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Review article

Review: Strategies for using satellite-based products in modeling $PM_{2.5}$ and short-term pollution episodes

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ABSTRACT

Short-term air pollution episodes motivate improved understanding of the association between air pollution and acute morbidity and mortality episodes, and triggers required mitigation plans. A variety of methods have been employed to estimate exposure to air pollution episodes, including GIS-based dispersion models, interpolation between sparse monitoring sites, land-use regression models, optimization models, line- or area-dispersion plume models, and models using information from imaging satellites, often including land-use and meteorological variables. There has been increasing use of satellite-borne aerosol products for assessing short-term air quality events. They provide better spatial coverage, but currently at the price of low temporal coverage and rather crude spatial resolution. This is a brief review on using satellite data for modeling short-term air quality and pollution events. The review can be pursued as a practical guide for modeling air quality with satellite-based products, as it includes important questions that should be considered in both the study design as well as the model development stages. Progress in this field is detailed and includes published models and their use in environmental and health studies. Both current and future satellite-borne capabilities are covered. It also provides links to access and download relevant datasets and some example R code for data processing and modeling.

1. Introduction

Estimation of exposure to air pollution is best divided into two main categories based on the length of exposure: long-term and short-term exposure. Long-term exposure is related to constant background concentrations of pollution or persistent exposure to air pollution in the day-to-day work-transport-home environment, or from the accumulation of many short-term exposure episodes. Long term exposures are more related to airborne particulate accumulation in the body and its chronic health effects (Hoek et al., 2013; Pope et al., 2004; Schwartz, 2000). Long-term analysis is importantly related to morbidity and mortality of a population. From an air-pollution control perspective, the benefit of a long-term analysis is to understand long-term spatial and temporal trends, improve planning and perceive the need for action for mitigation strategies. Short-term episodes have well-defined starting and ending days and times of the exposure period, and are usually related to natural disasters, e.g. wildfires, dust events and volcano eruptions, and severe pollution episodes. From a health perspective, short-term episodes can be related to acute health effects, mostly respiratory and cardiovascular outcomes (Just et al., 2002; Katsouyanni et al., 1996; Pope et al., 2006). Short-term studies of air pollution episodes lead to better causal understanding and simulation modeling of sources, transformation, and transport of air pollutants. This leads to improve state implementation plans and informed policy decision makers. There are two main reasons to understand short-term air quality episodes: one is to evaluate and improve complex source-receptor models, and second is to improve short-term air quality forecasting and signal imminent disaster response capabilities. Long-term models can perform well to quantify cumulative air pollution effects on a population, and yet not necessarily capture the fine details of extreme events. Short-term episodes motivate improved understanding of the association between air pollution, and acute morbidity and mortality episodes; in the United States they associate with air pollution exceedances triggering a mandate on regional agencies for improved remediation plans.

Atmospheric particulate matter (PM) in the respirable range, $PM_{2.5}$ (PM with an aerodynamic diameter less than 2.5 μm), is recognized as a major threat to human health (Brunekreef and Holgate, 2002; Dominici et al., 2006; Franklin et al., 2008; Kloog et al., 2013; Schwartz, 1996; Zanobetti et al., 2009). Epidemiological studies have been limited by the availability of relatively few $PM_{2.5}$ ground monitoring stations

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relative to the broad dispersal of affected populations. Hence, a variety of methods have been employed to estimate exposure to air pollution episodes, e.g., GIS-based dispersion models (Gulliver and Briggs, 2011; Ketzel et al., 2011), interpolation between sparse monitoring sites (Wong et al., 2004; Yuval et al., 2005), optimization models for NOx (Chen et al., 2016, 2018a; Yuval et al., 2013) line- or area-dispersion plume models (Gibson et al., 2013; Jones et al., 2006), and models using information from imaging satellites, often including land-use and meteorological variables (Just et al., 2015; Kloog et al., 2015; Ma et al., 2014, 2016; Sorek-Hamer et al., 2015; van Donkelaar et al., 2011, 2016; Zhang and Li, 2015). Sparse $PM_{2.5}$ monitoring networks may limit our ability to accurately assess human exposures to $PM_{2.5}$, since concentrations measured at an outdoor site may be less representative of the subjects' exposure as the distance from the monitor increases (Bell et al., 2007; Lee et al., 2011).

For this reason, there has been extensive development of techniques to make best use of satellite-borne aerosol products for assessing air quality. They provide better spatial coverage, but currently at the price of low temporal coverage and rather crude spatial resolution – especially if used for estimating personal exposure and to refer to variability among individuals that live in the same vicinity.

The use of Aerosol Optical Thickness (AOT) also referred to as the Aerosol Optical Depth (AOD), in short-term studies, is the focus of this review. AOD is a remotely sensed retrieval product, typically reported as a vertical column integral of extinction above the observed surface footprint. Methods using the MODerate resolution Imaging Spectroradiometer (MODIS) -based AOD to assess ambient PM levels for long and short term exposures showed early success in certain regions, while others remain very poorly characterized (Gupta et al., 2006; Hoff and Christopher, 2009; Koelemeijer et al., 2006; Liu et al., 2009; Martin, 2008; Zhang et al., 2009). Although it's near weekly overpass, the Multiangle Imaging SpectroRadiometer (MISR) sensor improves these capabilities to an extent (Liu et al., 2007), e.g. for estimating monthly PM averages (van Donkelaar et al., 2010), or examining spatiotemporal characteristics of the AOD-PM association during the DRAGON campaign over Central Valley, CA (Sorek-Hamer et al., 2020). MODIS-AOD products were found effective in predicting short-term $PM_{2.5}$ concentrations in China (Hua et al., 2019a; Zhao et al., 2018), particularly in creating continuous exposure maps, addressing an urgent need for a comprehensive, evidence-based assessment of the disease burden related to short-term $PM_{2.5}$ exposure (Li et al., 2019).

While satellite-borne AOD can be associated with ground-based PM concentrations, there can be strong contributions to AOD from particles encountered along the sensing pathway well above the planetary boundary layer with possibly different compositions. In addition, cloud cover severely limits the actual spatial coverage of AOD (Ford and Heald, 2016). Yet, in spite of these limitations (Jin et al., 2019), AOD has been employed extensively for assessing PM concentrations in different temporal and spatial study designs (e.g. (Franklin et al., 2017; Geng et al., 2018; Hu et al., 2014; Just et al., 2015; Kloog et al., 2014, 2015; Sorek-Hamer et al., 2015; van Donkelaar et al., 2015, 2016).

This review covers different modeling approaches using satellite remote sensing products to estimate short-term air quality and air pollution episodes. It will point out the advantages and limitations of using satellite data for this purpose, factors that need to be taken into account and questions that should be addressed in the study design stage. We then provide a summary of current satellite capabilities including examples, guided by R software code (R Core Team, 2016) for applying the models. It concludes with a summary of capabilities arising in future satellites and suggestions for future research directions.

2. Study design

The study design is a very critical stage for any research. A necessary first step is to take some time to address important questions regarding the research goals, the training, testing, and validation datasets, and the proposed methodology. This section will focus on the list of suggested questions to address in order to plan and prepare for a short-term air quality study framework including examples from published literature.

