary definitions, used by NASA and NOAA, are summarized in Table 3.) To use the data appropriately it is important that one understand the overall process to obtain the data, and the limitations and caveats inherent in each step. This is discussed below, and additional information is provided in the Supporting Information.

After conversion of the data from "sensor counts" into radiance units, the initial set of processing relates to the retrieval of geophysical quantities from the measured radiances. While the retrieval process is beyond the scope of this article (e.g., *8*), it is important to note that a priori information about the geophysical quantity of interest is often required to constrain the retrieval solution. For example, the a priori information could represent the climatological mean profile shape along with the variability of this shape.

Another factor to consider in the processing of satellite data is what is actually represented by the vertical profile of the data. Remote-sensing measurements have an inherent vertical resolution that depends upon the nature of the parameter being measured and the spectral characteristics of the measurement. The measured vertical profile represents a vertically averaged quantity of the true profile because the sensor itself has a finite field of view for the measurement. Conversely, models have their own set of vertical averaging characteristics, dictated by the way in which the model incorporates the vertical structure of the atmosphere. The proper way to treat these differences in vertical resolution is through the use of a sensor "averaging kernel". This is a mathematical representation of how the vertical structure of the atmospheric profile is mapped into the measured radiances (*8, 9*). This is expressed as a matrix where each row defines the averaging kernel for a particular retrieval level within the measured profile, and each element in this row represents the contribution of other levels in the atmospheric profile to the retrieved profile value. Thus, to compare the satellite profiles with model outputs, the measurement averaging kernel matrix is applied to the model output x' using

$$x'_{MODEL} \approx x_{a\ priori} + \mathbf{A}(x_{MODEL} - x_{a\ priori}) \qquad (1)$$

TABLE 3. Satellite data nomenclature

Data name	Description	Utility
RDR (raw data record)[a] or Level 1A[b]	Raw data downloaded from the sensor to the ground processing station. Whereas the file headers typically contain important ancillary data such as time, date, spacecraft and target location, and point angle, the data are usually in detector "counts" without any processing.	Of little use to scientists.
SDR (sensor data record)[a] or Level 1B[b]	Sensor data transformed from counts to engineering units. Calibration, bias correction, etc., applied. Data are directly linked to geospatial information such as latitude, longitude, date, and time.	Required for performing retrievals or investigating the radiometric impact of geophysical parameters.
EDR (environmental data record)[a] or Level 2[b]	Geophysical quantities derived from the SDRs, such as column ozone. Contains the necessary information about date, time, and Earth location. Usually has quality-control parameters listed (e.g., did the algorithm converge or is this potentially a bad data point?).	Data at the sensor spatial resolution can be used to perform one's own quality control and spatial/temporal regridding.
Level 3[b]	Data have undergone one or more postprocessing steps such as regridding to a standard spatial grid, spatial and/or temporal averaging, and/or subsetting for certain conditions (e.g., clear/cloudy).	Because the data are on a regularly spaced grid, they are useful for larger-scale studies, monthly means, etc.

[a] NOAA nomenclature. [b] NASA nomenclature.

The *x* vectors are a function of vertical pressure-based levels. The averaging kernel matrix (**A**) and the a priori are obtained along with the satellite retrieval and often depend on time and location. Circumstances such as proximity to large biomass fires or urban areas can render profiles significantly different from the true profile. The model profile may then be a better approximation of the true profile than the (measured) satellite data. In such cases, it may be appropriate to use the model vertical profile as the a priori profile, to retrieve the satellite data using this location/time specific profile, and to compare the new retrieved profile to the model results. This is often done on an ad hoc, rather than operational, basis for specific geographic regions or geophysical quantities (e.g., *10, 11*).

Use of satellite data in air quality modeling

Satellite remote-sensing data may be used to evaluate, initialize, constrain, and improve the performance of air quality models as discussed in this section.

Evaluation of air quality models. A large number of chemical species may be planned for retrieval during a satellite mission, but many of these are not retrieved because of either instrument or algorithm problems. Further, some data may not be validated and quickly made available for public dissemination. Validated tropospheric satellite data are commonly available only for O_3, CO, NO_2, SO_2, HCHO, and aerosol optical depth (AOD). Thus currently, tropospheric air quality models can be evaluated only for these species (*5–7, 12–22*). Data for halogens such as BrO may become more widely used as halogen chemistry starts to be taken into account in air quality models; atmospheric mercury deposition is one example. Satellite data for other species such as HNO_3 and glyoxal are becoming available (*23, 24*) but are sometimes limited by the time period of availability.

When using satellite data, we compare the model to data that offer a range of temporal and spatial resolutions. Most satellites involved in the remote sensing of air quality have a sun-synchronous polar orbit with once- or twice-daily measurements. Thus multiday averages at the time of the satellite observation, rather than 24 h averages, are more appropriate for comparison between the model and satellite data.

To ensure horizontal spatial compatibility between the modeling results and the satellite measurements, we need to first regrid the satellite data to the air quality model grid or the model results to the satellite grid. Although some recent sensors have a relatively fine spatial resolution, it may be more appropriate to use the Level 3 product available at a coarser resolution because that typically uses cloud-free measurements. For example, the MODIS AOD package on NASA's Terra has a $1° \times 1°$ spatial grid (*25*).

