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Using MODIS derived aerosol optical depth to estimate ground-level $PM_{2.5}$ concentrations over Turkey



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ABSTRACT

Satellite based particulate matter (PM) pollution monitoring on a regional basis is of importance due in part to the adverse health effects of PM. In this study, Moderate Resolution Imaging Spectroradiometer (MODIS) derived aerosol optical depth (AOD) data at 3 km and 10 km resolutions from both Terra and Aqua satellites were used, in conjunction with the surface in situ data, to improve the regional distribution of ground-level PM_{2.5} over Turkey. Five years (2011-2015) of heating season's (15th October to 14th May) in situ PM2.5 measurements from 7 monitoring stations in Ankara and 3 years (2013-2015) of the same data from 13 monitoring stations in Marmara Region were used. Linear and non-linear regression models were used to find the relationship between $PM_{2.5}$ and AOD data. To improve the correlations between $PM_{2.5}$ and AOD, the data points affected by free tropospheric long-range transport were removed from the analysis via back trajectory modeling analysis since long-range transport affects AOD more readily than surface PM_{2.5} data. Using non-linear models with the addition of meteorological parameters such as height of planetary boundary layer, surface temperature and surface wind speed improved the correlations significantly. The best non-linear model can explain 61% (n = 37, R^2 = 0.61, p < 0.001, RMSE = 0.337 µg/m³) of PM_{2.5} variations at the Edirne Keşan site. It was found that Terra worked better than Aqua. Furthermore, 10-km aerosol products gave better correlations with PM_{2.5} as compared to the 3-km products. With the aid of spatiotemporal model, PM2.5 distribution maps are created for the first time for Turkey.

1. Introduction

Atmospheric aerosols, liquid and solid particles suspended in air, have been in the focus of scientific interest for the last 2 decades due to their environmental impacts. Atmospheric aerosols, either released from anthropogenic and natural sources or formed in the atmosphere via secondary chemical reactions may contain inorganic ions (nitrate, sulfate and ammonia), carbonaceous aerosols (organic or black carbon), dust particles, and sea salt (Anderson et al., 2012; Fuzzi et al., 2015; Tsai et al., 2011). Particulate matter (PM) pollution adversely affects both ecosystems and human health in many ways. Particles enter the aquatic and terrestrial ecosystems by means of dry and wet depositions and alter the structure of ecosystems by means of reducing growth, changing chemical composition and biogeochemical cycles (Grantz et al., 2003). Black carbon plays an important role in climate change, and deposition of secondary inorganic aerosols can cause eutrophication (Fuzzi et al., 2015). PM can have detrimental effects on human health (Li et al., 2011). Particles with diameter less than $2.5 \,\mu m$ (PM_{2.5}) can enter bloodstream through the bronchial and pulmonary alveoli and create serious health effects on cardiovascular and pulmonary systems (Tsai et al., 2011; Wang et al., 2013b; Zhang et al., 2016). Exposure to particles in pregnancy or early childhood reduces the child weight (Kim et al., 2016). Another research states that exposure to particulate pollution increases the risk of obesity and metabolic syndrome (Wei et al., 2016). Effects of particulate pollution on human health are well discussed in literature (Anderson et al., 2012; Kim et al., 2015; Polichetti et al., 2009).

Due to its adverse effects, monitoring of particulate pollution has become increasingly important in recent years. It generally relies on air quality monitoring stations (AQMS). However, lack of spatial coverage of AQMS is an important challenge. On the other hand, Earth observation from the sensors of satellites (remote sensing) can be used as a complementary monitoring tool to determine the current level of air quality (Michaelides et al., 2018). Remote sensing is a cost effective

