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Daily estimation of ground-level $PM_{2.5}$ concentrations at 4 km resolution over Beijing-Tianjin-Hebei by fusing MODIS AOD and ground observations

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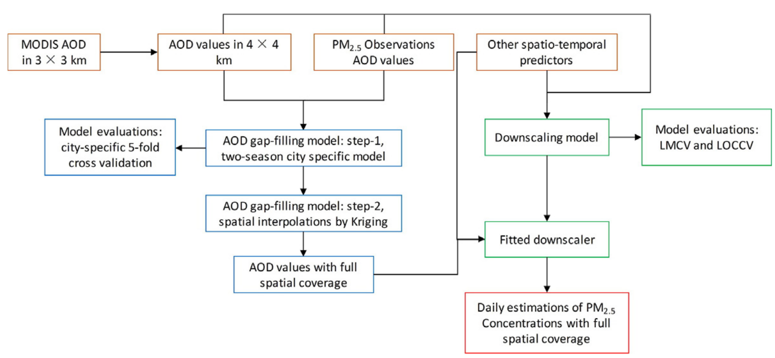
HIGHLIGHTS

- Fine resolution $PM_{2.5}$ concentrations are estimated in Beijing-Tianjin-Hebei area.
- Downscaling method modeled time and space varied $PM_{2.5}$-AOD associations.
- Missing AOD values were filled using a two-step approach.
- Derived $PM_{2.5}$ products have multiple potential applications with high accuracy.

GRAPHICAL ABSTRACT



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ABSTRACT

The satellite-borne Moderate Resolution Imaging Spectroradiometer (MODIS) aerosol optical depth (AOD) is widely used to estimate ground-level fine ambient particulate matter ($PM_{2.5}$) concentrations to evaluate their health effects. The associated estimation accuracy is often reduced by AOD missing values and by insufficiently accounting for the spatio-temporal $PM_{2.5}$ variations. In this study, we aim to estimate ground-level $PM_{2.5}$ concentrations at a fine resolution with improved accuracy by fusing fine-scale satellite and ground observations in the populated and polluted Beijing–Tianjin–Hebei (BTH) area of China in 2014. We employed a Bayesian-based statistical downscaler to model the spatio-temporal linear AOD-$PM_{2.5}$ relationships. We used a 3 km MODIS AOD product, which was resampled to a 4 km resolution in a Lambert conic conformal projection, to assist comparison and fusion with predictions by atmospheric chemistry models. A two-step method was used to fill the missing AOD values to obtain a full AOD dataset with complete spatial coverage. The downscaler has a good performance in the fitting procedure ($R^2 = 0.75$) and in the cross validation procedure ($R^2 = 0.58$ by random method and $R^2 = 0.47$ by city-specific method). The number of missing AOD values was serious and related to elevated $PM_{2.5}$ concentrations. The gap-filled AOD values corresponded well with our understanding of $PM_{2.5}$ pollution conditions in BTH. The prediction accuracy of $PM_{2.5}$ concentrations were improved in terms of their annual and seasonal mean. As a result of its fine spatio-temporal resolution and complete spatial coverage, the daily

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$PM_{2.5}$ estimation dataset could provide extensive and insightful benefits to related studies in the BTH area. This may include understanding the formation processes of regional $PM_{2.5}$ pollution episodes, evaluating daily human exposure, and establishing pollution controlling measures.

1. Introduction

Air pollution caused by fine particulate matter with aerodynamic diameters of 2.5 μm or less ($PM_{2.5}$) have become very serious in China in recent years (Ma et al., 2015; Zhang and Cao, 2015). Because of their tiny sizes, $PM_{2.5}$ can readily penetrate into human bronchi and lungs (Nel, 2005). Many epidemiological studies have shown that long-term exposure to $PM_{2.5}$ can cause human morbidity and premature mortality (Lelieveld et al., 2015; Pope and Dockery, 2006). Even short-term exposure to high-level $PM_{2.5}$ could have serious adverse effects on human health (Pope et al., 2011). Heavy pollution episodes frequently and periodically occur in China, especially in the Beijing–Tianjin–Hebei (BTH) area, with $PM_{2.5}$ concentrations reaching up to hundreds μg/m^3 (Huang et al., 2014; Ji et al., 2014; Lv et al., 2016a; Zhang et al. 2014). Since 2012, China has built a large-scale network to monitor ground-level $PM_{2.5}$ concentrations. In 2014, the average $PM_{2.5}$ concentrations in the densely populated BTH area exceeded 90 μg/m^3, nearly ten times the standard (10 μg/m^3) recommended by the World Health Organization. However, because of the network's sparse spatial coverage and aggregation within urban cores, significant uncertainties are associated with the direct use of the observations from the monitoring network in epidemiological studies.