- **Define goals** – *What are the study goals?* One can answer: "Create an air quality exposure metric". That is a very broad goal that is missing critical information: *Where When* and *What* is measured, and what is the required spatiotemporal resolution? Therefore, a more comprehensive response can be for example "Create daily 1 km air quality exposure metrics for NO_2 over California during the fires of summer 2018". A clear definition of the research goals will be a good guide through the next stages related to the data and methodology approaches that will be examined in order to achieve these goals. For example, Kloog et al. (2015) define their goal as examining the use of highly spatiotemporal resolved Multi-Angle Implementation of Atmospheric Correction (MAIAC) AOD data in Israel, exploring its $PM_{2.5}$ and PM_{10} predictions reliability. This definition includes a clear statement of the datasets that will be used in the study (i.e. MAIAC AOD, $PM_{2.5}$, PM_{10}) and their advantages (i.e. high spatiotemporal resolution), the study area (i.e. Israel), and what will be examined (i.e. $PM_{2.5}$ and PM_{10} prediction capabilities). Mhawish et al. (2019) define their research goal as evaluating the MAIAC AOD over South Asia using AErosol Robotic NETwork (AERONET) AOD, and further specifies that the evaluation includes a comparison to two operational MODIS AOD retrieval algorithms, and the performance will be conducted under varying conditions of aerosol loading, aerosol types, surface coverage, and viewing geometries. This definition incorporates a clear statement of the research goal, in general (i.e. evaluating the MAIAC AOD using AERONET AOD), and in more detail (i.e. comparing the MAIAC performance with two other AOD algorithms, and evaluating the performance under different well-defined conditions related to the aerosol type, viewing geometry etc.). This study goal definition includes the study area (i.e. South Asia), the datasets that will be used (i.e. MAIAC AOD and AERONET AOD), and in addition, the knowledge gap that this study will address (i.e. such a systematic analysis has not been reported before for South Asia). Chatfield et al. (2019) aimed towards the development of a "static model", which does not attempt to simulate transport and sources, but rather uses observational records related to vertical mixing and AOD over the San Joaquin Valley (SJV), California, during Winter 2012–2013. Understanding and clearly defining the scientific gap the study is seeking to address can be a good first step for defining the study goal.
- **Potential users** – As part of the process of defining goals, one should take into consideration who are the potential users. Different users might be interested in different spatiotemporal resolutions for different applications. It is recommended to interact and discuss the study goal/s with the potential user/s to better accommodate their needs, prior to conducting the research in general, and the modeling stage in particular. Some examples include Mhawish et al. (2019) who stated that their results are expected to be useful to the air quality and modeling communities, as well as for algorithm developers. Sorek-Hamer et al. (2015) mentioned that the use of satellite aerosol products to improve fine and coarse PM concentrations estimation capabilities over large arid regions, has a pronounced value for air quality management, environmental surveillance, and environmental health studies. Chatfield et al. (2019) that stated that mapping high $PM_{2.5}$ episodes in SJV, California, USA, can be used in pollution abatement actions and health studies, also mentioned that model outputs can be used for producing continuous air pollutant maps as a strong tool for both research and policy decision-makers. There are several related goals in producing $PM_{2.5}$ maps in short-term air quality episodes, and assessing their accuracy, e.g. allowing

air pollution professionals to understand particulate episodes and to improve sources and simulation details (e.g. transport error) for source-driven models. Understanding the application of the results and how they will be used is critical for the study design.

- **Identify data sources** – When it comes to data, we suggest addressing the following questions: *what datasets are required in order to achieve the study goal? What are the available data sources (ground/airborne/remote sensing)? Are the data available during the study period and cover the study area? Do the spatial and temporal resolutions of the data fit the research goals?* different goals will guide to use different sources of data, e.g. if the study goal is to create daily 1 km spatial maps of air pollution, a possible choice would be to use AOD products that are available at least daily with a spatial resolution of 1 km (e.g. MODIS-based MAIAC AOD product; Kloog et al., 2015; Stafoggia et al., 2019); but if the study goal is to characterize the composition and size of aerosols during a specific wildfire event one would likely use meaningful data products during the same air pollution event, e.g. MISR aerosol property products, airborne measurements, and available surface measurements, as applied in Friberg et al. (2018). When a certain dataset is included in a study, it is highly recommended to examine its availability during the specific air pollution episode examined, and over the geographic area of interest. For example, Chatfield et al. (2019) research goal is to use satellite-based MAIAC AOD for mapping high $PM_{2.5}$ episodes in SJV, California, USA (Nov 19, 2012–Feb 18, 2013), for use in pollution control and health studies. For the well-defined research goal, study area and time period, the following remote sensed datasets have been selected to be utilized in the study: (MODIS-based) MAIAC AOD – with a spatial resolution of 1 km and a daily overpass (~1:30 pm, local time), allowing a time sequence of mapped aerosols at 1 km for cloud-free days, and DSCOVER-AQ NASA airborne data available on campaign specific days during winter 2013 over Central Valley, CA, USA. Aircraft data from the DSCOVER-AQ period was chosen since it can provide information about the aerosol vertical distributions and composition in the selected time period. When importing the MAIAC data from its source website (https://search.earthdata.nasa.gov/search) the time period and study area were selected in order to import only the relevant dataset for the study. Chatfield et al. (2019) wanted to identify how many MAIAC AOD - EPA $PM_{2.5}$ collocations are available (i.e. available MAIAC data over PM site locations, when PM data is available within ± 1 hour around the satellite overpass time). This was examined by plotting the collocations as a time series (x-axis) by EPA $PM_{2.5}$ sites (y-axis) over the whole study period (Fig. 1). In addition to data availability this plot illustrates the variability of the data in time and in space.
- *Code for examining the spatiotemporal extent of a dataset (*i.e. *producing* Fig. 1*) can be found in the following link:* https://github.com/mshamer/ShortTermStrategies.git *(Fig. 1.zip, README Fig. 1)*

A literature review with search terms related to the defined research goal/s is essential in order to better understand what had been already done to date, and which datasets are available over the study area and during the study period. Finally, after deciding which variables will be included in the analysis, one should become familiar with the options of obtaining target data to train, test and validate the model. Table 1 provides a short list of currently available links to relevant potential ground based/airborne/remote-sensing datasets, which can be filtered by time and location. This list can serve as a starting point for examining available data sources for a study.

Another source of data can be modelled datasets such as GEOS-Chem and CMAQ model outputs. GEOS-Chem is a global 3-D model of atmospheric chemistry driven by meteorological input from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office. It is applied by research groups around the world to a wide range of atmospheric composition problems (Bey et al., 2001; Philip et al., 2014). The Community Multiscale Air Quality Modeling System (CMAQ; colloquially pronounced see-mak) is an active open-source development project of the U.S. EPA that consists of a suite of programs for conducting air quality model simulations. CMAQ combines current knowledge in atmospheric science and air quality modeling, multi-processor computing techniques, and an open-source framework to deliver fast, technically sound estimates of ozone and particulates, as well as other pollutants (https://www.epa.gov/cmaq; Appel et al., 2017). More recently, the GEOS-5 assimilation system for meteorology has been extended to give prompt assimilations of respirable aerosols and other trace constituents like Ozone. The GEOS FP, provides analyses and forecasts produced in real time, using the most recent validated GEOS system (Lucchesi, 2018) has much simpler descriptions of transformation mechanisms than GEOS-Chem, also based on GEOS products, but it does feature higher resolution and prompt descriptions of best-estimate aerosol model.

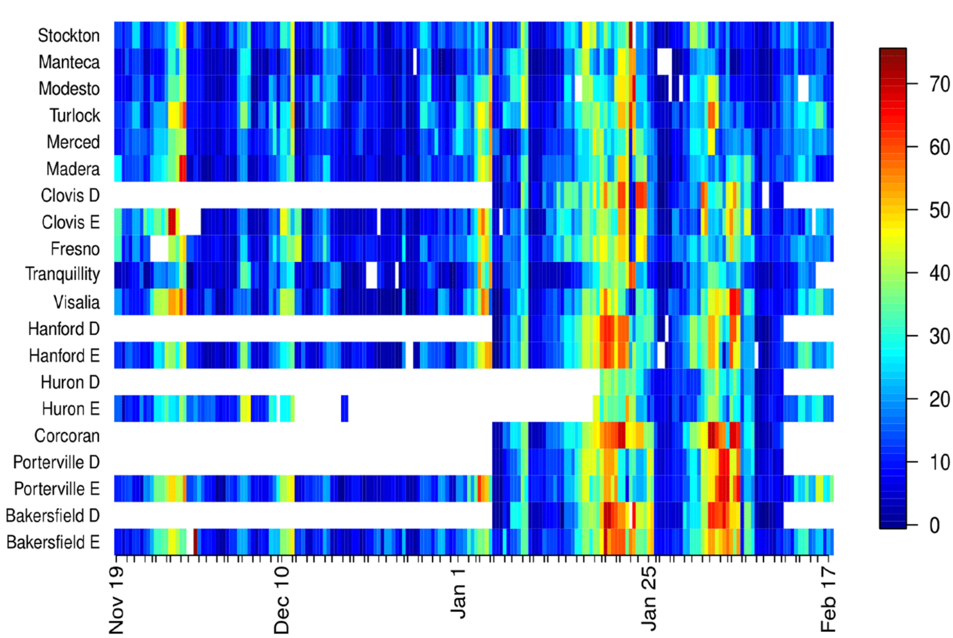

Fig. 1. Availability and spatiotemporal variability of observed $PM_{2.5}$ in the SJV, CA during winter 2012–2013 (Chatfield et al., 2019). *Y* axis: EPA $PM_{2.5}$ sites in the SJV, roughly north to south. *X* axis: date (Nov 19, 2012-Feb. 18, 2013); the color scale indicates afternoon $PM_{2.5}$ measurements (μg/m^3). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Selected data sources for air-quality studies using satellite-borne data.