One of the key advantages of using satellite data for evaluation of air quality models is the availability of data aloft. These data may be available as a total atmospheric column, tropospheric column, and/or vertical profiles. Several studies have compared air quality model simulations with satellite retrievals of ozone column (*15, 22, 26*), tropospheric NO_2 column and profiles (*12, 27, 28*), CO column and profiles (*20, 29*), total and tropospheric column AOD (*6, 13, 30*), and HCHO column (*19, 24*). Figure 2 presents an example of air quality model evaluation using satellite retrieval; here monthly mean tropospheric NO_2 column densities for January 2001 from GOME and the community multiscale air quality (CMAQ) model (*19*) are compared.

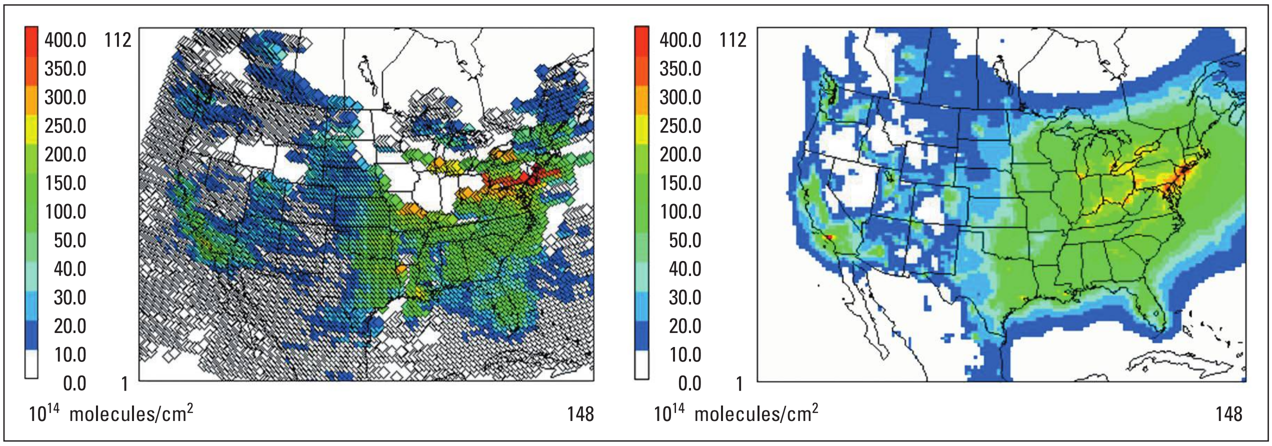

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FIGURE 2. Comparison of monthly mean tropospheric NO_2 column densities in January 2001 from satellite retrieval (GOME; left) and air quality model (CMAQ; right) (from Ref. *19*).

As discussed above, the satellite averaging kernel is applied to the model outputs before comparison with the retrieval. Also, the selection of the tropopause and additional processing are important during the comparison of model-derived column quantity (e.g., tropospheric column ozone) with the satellite retrieval (*17*).

There may be errors in the satellite data due to factors such as sensor calibration, bias in the spectroscopic parameters used in the retrieval algorithm, and/or the choice of a priori constraints used to stabilize the retrieval algorithm. In general, satellite data should be used as a quantitative benchmark in the performance evaluation of air quality models only after the satellite retrievals have been independently validated against other data such as those from aircraft, sondes, and ground-based measurements. Such validation is routinely performed by the satellite data retrieval teams before releasing the measurements to the public.

Boundary and initial conditions. Boundary conditions can have a significant influence on the simulated pollutant concentrations, particularly for pollutants that have a long atmospheric lifetime, such as $PM_{2.5}$ in the absence of precipitation. In situ measurements available to provide those boundary conditions are generally sparse and limited to surface locations. Global-scale models are typically used to provide concentrations at the boundaries of a regional model; however, there may be significant uncertainties associated with their simulated concentrations. Satellite data provide the spatial coverage needed for the boundary and initial conditions of regional air quality models, particularly aloft, over the oceans, and in areas where data may not be available. Global air quality models can be used to provide the vertical profile of lateral boundary conditions for regional air quality models while the column integrated values are constrained by the satellite retrieval.

Satellite measurements, when used as boundary conditions, can be used to account for the contributions of pollutants transported over long distances, for example, from Asia over the Pacific Ocean to the U.S. This phenomenon of long-range transport has been demonstrated in several studies such as CO data from MOPITT (*31*), O_3 data from TES (*32*), AOD data from MODIS (*4*), and so forth. A combination of satellite measurements and air quality modeling of O_3 and CO can be used to quantify the continental outflow of these pollutants (*32*).

Initial concentrations of chemical species such as O_3 and CO may have a non-negligible effect on simulations that cover a time period of a few days or less. A "spin-up" simulation period is typically used to minimize the effect of the initial conditions, but using available data can nevertheless improve the initialization of an air quality model, particularly when conducting air quality forecasting (*7*). For example, one approach used consists of assimilating the satellite data into the model at regular intervals (e.g., 3 h) using an analysis that leads to the creation of a new reanalysis field of initial conditions that is an optimized combination of the model output and satellite information.