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way of observing ground level air pollution when in situ monitors are unavailable or too sparse (Hu et al., 2014). The Moderate Resolution Imaging Spectroradiometer (MODIS) instrument (installed onboard NASA's two Earth Observing System (EOS) satellites: Terra and Aqua) is widely used for aerosol monitoring purposes. Aerosol Optical Depth (AOD) (also referred to as Aerosol Optical Thickness, AOT) is the integral of extinction coefficient of aerosol column from the surface to the top of the atmosphere. On the other hand, in situ measurements of PM represent the surface loading of aerosols (Guo et al., 2009). The presence of aerosols in an atmospheric column changes the measure of the light extinction of sunlight at a certain wavelength due to scattering and absorption (Zhang et al., 2016). Therefore, AOD and PM is directly related and certain conversion factors are needed (Guo et al., 2009; Kloog et al., 2015, 2014). In order to find a better relationship between AOD and PM_{2.5}, multivariate regression models are recently used with the addition of local meteorological parameters such as cloud cover, planetary boundary layer height, relative humidity, wind speed, wind direction and surface temperature (Guo et al., 2017; Lin et al., 2015). Some other researchers included land use information (such as forest cover, topography, elevation, open spaces, and urban percentage), emission inventory and site specific factors (like surface reflectivity, population density, and traffic density) as well in multivariate regression models (Hu et al., 2014; Kloog et al., 2011; Liu et al., 2007; Ma et al., 2016; Sorek-hamer et al., 2015; Xie et al., 2015). Song et al. (2015) used MODIS AOD data, meteorological variables, coordinates and other pollutants (CO, SO2, NO2 and O3) as independent variables in their generalized addictive model to predict PM2.5 concentrations in Xi'an City of China. Moreover, other satellite derived data such as MODIS fine mode fraction (FMF) can also be included in the statistical analysis (Zhang and Li, 2015).

As a European Union (EU) candidate country, Turkey has been trying to reach the air quality standards as stated in EU Directives. The Ministry of Environment and Urbanization is aimed at reaching the attainment of criteria pollutants in 2019 and 2024 for harmonization of air quality legislation with EU. In last two decades, air quality monitoring stations have been established in every city in Turkey. However, most of these stations are located in urban areas, and the rural coverage is quite limited. Moreover, old stations only measures PM₁₀ (Particulate Matter with aerodynamic diameter less than 10 µm) and SO₂ (Sulfur dioxide) as pollutants. Only a few AQMS, located in Ankara and newly established stations in Marmara region, measure PM2.5. The other parts of the Turkey lack of PM2.5 records. Moreover, there is not a standard for PM_{2.5} neither in Turkish air quality legislations nor in Turkish Air Quality Index. United States Environmental Protection Agency (EPA), World Health Organization (WHO) and European Union threshold values for $PM_{2.5}$ are 35 $\mu g/m^3,$ 25 $\mu g/m^3$ and 25 $\mu g/m^3$ respectively (24 h averaging time).

In literature, although there are several studies related with PM_{2.5} measurement in Turkish cities, only two of the published studies use remote sensing technology. Some of these studies dealt with chemical composition (Kendall et al., 2011; Onat et al., 2013; Pekey et al., 2010; Szigeti et al., 2013), and others focused on source apportionment (Koçak et al., 2007; Yatkin and Bayram, 2008), size characterization (Karaca et al., 2005) or traffic related emissions (Gaga et al., 2018; Onat et al., 2019). PM_{2.5} levels measured in these studies are briefly summarized in Table 1. To our knowledge, there are only two studies that focus on atmospheric PM in Turkey by means of MODIS data. One paper investigates the contribution of Saharan dust in PM₁₀ concentrations in Turkey (Kabatas et al., 2014). The other study tried to find correlation by simple linear regression between Terra MODIS AOD and daily average PM_{2.5} concentrations at Marmara Region (Öztaner et al., 2015). It can be concluded that PM_{2.5} monitoring by remote sensing is a quite new subject in Turkey. This is the first comprehensive study which uses remote sensing techniques in greater detail for PM_{2.5} monitoring in Turkey. The aim of this paper is to find a relationship between MODIS AOD data and ground based measured PM_{2.5} concentrations in Turkey.

The organization of this paper is as follows. In Section 2, the study area is described and the methods of gathering and processing data (satellite observations, ground based measurements and meteorological data both for regression models and back trajectory analysis) are outlined. Results and Discussion (Section 3) contains the analysis of $PM_{2.5}$ measurements, analysis AOD retrieval rates, back trajectory modeling results and statistical relations between $PM_{2.5}$ and AOD. The conclusion is given in Section 4.