Source	
Satellite data	NASA – e.g. MODIS, MISR, OMI
	https://worldview.earthdata.nasa.gov/
	NOAA – e.g. VIIRS, GOES-R
	https://www.avl.class.noaa.gov/saa/products/catSearch
	EUMESTAT – e.g. SEVIRI, IASI, AVHRR, GOME-2
	https://www.eumetsat.int/website/home/Data/Products/Atmosphere/index.html
AERONET data	Ground based remote-sensing network for measuring aerosol products
	https://aeronet.gsfc.nasa.gov/new_web/data.html
Ground monitoring data	openaq - aggregate physical air quality data from public data sources, global.
	https://openaq.org
	EPA – pre-generated data files of hourly and daily pollutant concentrations , USA
	https://aqs.epa.gov/aqsweb/airdata/download_files.html
Field campaign Airborne data	LaRC database
	https://tad.larc.nasa.gov
	JPL database
	https://airbornescience.jpl.nasa.gov/data-nasa/
	ESPO data archive – ORACLES, AIRMSPI
	https://espoarchive.nasa.gov/archive/browse/oracles
USGS	https://www.usgs.gov/products/data-and-tools/overview
Meteorological data	https://climatedataguide.ucar.edu/
	https://rapidrefresh.noaa.gov/hrrr/
Modelled data	GEOS-Chem http://geos-chem.org
	CMAQ https://www.epa.gov/cmaq
	GEOS-5 High-resolution assimilated AOT https://cds-cv.nccs.nasa.gov/GMAO-V/

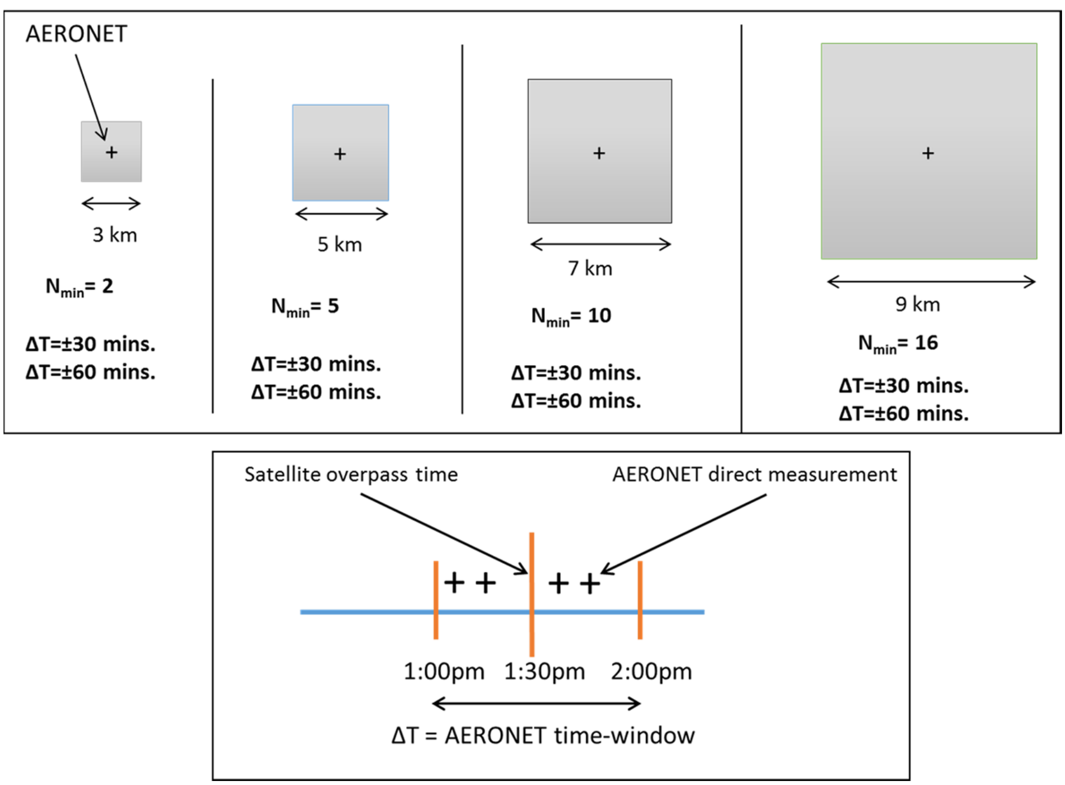

Fig. 2. Example for defining a spatiotemporal collocation methodology including a spatiotemporal sensitivity analysis.

- **Define model grid and collocation method –** based on the datasets chosen to be used in the study, define both the spatial and temporal grids of the model. In order to make sense of using several datasets, especially a combination of remote sensing (i.e. satellite) and ground monitoring data, the collocation methodology should be carefully designed. To better understand collocation approaches, we provide the following example; if a researcher is using the Visible Infrared Imaging Radiometer Suite (VIIRS) AOD 6 km product, AERONET AOD observations, and ground monitored $PM_{2.5}$ concentrations, the thinking process should adhere to the following questions (Fig. 2): Since we have spatial remote sensing data and point location ground level data, *what is the spatial buffer around the point location that represents both datasets? what is the temporal period that will best represent them? Do we want to use the closest pixel or analyse a certain spatial extent centred at the ground location?* Ichoku (2002) tried to answer these questions when he validated satellite-borne MODIS 10 km AOD products using AERONET AOD data, suggesting a spatial buffer with a pixel ratio of 1:5 (i.e. 50 × 50 km window-size around the point location) and ± 30 min from the satellite overpass. This choice of the buffer window-size

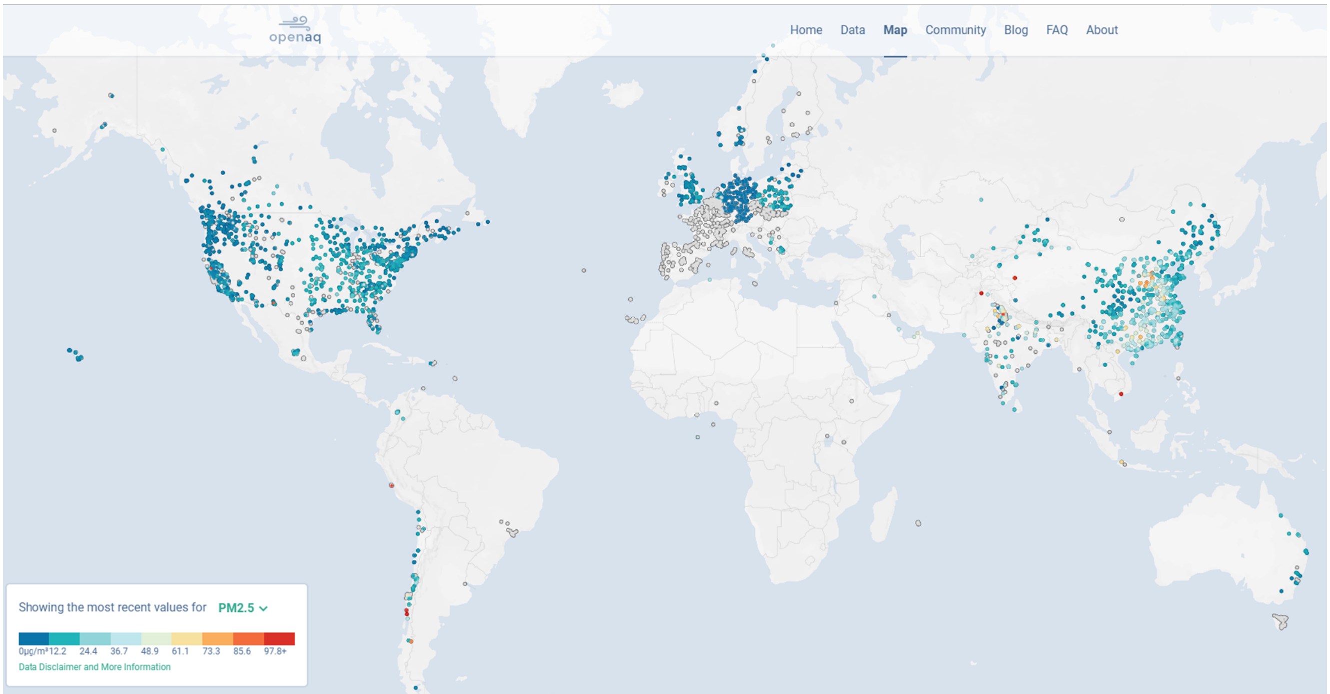

Fig. 3. $PM_{2.5}$ global monitoring network available through OpenAQ (https://openaq.org).

was explained by the average travel speed of an aerosol front that is on the order of 50 km/h, which would match a 1-hour sunphotometer dataset. This pixel ratio has been preserved for the validation of MODIS AOD 3 km products only as a circular buffer (Remer et al., 2013). For our example, this means that for a single VIIRS satellite overpass we can use (an average of all) AERONET/$PM_{2.5}$ measurements that are within 30 or 60 min before and after the overpass time. For the spatial buffer we can use the 1:5 ratio (i.e. 15 km diameter around the point location) or run a sensitivity analysis (Fig. 2) for finding the best spatiotemporal representation, i.e. maximum observations fall within an error envelope. Further collocation methods, such as kriging and other spatial statistic methods, are also available (Jinnagara Puttaswamy et al., 2014) and may well be considered. Another condition that should be taken into account is the allowed minimum number of observations in the defined temporal resolution (e.g. Nmin = 10 within ΔT) and in the spatial extent (e.g. Nmin = 10 sites within the study area). For a short-term air quality model, it is critical to have sufficient number of observations such that conclusions can be drawn from the data. How much is sufficient? That is a good question. The answer will be study-specific and dependent on the methodology used and the research goals.