Inverse modeling and data assimilation

Satellite data can be used for inverse modeling or data assimilation. For inverse modeling, a set of inputs is estimated by minimizing the difference between the model output and the satellite data. For data assimilation, satellite data can either refine model inputs (i.e., initial conditions) or correct model output such as concentrations of chemical species.

Estimation of input data. The most common application of inverse modeling to chemistry transport models (CTMs) has been to estimate emission data. Some approaches have ignored atmospheric transport by assuming that the atmospheric processes of interest (i.e., chemical reactions) occur mostly at spatial scales shorter than the model spatial resolution (>100 km). In those cases, such as the estimation of NO_x emissions from NO_2 data (*33, 34*) and the estimation of isoprene emissions from HCHO data (*35*), the species measured is a product species and the column density of that species is assumed to be related to the emission rate of the species of interest in that column through linear chemistry relationships. That is, it is assumed that the chemical species corresponding to the satellite data is mostly governed by oxidation of the emitted species of interest. The chemistry relationships are obtained from the model simulation and, therefore, vary among the columns. Examples include NO_2 fraction of NO_x and loss of NO_x via chemical reactions or yield of HCHO from isoprene oxidation.

The estimation of emissions from satellite measurements has also been conducted by taking into account both transport and chemistry using a variational approach. For example, CO emissions with good spatial resolution were optimized using CO column densities from the MOPITT satellite with GEOS-Chem (*36*). NO_2 column densities from SCIAMACHY were used to optimize NO_x emissions with CMAQ (*37*).

In addition to emission estimation, inverse modeling can also be used to estimate boundary conditions of regional-scale CTMs, for example, with a variational analysis similar to those used with ground-level measurements (*38*) but extended to the entire column. However, since satellite data have a large spatial coverage, they can be used as direct inputs (see above) to provide information on boundary conditions and, therefore, their use in an inverse modeling exercise seems superfluous.

Data assimilation. Data assimilation is primarily of interest in two areas: (1) in dynamic mode for air quality forecasting or hindcasting; and (2) in static mode for data fusion. For the latter, "fusion" is a postprocessing step involving the combination of the model simulation's results and measurements.

For data assimilation into an ongoing air quality simulation, both concentrations and optimized emissions can be assimilated to improve model performance. In the case of concentrations, assimilation of satellite data for O_3, NO_2, and AOD—a PM surrogate—will directly improve the performance of air quality simulations for these pollutants. Note, however, that the assimilation of AOD data will only be useful if the model already correctly characterizes the major PM concentration patterns. These are PM aloft due to biomass fires, desert dust, or volcanic eruptions and PM in the planetary boundary layer due to surface emissions from anthropogenic sources and vegetation. In the case of emissions, the ability to perform the inverse modeling in a near-real-time manner will be the limiting step for air quality forecasting, although this is not an issue for hindcasting.

There are some specific areas where such data assimilation will be key because satellite data provide information that is not directly available from other sources. For example, AOD measurements can provide valuable information on the magnitude and extent of biomass fires, and SO_2 measurements can help characterize volcanic eruption plumes. The multiangle imaging spectroradiometer (MISR) provides over dark water valuable information on particle size distribution and shape; such information can be used for models that simulate PM with such characteristics (i.e., modal or sectional size distribution and external PM mixtures).

An example of data assimilation is the use of a Kalman filter to assimilate CO and O_3 data from the Aura tropospheric emission spectrometer (TES) in GEOS-Chem (*39*). The revised O_3 simulation affected the NO_x chemistry, which in turn changes the NO_x/NO_2 relationship that is used in the retrieval of NO_2 satellite data to estimate NO_x emissions. This result highlights the complex relationships between various chemical species in a nonlinear system and the benefits (i.e., lower errors) that can be gained by conducting satellite data assimilation jointly for several chemical species.

For data fusion, satellite data will be most useful to improve concentration maps of air pollutants such as O_3, NO_2, and PM (using AOD). Some applications have already been performed with AOD data (*30, 40*) or are ongoing for display of air pollutant concentration maps or use in epidemiological studies.

Concluding remarks

Satellite remote-sensing retrievals provide valuable information on the tropospheric concentrations of some chemical species. These measurements offer significant potential to improve the performance of air quality simulations through input data optimization, data assimilation, and postsimulation data fusion and model evaluation. Although the current number of chemical species and other air-quality-related products available in satellite retrievals is small, the number is steadily increasing. Such products are useful not only in the absence of ground-level and airborne in situ data but also to refine or corroborate such data. Opportunities abound for collaborative studies between the remote-sensing and air quality modeling communities to mutually seek ways to use models and data effectively.

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Supporting Information Available

Additional text and tables on air quality products from instruments on Canadian and European satellites, accuracy of sensors, uncertainties in satellite data and their processing, and a list of acronyms used in the article. This information is available free of charge via the Internet at http://pubs.acs.org.

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