2. Materials and methods

2.1. Data

In this study, four different types of datasets are used: (1) PM_{2.5} mass concentrations of ground measurements, (2) Aerosol Optical Depth data from MODIS onboard Terra and Aqua satellites, (3) National Centers for Environmental Prediction (NCEP) Climate Forecast System Reanalysis (CFSR) meteorological data, and (4) Global Reanalysis Data for back trajectory analysis.

2.1.1. Study area and PM_{2.5} measurements

As stated in previous section, PM_{2.5} monitoring is a quite new concept for Turkey. At the end of 2015, the air quality of Turkey is continuously being monitored by 195 stations and 4 mobile stations. However, there are only 20 stations measuring PM_{2.5}. 7 of these stations, located in Ankara - the capital city of Turkey, have been recording PM_{2.5} since 2010. Newly installed 13 stations have been measuring fine particulate matter since 2013 in Marmara Region. The names and coordinates of the stations in Ankara and Marmara Region are listed in Tables 2 and 3 respectively. Table 3 also contains some spatial information that will be used in a spatiotemporal model. Station coordinates, elevation data, and county area information were obtained from the Ministry of Environment and Urbanization. Population information was taken from the Address Based Population Registration System. Finally, daily number of vehicles was gathered from the Traffic Volume Maps published by the General Directorate of Highways. Both highways and state ways were taken into account. The word "MTHM" in the station names stands for Marmara Clean Air Center. Fig. 1 shows the locations of these stations. Ankara, the capital city of Turkey, is a highly urbanized city with continental climate (cold and semi-arid). İstanbul, Bursa, Kocaeli and Tekirdağ are highly industrialized cities in Marmara region. Marmara (Transitional) Climate and Black Sea Climate (near the Black Sea shore line) are observed in this area. Moreover, continental climate is seen in inner parts of this region.

Ground level $PM_{2.5}$ mass concentration data are obtained from Turkish Air Quality Monitoring Stations Web Site (NAQMS, 2016). Daily and hourly measurements are accessible via web site. Hourly $PM_{2.5}$ measurements of 20 stations were downloaded.

2.1.2. Remote sensing data

Both Terra and Aqua satellites rotate around the Earth in sun-synchronous, near polar, circular orbit (705 km). Terra was launched on 18 December 1999, and Aqua was launched on 4 May 2002 (Kloog et al., 2011; Papadimas et al., 2009; You et al., 2016). Terra and Aqua satellites have been observing Earth since February 2000 and June 2002 respectively (Levy et al., 2010; Wang et al., 2013a,b). Aqua passes the equator at 13:30 local solar time (afternoon orbit) in the south-north direction (ascending mode) and Terra passes the equator at 10:30 local solar time (morning orbit) in the opposite direction (descending mode) (Emili et al., 2010; Li et al., 2011; Papadimas et al., 2009). MODIS instruments are capable of retrieving data in 36 spectral bands from blue to thermal infrared part of the spectrum ($0.41-14.4 \mu$ m). The swath width of MODIS is about 2300 km. The temporal resolution of MODIS is 2 days globally, 1 day at mid-latitudes (greater than 30°) (Liang et al., 2006; Wang et al., 2013a,b).

In this study, MODIS AOD products which is also referred to as AOT

Table 1

PM_{2.5} levels in some Turkish cities.