Satellite-based algorithms have been validated globally with data from available AERONET or similar ground-based remote sensing networks. Each algorithm has its own accuracy level, for example ± (0.05 + 15%) for MODIS Dark Target 10 km AOD product (Levy et al., 2013) and ± (0.05 + 10%), for MODIS MAIAC 1 km AOD product (Lyapustin et al., 2018). This section emphasizes the importance of spatiotemporal colocation in order to correctly fuse different data sources of remote sensing (i.e. satellite) and ground monitoring data. Fig. 2 is given only as an example for defining a spatiotemporal collocation methodology including a spatiotemporal sensitivity analysis and its theory is applicable when collocating satellite data with any ground observing sites/network, e.g. AERONET, ground $PM_{2.5}$ monitoring stations.

For example, the primary goal of Shtein et al. (2018) is to estimate PM_{10} and $PM_{2.5}$ concentrations in Israel on daily and intra-daily temporal resolutions. They designed their model grids according to the variability in the satellite overpass times. The mean overpass time over the study area for Aqua and Terra is 1:05 pm, and 10:50am, local time, respectively. For the intra-daily (hourly) model that estimates PM around the satellite overpass time they used a range of two standard deviations in time, 1 hr and 1.5 hr, for Aqua and Terra, respectively. Namely, averaged $PM_{2.5}$ concentrations from observations during 10 am and 4 pm for Aqua, and during 8 am and 2 pm for Terra. The wide time window used for the intra-daily models was chosen after evaluating the sensitivity of the model to different time window widths. They worked with exact pixel collocation and did not discuss a spatial analysis of the collocation grid. In another example, Franklin et al. (2018) temporally matched AERONET and MISR data as a pre-processing step toward ground PM estimation in Mongolia. They used all AERONET observations within a 15 min time window around the Terra satellite overpass, and took the closest spatial match (within 4.4 km) to the AERONET site for MISR observations in three different paths. Lyapustin et al. (2018) used MAIAC AOD data in a 25 km window around the AERONET site location as the collocation approach. This relatively coarse spatial resolution grid fits the study goals, which are obtaining a global validation for the MAIAC AOD algorithm over AERONET sites.

- **Obtain data** – There are numerous sources for obtaining relevant data, e.g. satellite data, ground monitoring data, AERONET data, field campaign airborne data, meteorological data, and assimilated model estimates (Tables 1 and 3). As an example, data from ground PM monitoring stations can be found in separate websites based on the local authority datasets or in aggregative sites as ‘OpenAQ’. The ‘OpenAQ’ website (https://openaq.org) aggregates regulated ground monitoring data from public sources and has a near global coverage (Fig. 3). This map can be a starting point for understanding availability of ground measurements over the studied region and during the anticipated episode.

Despite the spatial limitations of using $PM_{2.5}$ ground monitoring networks (Martin et al., 2019), the Bloomberg Global $PM_{2.5}$ Tracker for mapping polluted cities around the world, was built pulling data from the OpenAQ platform, for addressing the global threat of long-term exposure to polluted air (https://lnkd.in/e4r534X), among other studies that used this data source (Hasenkopf et al., 2016; Pinder et al., 2019). While PM data is usually in the format of text files, satellite data, downloaded from selected sources come in Hierarchical Data Format (HDF4 or HDF5, very distinct formats requiring different software) or NetCDF (nearly identical data format to HDF5 but accessed with different calling interfaces) formats that can be imported and read in bulk using different software tools as MATLAB, R, Python, and Google Engine. Pre-processing and normalizing the data is an important stage that includes knowing the data, its availability, trends in time and space, and analysing anomalies.

- *Code for reading hdf4 with rgdal in R (for PC and Linux):* https://alexandrashtein.github.io/Basel-workshop/DB_building_for_PM_model.html
  RGDAL: https://cran.r-project.org/web/packages/rgdal/index.html

- *Previewer/Reader tool for HDF4, HDF5, NetCDF and Grib Format data with options for conversion: Panoply* https://www.giss.nasa.gov/tools/panoply/download/ (best used with NetCDF operators, best augmented by NCO tools for elementary operations on NetCDF files (http://nco.sourceforge.net)
- **Select methodology** – Choosing a modeling approach depends on several factors, primarily on the level of details required for fulfilling the goals of the study, the available datasets for training, testing and validating the model, and on the physical and dynamic nature of the atmospheric systems that are analysed. The physical nature of the studied episode depends on the characteristics of the pollutants of interest and their sources, the averaging time determined for the pollutant concentrations, and the points determined for model validation. There is no one 'right or wrong' model to use. As a basis for selecting the study methodology, following, we present the rationale behind commonly used methods in satellite-based air pollution studies.

Linear regression models, can describe the raw association between AOD and PM2.5 measurements. However, they are not able to take into account spatiotemporal affects and additional variables that have been found to affect this relationship and contribute to the modeling quality (e.g. meteorological parameters, traffic and land use data). These variables can be integrated into a *Multivariate linear regression*, e.g. Zhao et al. (2018). Whereas multivariate linear regressions can account for multiple variables, in many cases the relationships between the independent variables and the dependent variable are not necessarily linear. *Generalized Additive Models (GAM)* were used to reflect a non-linear association while constructing a regression of smooth functions of the independent variables (Hastie et al., 2009; Wood et al., 2016). GAM has been used in different study areas and datasets demonstrating relatively good results (Franklin et al., 2017; Hua et al., 2019b; Liu et al., 2009; Sorek-Hamer et al., 2013, 2020). The shortcoming of the GAM approach is that for large databases it is cumbersome since it is not selective, namely, it fits all the predictors, which is generally inefficient for a large number of predictors. In addition, interaction between variables can be included manually, and not examined automatically by the model (Sorek-Hamer et al., 2013).

- Example code for applying GAM can be found in the following link: https://github.com/mshamer/ShortTermStrategies.git (GAM-example.R)

An alternative method, that automatically takes into account interactions and performs variable selectivity by its contribution to the prediction, is the *Multivariate Adaptive Regression Splines (MARS*; Friedman, 1991). This approach has shown promise in previous studies (Moisen and Frescino, 2002; Muñoz and Felicísimo, 2004). It combines the strengths of regression trees and smoothing spline fitting by replacing the step functions normally associated with regression trees with piecewise linear basis functions (Sorek-Hamer et al., 2013). MARS has an exceptional analytical speed outperforming the GAM, and its simple rule-based basis functions facilitate the prediction of the response variable distribution using independent data when a big dataset with a large number of variables is used.

While accounting for additional predicting variables, the day-to-day variation in the AOD-PM association was found to be important, and introduced a new method to this field, the *Linear Mixed Effects Model* (LMEM; Lee et al., 2011). This approach can fit when the data is available daily to reflect this variation. A key decision of the LMEM modeling process is specifying model predictors as fixed or random effects. Unfortunately, the distinction between the two is not always obvious. Generally, absolute rules for how to classify a term as a fixed or random effect are not useful because it depends on the goals of the analysis and the available data. Harrison et al. (2018) provide an overview that can serve as a widely accessible code of the best practices using the R package lme4 (Bates et al., 2015) for applying LMEMs to complex problems and model structures.