Aerosol optical depth (AOD) measures the light extinction caused by the presence of atmospheric aerosols. The AOD data observed by satellite-based instruments, such as the Moderate Resolution Imaging Spectroradiometer (MODIS), have been widely used to derive ground-level $PM_{2.5}$ concentrations (Liu et al., 2005; Van Donkelaar et al., 2011). Early studies used linear relationships between AOD and $PM_{2.5}$ to generate these estimations, in combination with employing other spatiotemporal predictors (Liu et al., 2005; Van Donkelaar et al., 2006). More recently, more complex models have been proposed to describe the varied relationships between AOD and $PM_{2.5}$ levels, such as geographically weighted regression (GWR) models (Ma et al., 2014), linear mixed-effect models (Lee et al., 2011), generalized addictive models (Liu et al., 2009), remote sensing formulas (Li et al., 2016; Lin et al., 2015; Zhang and Li, 2015), multi-stage models (Ma et al., 2015) and the complex statistical downscaling method (Chang et al., 2014). The downscaling method accounts for varied spatio-temporal relationships between AOD and $PM_{2.5}$ in a linear regression setting. Given the spatially heterogeneous compositions of atmospheric aerosols, this Bayesian-based downscaling framework is able to better model the AOD-$PM_{2.5}$ relationships.

In almost all previous studies in China, the AOD datasets with a coarse spatial resolution (e.g. 10 km MODIS AOD from Collection 5) have been used. To our knowledge, only a few studies have used the 3 km MODIS AOD products from Collection 6 retrievals (Ma et al., 2016; Xie et al., 2015; You et al., 2016). These finer resolution estimations of ground $PM_{2.5}$ levels would provide more detailed spatial information than the 10 km dataset. Therefore, application of the fine resolution AOD dataset at a 3 km resolution at the regional scale could provide insightful information for our understanding of $PM_{2.5}$ pollutions and contribute to human exposure studies.

A possible bias associated with the use of satellite-based AOD values to estimate $PM_{2.5}$ concentrations often arises from missing AOD values. Such missing data may be caused by high surface albedo, clouds and, potentially, extremely high particulate pollution levels (Engel-Cox et al., 2004). To reduce the bias, several methods have been proposed in previous studies, such as simple interpolation from retrieved AOD using the Kriging method (Ma et al., 2014) and correction factors based on the ratio of observations to estimations (Van Donkelaar et al., 2012; Zheng et al., 2016). In addition, the interpolated fields from $PM_{2.5}$ observations have been used to help obtain spatially continuous estimations of $PM_{2.5}$ concentrations (Kloog et al., 2011). Most of these gap-filling or prediction correction methods are not based on daily data. Therefore, their application would be constrained when studying daily ground-level $PM_{2.5}$ concentrations.

In the current study, we applied the 3 km MODIS AOD dataset over the BTH area of China in 2014 (from January 10 to December 30). We established a two-step method to fill the missing AOD values, to obtain a full AOD dataset with complete spatial coverage. We then employed a statistical downscaling method to model the spatially and temporally varied AOD-$PM_{2.5}$ relationships. The daily fine-scale estimations with complete spatial coverage were finally generated.

2. Data and methods

2.1. Study area

Estimation of ground-level $PM_{2.5}$ concentrations was carried out over a gridded area of BTH with a spatial extent of 35.86 to 41.52°N latitude and 114.23 to 117.79°E longitude (Fig. 1). The resolution of grid cells was determined to be 4 × 4 km under the Lambert conic conformal projection. The setting of the grid was determined for the convenience of inter-comparison and fusion with simulations of atmospheric chemistry models such as the Community Multiscale Air Quality model (CMAQ). There were 81 grid cells in the *x* direction and 151 cells in the *y* direction (12,231 cells in total). The original 3 km AOD dataset was resampled to the 4 km grid using a nearest neighbor method.

2.2. Data

2.2.1. Ground monitoring $PM_{2.5}$

The technique workflows revolving the data and methods adopted in this study were depicted in the Fig. S1 in the supplementary material. The hourly $PM_{2.5}$ observations were collected from the real-time data publishing platform (113.108.142.147) maintained by the China Environmental Monitoring Center (CNEMC), affiliated to the Chinese Ministry of Environment Protection (MEP). Daily mean $PM_{2.5}$ concentrations were calculated using the 24-hour mean of hourly measurements within a day. There are 94 monitoring sites in total (Fig. 1) in 16 prefecture-level cities within our study area. They are assigned to 82 4 × 4 km grid cells, indicating the existence of multiple monitoring sites in a single grid cell. We used the mean $PM_{2.5}$ concentrations of the monitoring sites that are located in a single grid cell, to avoid inconsistency of the $PM_{2.5}$–AOD relationships. In this we, we had a total of 28,836 $PM_{2.5}$ observations.

2.2.2. MODIS AOD data

The MODIS instruments, aboard two sun-synchronous satellites Terra and Aqua, provided two observations at approximately 10:30 a.m. and 1:20 p.m. local solar time. We used the collection 6, level 2 product (MOD_3K and MYD_3K) at a 3 km resolution. Using dark target algorithms, the MODIS AOD over land is retrieved using the spectral information at three channels of 0.47, 0.66 and 2.12 μm (Remer et al., 2005) to acquire signals of atmospheric aerosols in the vertical direction. The 3 km products use averages within a window of 6 × 6 pixels rather than 20 × 20 pixels of the 10 km products (Munchak et al., 2013). The MOD_3K and MYD_3K products from Jan.