- *Code for applying a basic LMEM:*

Model	Statistical model	R code
M1	$PM_{ij} = u + \beta AOD_{ij} + \varepsilon_{ij}$	M1 < - lmer (PM ~ AOD)
M2	$PM_{ij} = u + v + \alpha AOD_{ij} + \varepsilon_{ij}$	M2 < - lmer(PM ~ 1 + (1|AOD))
M3	$PM_{ij} = u + \beta AOD_{ij} + v_i + \alpha_i AOD_{ij} + \varepsilon_{ij}$	M3 < - lmer(PM ~ AOD + (1 + AOD|DOY))

where, the dependent variable PM_{ij} is the daily average PM concentration in day i and station j, u and β are the fixed intercept and slope, respectively, and v and α are the random intercept and slope, respectively. $v_i$is the random intercept on day i, $\alpha_i$is the random slope of AOD_{ij} on day i, and ε_{ij} is an error term that represents the unexplained variance of the PM in day i at station j. Fitting AOD as a fixed effect in model M1 assumes the AOD retrievals are all independent of one another, and share a common residual variance (similar to a linear regression, lm(PM ~ AOD)). Conversely, fitting AOD as a random effect model in model M2 assumes that the retrieved AOD means are only a subset of the realised possibilities drawn from a 'global' set of population means that follow a normal distribution with its own mean and variance. Therefore, LMEMs model the variance hierarchically, estimating the processes that generate among-AOD variation in means, as well as variation within AODs. In M3, the fixed effects represent the average relationship between AOD and PM during the study period across all ground monitoring stations, and the random effects represent the daily variability of the regional AOD–PM relationship by day of year (DOY). LMEM has been widely used (Chatfield et al., 2019; Chen et al., 2018b; Kloog et al., 2014, 2015; Stafoggia et al., 2017; Zhang et al., 2019).

When observing large spatial regions, a Geographically Weighted Regression (GWR) has been used, usually in support of other statistical approach, accounting for the spatial effects in the AOD-PM association (Bertazzon et al., 2015; Ma et al., 2014; van Donkelaar et al., 2015, 2016; Yao et al., 2019).

- Example code for *applying GWR can be found in the following link:* https://github.com/mshamer/ShortTermStrategies.git *(GWR-example.R, README GWR-example)*

In recent years, the application of *Machine Learning (ML)* methods has been introduced to this field, using Gradient Boosting, Neural Networks, and Random Forest models, among others (Chen et al., 2019a; Di et al., 2019; Franklin et al., 2018; Hu et al., 2017; Stafoggia et al., 2019; Zamani Joharestani et al., 2019). ML models are usually a 'black box', therefore, it is very important to clearly understand what the model does, what are the assumptions it's based on, and how to interpret results. ML models must be repeatedly re-evaluated and re-fit, since they are blind to changing underlying physical causation.

After running an initial model, refining predictors and checking model fit, the main goal/s of the study will define the next steps. If the study is a truly exploratory analysis, or developing a prediction model, some sort of a stepwise approach can be suitable (Siwek and Osowski, 2016), hierarchical modeling (Blangiardo et al., 2019) or SHapley Additive exPlanations (SHAP) (Lundberg and Lee, 2017) as a unified approach to determine the 'best' predictors with the highest contribution to the model. For example, Sorek-Hamer et al. (2013) applied a multi-stage approach to determine both the best predicting variables and the best satellite-based model, for predicting ground $PM_{2.5}$ concentration in Central Valley, CA. As a first step they applied a Generalized Boosting Method (GBM) for choosing the variables that would optimize the model and lead to the best prediction results. The boosting approach, emerged in the field of ecology, was introduced by Freund and Schapire (1996) and recently used in air quality studies (Chen et al., 2019b; Di et al., 2019; Velasco and Johnson, 2019). Boosting was used hereafter as a procedure for decreasing the number of predictor variables instead of using a heuristic stepwise choice. Ten variables were initially used for applying the boosting, with and without interactions between variables, which resulted in four main variables that had the highest relative relationship with the response variable (i.e. $PM_{2.5}$).

Regardless of the selected methodology, it is recommended, for any approach, to have a well explored baseline for camparison, for example, commonly used is a linear regression.

3. Limitations of using satellite-borne data for modeling short-term episodes

Satellite data have a spatial advantage over point sources, yet it is important to understand the limitations and pitfalls of using this type of data when examining AOD-$PM_{2.5}$ short-term associations. The main limitations include (1) integration of the whole atmospheric column; (2) available under cloud-free conditions; (3) columnar RH conditions; and (4) instantaneous snapshot, i.e. satellite overpass time.

Satellite data are available in cloud free conditions since clouds usually mask the ability to retrieve information from Earth (Ford and Heald, 2016). Strong dust or smoke events can behave as a masking phenomenon and similarly limit retrieval capabilities. For example, collocations of satellite-borne AOD from MOIS-based MAIAC AOD and ground monitored PM concentrations were available during only 36% of the days over Israel during 2003–2013 (Kloog et al., 2015); over other locations in Europe and the USA during 2009–2011, AOD-PM collocations availability varied from 32% to 65% (Sorek-Hamer et al., 2017). Most Low Earth Orbit satellites (LEO) have no more than one or two daily overpasses which might not capture the whole diurnal cycle of aerosol loading in the atmosphere. It is essential to understand the level of details necessary for a study. There is a great difference between modeling repeated episodes of exposure for two years in a region, compared to modeling one specific air pollution episode. If the short-term study has sufficient length, the spatial and temporal availability of data from ground-monitoring sites that serve as the ground-truth for model evaluation, are critical. Insufficient ground data caused by spatial imbalance in site deployment and the sparsity of stations, especially in rural areas and developing countries, may largely affect the ability to perform a full model evaluation. Although satellite data can widely cover both urban and rural areas, the availability of ground measurements can highly influence the model quality, Recently, low cost sensors have been deployed for use in air quality modeling purposes (Gupta et al., 2018; Li et al., 2020). Caution should be taken when using such networks in regards to instrument calibration and accuracy (Castell et al., 2017). Examining the contribution of temporal variables is important: month, day of the year, day of the week, season (pre- or manually-defined), as temporal effects are often dominant (Brunello et al., 2019; Sorek-Hamer et al., 2020). For local episodes, a combination of all available data sources can be a sufficient approach for obtaining the data. Furthermore, most satellite datasets represent an integration of the whole atmospheric column, without information on the vertical distribution of the pollutants. This is a critical piece of information that is rarely available (in space and time), and can attribute the columnar AOD to certain heights of the atmospheric layers, namely, will enable a better vertical association between these variables. Therefore, additional data such as meteorological data (e.g. planetary boundary level, temperature, RH, wind direction and speed), and vertical layering of aerosols from Light Detection and Ranging (LIDAR) instruments can support the analysis and increase the ability to understand the dynamics of the atmospheric system through a relatively short time period. Different RH conditions are well known between the AOD retrievals and the PM measurements. Filter-based ground monitoring PM sites are controlled approximately around 30%-40% RH, while the columnar AOD is affected by the (non-controlled) columnar atmospheric RH conditions. In addition, most LEO satellites provide daily snapshots, at a certain overpass time (nearly) every day during daylight time, which cannot necessarily capture certain events that occur during the day and night nor the diurnal variation of certain phenomena. Geostationary (GEO) satellites will significantly improve the temporal resolution, availability, and capabilities of satellite data with the forfeit of a slightly lower spatial resolution (Table 3).

4. Evolution of short-term modeling

Early studies such as Engel-Cox et al. (2004) demonstrated the capabilities of Earth-observing satellites in conjunction with ground-based data for estimating urban-scale air quality monitoring. Specifically, an assessment of the integrated use of ground-based and satellite data for air quality monitoring was conducted, including several short case studies. In the following decade, a rapidly increasing number of studies and new methods have been introduced. In the early studies, the relationship between AOD and $PM_{2.5}$ concentrations was generally established via a simplistic *Linear regression model*, which can reflect the association between these two measurements under lab conditions, i.e. clean and static environment, applied under the assumption that it is stable within a certain spatiotemporal range. The studies' extent varied from days to years, and from cities to continents, with the regression coefficients varying in the range of 0.2–0.98 (season and location specific). In general, the precision of the AOD retrievals was found to be ± 20% and the prediction of $PM_{2.5}$ by AOD was in the order of ± 30% in the most meticulous studies (Hoff and Christopher, 2009). Inconsistent results indirectly showed that improvements are needed for models that use AOD as the main variable for the prediction of $PM_{2.5}$. Based on this premise, different modeling approaches and additional variables have been introduced to this field (e.g. meteorological parameters, such as boundary layer height, temperature, relative humidity, and wind velocity, traffic and land use data). These properties of particles can significantly affect the degree of vertical mixing and explain the moisture absorption level of the aerosols. To comprehensively consider the synergistic effects of all these variables, under the assumption that these are linear effects, *Multivariate linear regression* has been used Zhao et al. (2018), specifically including the effects of the boundary layer height and relative humidity (Liu et al., 2009), land use information (Kloog et al., 2014), and other co-measured satellite-borne products (Koelemeijer et al., 2006; Liu et al., 2005, 2007; Strawa et al., 2013). A study in China established a multi-parameter remote sensing formula for dry $PM_{2.5}$ mass concentration near the ground, incorporating AOD, the Planetary Boundary Layer (PBL) height, and the Relative Humidity (RH) to derive the columnar volume to extension ratio of fine particles during winter 2013 (Zhang and Li, 2015). While PM concentrations in the study region ranged from 5 to 540 $\mu g/m^{3,}$ the model obtained a Mean Absolute Error (MAE) of 64 μg/

Table 2
Summary of selected studies using satellite data and models for estimating short-term air quality and pollution episodes (STE-short term exposure, STE-U-short term exposure in an urban environment, BB-biomass burning).

Event Type	Time Period	Location	Model	R^2	RMSE [μg/m^3]	Remote sensing Instrument/s	Ref
STE	2003	New England region, USA	Mixed Effects Model	0.95	2.5	MODIS	(Lee et al., 2011)
BB	Summer 2010	Russia	$PM_{2.5}$ = η x AOD Eq. 1[a]	0.85	NA	MODIS	(van Donkelaar et al., 2011)
STE	12.2012–11.2013	China	GWR	0.64	32.98	MODIS, MISR	(Ma et al., 2014)
STE-U	3.2013–4.2014	Beijing, China	Mixed Effects Model	0.81	17.85	MODIS	(Xie et al., 2015)
STE	10.2013–12.2013	China	Columnar volume-to-extinction ratio of fine particulates	0.5	64 (MAE)	MODIS	(Zhang and Li, 2015)
BB	Apr-Sep. 2011–2014	Colorado, USA	Bayesian ensemble model	0.66	2	MODIS	(Geng et al., 2018)
STE-U	2003–2005	Southeastern USA	Bayesian Model Averaging	0.83	3	MODIS	(Murray, 2018)
STE	Winter 2012–2013	Central Valley, CA, USA	Mixed Effects Model	0.9	7	MODIS	(Chatfield et al., 2019)
STE	2013–2015	Italy	spatiotemporal land-use random-forest	0.86	0.02	MODIS	(Stafoggia et al., 2019)
STE	2014	Beijing, China	TFERGWR	0.8	less than27%	VIIRS	(Yao et al., 2019)

[a] η is determined from the ratio of simulated $PM_{2.5}$ to simulated AOD at satellite overpass. It is a function of aerosol size, aerosol type, relative humidity, and the vertical structure of aerosol extinction.

m^3. Specifically for modeling air pollution episodes, biomass burning has been studied in specific fire events (van Donkelaar et al., 2011) and seasons (Geng et al., 2018).

Since many time-varying parameters, such as local meteorological variables (e.g. temperature, RH), the vertical $PM_{2.5}$ concentration profile, and the particle optical and other thermo-physical properties may affect the AOD-$PM_{2.5}$ association, it is reasonable to expect that the latter may vary on a timely basis. To account for the daily variability LMEM has been applied (Chatfield et al., 2019; Kloog et al., 2015; Stafoggia et al., 2017; Xie et al., 2015), which enables calibration of the model for time varying variables ("daily calibration"). Using the LMEM showed significant improvement over China, with R^2 (RMSE) of 0.47 (32.09 μg/m^3) and 0.81 (17.85 μg/m^3), applying a linear regression and a LMEM, respectively. The results had a clear seasonal effect, with better results in the warm season than in the cold season (Xie et al., 2015). Using a similar approach, Chatfield et al. (2019) introduced the use of the Column Water Vapor (CWV) and its usefulness with a daily calibration of the AOD/CWV ratio relationship to $PM_{2.5}$. They examined the contribution of additional predictors on the baseline model using only AOD. The base model resulted in a linear regression coefficient of 0.4 compared to 0.9 (RMSE = 7 μg/m^3) when applying the LMEM using the AOD/CWV ratio in both the random and fixed effects parts of the model.

In recent years machine learning has been introduced to the field, mainly for long-term studies as large datasets are required for the modeling process (Alvarez-Mendoza et al., 2019; Bellinger et al., 2017). For example, Random Forest (RF) has been used in air quality models (Hu et al., 2017; Mhawish et al., 2020; Stafoggia et al., 2019), not necessarily incorporating satellite data (Brunello et al., 2019; Kamińska, 2018) for examining the effect of temporal variables on air quality modeling, using the R software package 'randomForest' (Liaw and Wiener, 2016). Moreover, "Geomatic" modeling which is the contraction of the terms "geography" and "computer informatics" has been recently introduced to the air quality field (Bajpai et al., 2019). It is a set of technologies for modeling, representing and analyzing the territory to make virtual representations: geolocation, spatial imagery, databases, GIS (geographic information system) and Web technologies.

- Example: *code for applying RF can be found in the following link:* https://github.com/mshamer/ShortTermStrategies.git *(RF-example.R, README RF-example)*

While many studies have used MODIS satellite products, MODIS is coming toward its limits and a shift for new sources is required. VIIRS onboard the Suomi National Polar-orbiting Partnership (S-NPP), was launched in 2011 and another VIIRS on NOAA-20 (also known as Joint Polar Satellite System; JPSS-1) was launched in 2017. They continue the MODIS legacy, at least for afternoon sampling. The ESA Sentinel 3 satellites and future MetOP satellites carry on the MODIS approach for morning sampling (~10am local solar time). Yao et al. (2019) utilized the VIIRS high resolution IP AOD product for examining short-term exposure in Beijing, China. They used a nested spatiotemporal statistical model that consists of a nested time fixed effects regression model and a series of Geographically Weighted Regression (GWR) models. GWR has been used in this type of studies showing that the meteorological and land use information can strongly improve model performance (Ma et al., 2014). Results indicate that the $PM_{2.5}$-AOD relationship presents strong temporal heterogeneities. Varying intercepts with a shorter time interval, available, for example, from geostationary satellites, will probably be able to capture this temporal behavior (Yao et al., 2019).

Application of modeling with satellite AOT columns from different satellite platforms has been used in different field campaigns, combining satellite and airborne datasets. Several Distributed Regional Aerosol Gridded Observation Networks (DRAGON) field campaigns have been deployed in different locations and times (Holben et al.,

Table 3
Summary of selected current and future satellites to leverage current capabilities in short-term air quality research studies.

Satellite	GEO/LEO	Instrument	Launch	Spatial coverage	Spatial res. [km]	Temporal res. [min]
Aqua/Terra	LEO	MODIS	2002/2000	Global	1/3/10	Daily
Aqua/Terra	LEO	MODIS	2002/2000	Global	1/3/10	Daily
Terra		MISR				Every 7–9 days
Aura	LEO	OMI	2004	Global	13x24	Daily
S-NPP	LEO	VIIRS	2011	Global	0.75/6	Daily
Sentinel-5	LEO	TROPOMI	2017	Global	7	Daily
Himawari	GEO	AHI	2014	Japan	0.5–2	0.5–10 min
GOES-16	GEO	ABI	2016	East pacific	0.5–2	0.5–15 min
GOES-17	GEO	ABI	2018	West pacific	0.5–2	0.5–15 min
GEO-KOMPSAT-2B	GEO	GEMS	2018	Korea	5x15	Hourly
MTG-S	GEO	Sentinel-4	~2021	Europe	8.9x11.7	Hourly
Intelsat 40e	GEO	TEMPO	~2022	USA	2.1x4.5	Hourly
(OTB)-2	LEO	MAIA	~2022	Global	1	Daily

* http://www.wmo-sat.info/oscar/instruments.

2018). One of the AERONET field campaigns was established in CA central valley in 11/2012–4/2013. This short-term network provides a rich aerosol ground measurement dataset with 8 sites in the CA Central Valley. For periods within the short-term field campaign, DISCOVER-AQ, model fit was able to achieve $R^2 \sim 0.8$. These results were achieved using separate sub-regions of the Central SJV. They highlight the complexity of composition and a source-driven simulation (Friberg et al., 2018). Another modeling approach combines satellite data with numerical modeling simulation (CMAQ) for applying Bayesian models. This method shows promise in South eastern USA (Murray, 2018) and it was able to capture elevated $PM_{2.5}$ concentrations over large fire episodes in Colorado (Geng et al., 2018).

All the models reviewed in this section, demonstrated improved results compared to the outputs of a linear regression model. A summary overview of selected studies is listed in Table 2.

5. Interpretation of results

After obtaining results, their interpretation will define the next steps. There is no ‘one’ response or interpretation approach, as it is expected to differ between studies based on the datasets, study goals and methodologies examined. For example, Sorek-Hamer et al. (2013) approach of applying boosting, resulted in four main variables contributing to the $PM_{2.5}$ prediction. These variables were used as input to both non-linear GAM and MARS models. Although these models used the same input datasets, they provided different results, since they fitted different functions to the variables. The results were presented in terms of R-square, Root mean squared error (RMSE), and Normalized RMSE (NRMSE) between the predicted and observed $PM_{2.5}$ concentrations, and they were compared to a raw linear baseline. Furthermore, they examined the distribution of these statistics among all 100 cross-validation (CV) runs and the relationship between them, e.g. the correlation between the R-square and the NRMSE showed that the error measures, which examine the model performance, behave in a linear trend, indicating that with more explained variability the model residual errors decrease. CV is a model validation technique usually given a dataset of known data on which training is run (training dataset), and a dataset unseen by the model against which the model is tested (called the validation dataset or testing set). One round of CV involves partitioning a sample of data into train-test subsets, performing the analysis on the training subset and validating the analysis on the testing subset. CV combines measures of fitness from all runs, to derive a more accurate estimate of model prediction performance (Cawley and Talbot, 2010). This study (Sorek-Hamer et al., 2013) suggests that some non-linear techniques offer similar levels of modeling performance. The choice of a specific methodology approach should take into account factors such as computation speed, ability to ignore predictors of marginal relevance, transparency of the fitted relationships, and the ease with which model results can be transferable into other analyses. Based on these criteria, MARS was found to be a good candidate for the task of retrieving $PM_{2.5}$ from satellite remotely sensed aerosol products during the specific time period and over the study area. Results can be much localized depending on the specific characteristics of the studied region. For example, although many studies demonstrated promising improvements using satellite-based AOD data, we found marginal (Fig. 4) or no contribution (Zamani Joharestani et al., 2019) to the explained variation. While the efficacy of AOD as an explanatory variable in large-scale studies is clear, due to its continuous spatial coverage, on a local scale, both spatial and temporal factors might affect its ability to capture air quality structures, especially when pollution levels are relatively low. This should be examined on a case-by-case basis as it is a very local phenomena, affected by local environmental characteristics.

Interactions between variables can be examined and other types of non-linearity relationships can be explored for dropping insignificant variables. It is highly recommended to check for and resolve data issues. That includes multicollinearity, outliers, and missing data. Data issues occur within the context of the model. Following the application of the model, finally the results can be interpreted. As mentioned earlier, R-square is a common statistic yet it doesn’t provide enough information on its own. It is therefore recommended to use several statistics of the estimation error (e.g. Mean Absolute Error (MAE), RMSE, NRMSE; Eqs. (2)–(4)) and examine the temporal and spatial effect of variables and the spatiotemporal variance of the error. NRMSE is a function that allows the user to calculate the normalized root mean square error as an absolute value between predicted and observed values using different

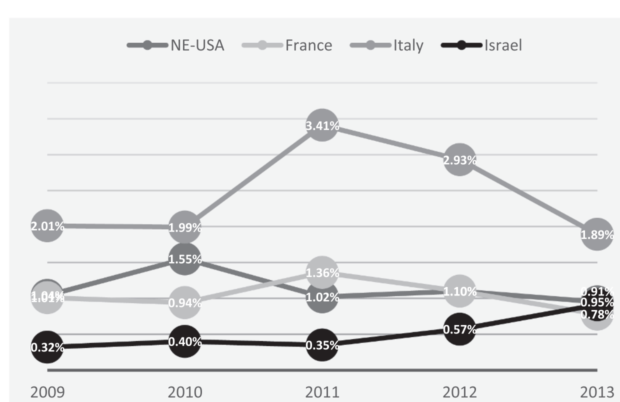

Fig. 4. Results of analysing AOD contribution in different locations using a LMEM. Each line represents a location (i.e. NE-USA, France, Italy, and Israel); each circle shows the annual contribution (in percentages) of the satellite-based AOD to the $PM_{2.5}$ estimation over a certain location at a specific year.

type of normalization methods. It is advisable for a comparison across indicators (Sorek-Hamer et al., 2013).

	Statistical Equation	R code

Eq. 2	$MAE = \frac{1}{n}\sum \lvert y - \hat{y} \rvert$	error <- actual - predicted
		(both numeric vectors)
		# Function that returns Mean Absolute Error
		mae <- function(error)
		{
		mean(abs(error))
		}

Eq. 3	$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum (y - \hat{y})^2}$	# Function that returns Root Mean Squared Error
		rmse <- function(error)
		{
		sqrt(mean(error^2))
		}
		# Another option is through the Metrics package:
		Install.packages("Metrics")
		Require(Metrics)
		rmse(actual, predicted)

Eq. 4	$\mathrm{NRMSE} = \frac{RMSE}{SD(y)}$ $\mathrm{NRMSE} = \frac{RMSE}{Mean(y)}$ $\mathrm{NRMSE} = \frac{RMSE}{Max(y) - Min(y)}$ $\mathrm{NRMSE} = \frac{RMSE}{Q1(y) - Q3(y)}$	Install.packages("INDperform") Require(INDperform) nrmse(pred, obs, method = "sd", trans-formation = "none", trans_function = "none") Method = A character string indicating the value to be used for the normalization of the RMSE. The default is the standard deviation (sd). Alternatively, the "mean" can be used, "maxmin" (difference between the maximum and minimum observed values) or "iq" (interquartile, the difference between the 25th and 75th percentile of observations)

Since satellite data have a significant spatial component, it is also important to interpret the spatial distribution of the prediction error. This type of spatial mapping will reveal spatial patterns of the model error and define dependency on spatial terms, e.g. Sorek-Hamer et al. (2020). These results illustrate how the communication of uncertainties can help, providing more confidence in the final valuation of the air quality impact. Another example addresses the challenges in using remotely sensed AOD to characterize $PM_{2.5}$, as they were especially evident in the wintertime in SJV, CA. This region experiences a unique climatology, related to high-albedo surfaces and very shallow vertical mixing layers. Chatfield et al. (2019) found success with a LMEM and a characterization of vertical mixing, by incorporating specific understandings of the region's climatology. This technique has been described as a "static estimation", not dependent on well-mapped source strengths or on transport error. Fig. 5 visually demonstrates a strong agreement between the modelled PM and the observed PM concentrations, in magnitude and pattern.

The accuracy of air pollution models can only be demonstrated by comparison with ground evidence or other modeled information. Unfortunately for health issues or crop planning, such evidence is neither always available nor easy to collect, as many factors are contributing and competing in determining those outcomes. It is challenging to disentangle and separate only the contribution of air pollution. It is therefore very important that the highest available level of accuracy (i.e. quality assurance flag) is guaranteed for the data that are used to run the models, and that the results are provided with meaningful confidence intervals (Solazzo et al., 2018).

6. Future directions

- **Geostationary satellites –** New generation of geostationary satellites to measure tropospheric ozone, aerosols, and their precursors, have been recently launched or are under development, and will be launched by multiple space agencies in the upcoming years. Geostationary satellites provide the ability to measure these constituents at high spatial and temporal resolution, but only viewing a certain part of the globe. Coordination through a constellation framework will provide a global perspective otherwise impossible to achieve. GeoNEX was established to achieve this goal. High temporal resolution products will provide more data for short-term analysis and will expand capabilities in this field of research. GeoNEX is a collaborative effort for generating Earth monitoring products from the new suite of geostationary satellite sensors. In collaboration with scientists at NOAA, NASA and other international organizations, GeoNEX serves as a platform for scientific partnership, knowledge sharing and research for the Earth science community (https://www.nasa.gov/geonex). GeoNEX currently offers 1 km gridded products from both LEO and GEO satellites (e.g. GOES 16/17, Himawari 8/9). New sensors on geostationary satellites have great promise for planetary monitoring. In particular, the new capabilities of NOAA's GOES and JAXA's Himawari have significant spectral, radiometric, temporal and scan rate improvements. For example, GOES sensors have three times more spectral channels, four times better spatial resolution and five times faster scan rate than earlier versions (Fig. 6).

The new geostationary-based datasets will significantly increase the size of the available datasets to analyze for short-term studies and enable utilizing more sophisticated Deep learning approaches. In addition, the main goal of NASA's MAIA (Multi-Angle Imager for Aerosols) LEO mission is similarly to deliver new daily data, mapping $PM_{2.5}$ exposures sufficient for health effects studies (Diner et al., 2018).

- **Vertical distribution** – The vertical distribution and layering of aerosols is critical for understanding how well AOD represents aerosols that reside at heights (from the ground) relevant for human exposure. Very few tools have been available for conducting research that co-located remote sensing products and information about the vertical distribution. Lidar provides a very helpful view of complexities of submicron particle abundance and properties within the mixed layer and the uniformity of the mixed layer top (Sawamura et al., 2017). LIDAR measurements are available from different ground based networks, e.g. MPLNET, EARLINET, and can be accessed by the following links https://mplnet.gsfc.nasa.gov/data, https://www.earlinet.org/index.php?id=125, respectively, and somewhat limited from space (i.e. Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation; CALIPSO). AOD correction using CALIPSO can be investigated despite its limited spatio-temporal resolution. 3D modeling is a promising direction with data playing a larger part in assimilations.
- **Night time light** – Recently, Night time light (NTL), based on the Day/Night Band (DNB), a product retrieved from VIIRS, aboard the S-NPP satellite, has been found to explain some of the variance in PM concentrations (Zhang and Hu, 2017) and spatiotemporal trends in urbanization and in air pollution (Wang et al., 2016), yet it hasn't been extensively studied. The DNB collects global low-light imaging data detecting electric lighting present on the Earth's surface with a spatial resolution of approximately 750 m (Elvidge et al., 2017; Wu and Wang, 2019). Since most of these lights have been recognized from human settlements, NTL was found to be a good indicator of urbanization and human activity, which can affect $PM_{2.5}$ concentrations predictions and spatial trends in poverty (Andreano et al., 2020; Jean et al., 2016). The commonly used monthly mosaic of NTL VIIRS imagery is a preliminary product, calibration and filtering to remove light detections associated with fires, gas flares, volcanoes, and background noise, is recommended, before they are used to estimate environmental and socioeconomic variables (Li et al., 2013; Wu et al., 2018).

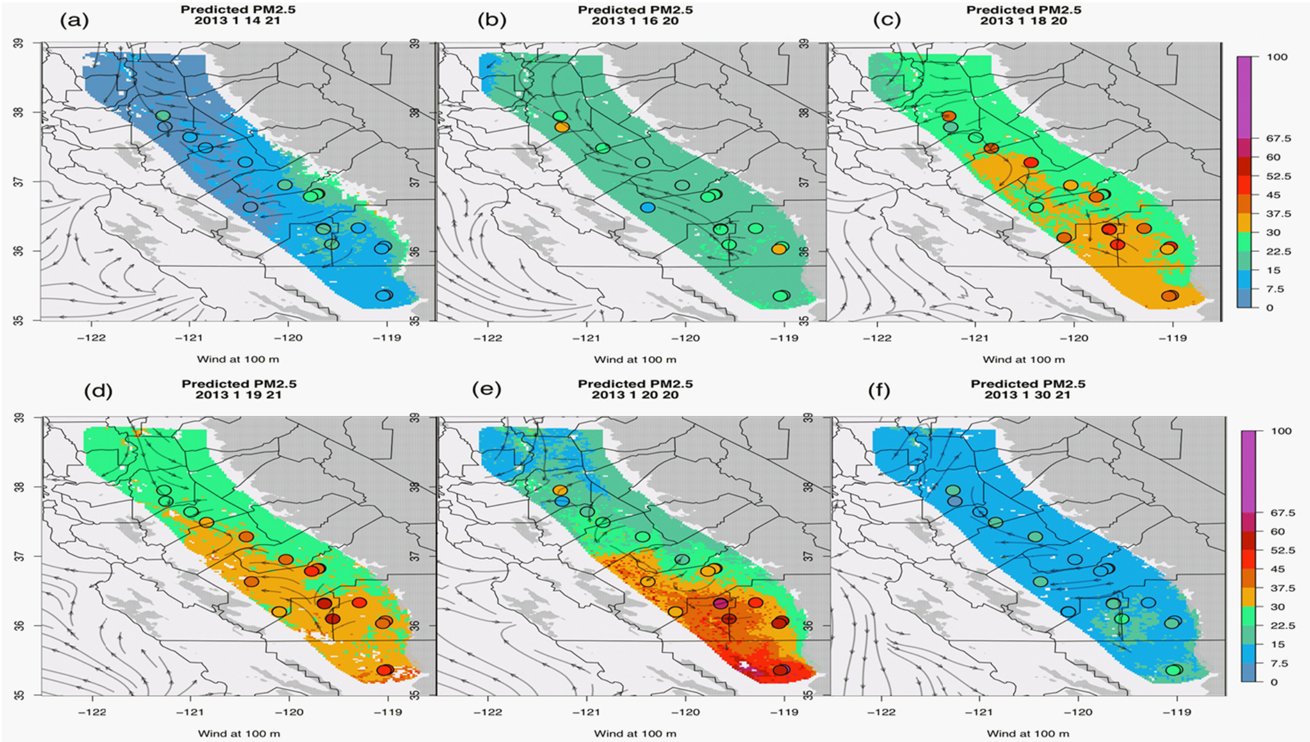

Fig. 5. Estimated surface $PM_{2.5}$ at 1 km indicated overpass times for the first wintertime episode in the San Joaquin Valley. Winds at 360 m agl are also shown. Estimated RMS error is 7 μg/m^3 with a similar limit of detection. Filled circles show $PM_{2.5}$ stations (Chatfield et al., 2019).

7. Summary

To conclude, using satellite data for modeling short-term air quality has been widely used despite its known limitations. If this is the general direction of the study, make sure to have clear and detailed study goals and to know the data. Spend time on preprocessing and documenting the assumptions, understand climatology and the environment of the study period or the air pollution event. Design the study carefully, develop modeling strategies including a validation plan, interpret results and provide new insight on air pollution to the field. Remember to put some thought into the availability of datasets, spatiotemporal variability, local and regional met conditions, and cross validation methods. Be careful in interpreting the results and investigate spatiotemporal trends in error. For future steps, the use of geostationary satellites will provide better temporal availability which might enable to utilize deep learning approaches. Night time light and data related to the vertical distribution can be very effective and improve current state of modeling both long-term and short-term air quality. Satellite-borne data have the capabilities to improve the temporal and spatial coverage of fine particle exposure estimates. With proper adjustment of meteorological factors, satellite AOD might be considered as a direct tool for estimating acute health impacts of ambient particles without prior calibrating to the sparse ground monitoring networks (Wang et al., 2013), yet with a strong validation plan.

CRediT authorship contribution statement

Meytar Sorek-Hamer: Conceptualization, Data curation, Writing - original draft. **Robert Chatfield:** Conceptualization, Visualization. **Yang Liu:** Conceptualization, Writing - review & editing.

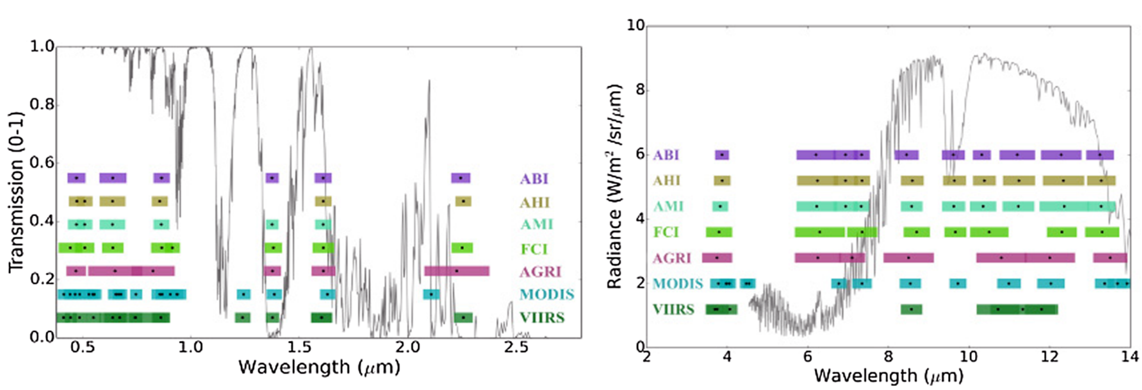

Fig. 6. Comparison of spectral band positions across LEO and GEO sensors alongside those of polar-orbiting missions for land surface monitoring, NASA's MODIS and NOAA's VIIRS. The black line is solar transmittance (left) and radiance (right) from HITRAN (https://www.nasa.gov/geonex). ABI – Advanced Baseline Imager on GOES-16/17 (United States). AHI – Advanced Himawari Imager on Himawari 8/9 (Japan). AMI – Advanced Meteorological Imager on GEO-KOMPSAT2 (South Korea). FCI – Flexible Combined Imager on MTG (Europe). AGRI – Advanced Geosynchronous Radiation Imager on Fengyun-4 (China). MODIS – Moderate Resolution Imaging Spectroradiometer (United States). VIIRS – Visible/Infrared Imaging Radiometer Suite (United States).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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