İstanbulnear the Büyükçekmece LakeJuly 2002–July 200320.8Karaca et al. (2005)MersinErdemli (36° 33′ 54″ N, 34° 15′ 18″ E)April 2001–April 20029.7Koçak et al. (2007)Zonguldak41.4508° N, 31.7726° EDecember 2004–October 200529.1Tecer et al. (2008)Kocali15 different locationsMay 31–June 29, 2006 December 16, 2006–January 20, 200723.5 (summer) 21.8 (winter)Pekey et al. (2010)ErzurumErzurum Regional Directorate of HighwaysFebruary 2005–February 200613Bayraktar et al. (2010)BursaNilüferMay 2007–April 200853Kendall et al. (2011)İstanbulMaslak (47°30.6′ N, 19°1.8′ E)June 2010–May 201140Szigeti et al. (2013)İstanbulKültür University Campus24 April–24 May 200940.5Onat et al. (2013)	City	Locations	Period	$PM_{2.5}$ concentration (µg/m³)	Reference
	İstanbul Mersin Zonguldak Kocaeli Erzurum Bursa İstanbul İstanbul	near the Büyükçekmece Lake Erdemli (36° 33' 54" N, 34° 15' 18" E) 41.4508° N, 31.7726° E 15 different locations Erzurum Regional Directorate of Highways Nilüfer Maslak (47°30.6' N, 19°1.8' E) Kültür University Campus Parkär Aliaža	July 2002–July 2003 April 2001–April 2002 December 2004–October 2005 May 31–June 29, 2006 December 16, 2006–January 20, 2007 February 2005–February 2006 May 2007–April 2008 June 2010–May 2011 24 April–24 May 2009 July 2000, April 2010	20.8 9.7 29.1 23.5 (summer) 21.8 (winter) 13 53 40 40.5 28.2	Karaca et al. (2005) Koçak et al. (2007) Tecer et al. (2008) Pekey et al. (2010) Bayraktar et al. (2010) Kendall et al. (2011) Szigeti et al. (2013) Onat et al. (2015)

Table 2

Air quality monitoring stations in Ankara.

AQMS Name	StID	Latitude	Longitude
Ankara Bahçelievler	S01	39.91806	32.82278
Ankara Demetevler	S02	39.96750	32.79556
Ankara Dikmen	S03	39.89639	32.84056
Ankara Kayaş	S04	39.92528	32.92667
Ankara Keçiören	S05	39.96722	32.86278
Ankara Sihhiye	S06	39.92752	32.85947
Ankara Sincan	S07	39.97194	32.58500

products are used (Kloog et al., 2014). MODIS AOD data give possibility to estimate ground level PM pollution. MODIS AOD is more sensitive to $PM_{2.5}$ at 550 nm. Although most studies focused on $PM_{2.5}$, some studies centered upon PM_{10} since $PM_{2.5}$ monitoring is rare except North America and Western Europe (Streets et al., 2013; Wang et al., 2013a,b).

MODIS Dark Target aerosol product has a spatial resolution of 10 km at nadir and labeled as Level 2 (MOD04_L2 for Terra and MYD04_L2 for Aqua). MODIS Dark Target aerosol products have become quite popular among the air quality community for estimating particulate pollution. Because of coarse resolution, it was difficult to identify the local effects in exposure studies. Therefore, a new MODIS aerosol product with finer resolution was needed. The MODIS team released the Collection 6 dataset with AOD products of a 3 km resolution in 2014. New Level 2 files with 3 km resolution are label as MOD04_3K and MYD04_3K for Terra and Aqua respectively (Remer et al., 2013; Xie et al., 2015). In this study, MODIS AOD data retrieved from Terra and Aqua satellites are used with both 10 and 3 km resolutions.

Aerosol products are processed and archived by MODIS Adaptive Processing System (MODAPS) at NASA's Goddard Space Flight Center. These files can be downloaded freely from Goddard Space Flight Center web site (NASA, 2016). AOD data uses Hierarchical Data Format (EOS- HDF) which has lots of Science Data Sets (SDS) (Levy et al., 2010; Wang et al., 2013a,b). In literature, several SDS are used for estimation of particulate matter: Optical Depth Land And Ocean (Cheng et al., 2012; et al., 2007; You al., 2016), Lin et Image_Optical_Depth_Land_And_Ocean (at 550 nm with Quality Assurance Confidence Flag = 2 and 3) (Ma et al., 2014), Corrected_Optical_Depth_Land and Effective_Optical_Depth_Average_Ocean (Bennouna et al., 2011). Some studies suggest using quality flags for daily data analysis (Gupta and Christopher, 2008). Among these Science Data Sets (SDS), Optical Depth Land And Ocean, which uses the Dark Target algorithm, measures AOD at 0.55 µm for both Ocean (best) and Land (corrected) with best quality data (QA Confidence Flag = 3). These SDS data are available for both 3-km and 10-km aerosol products. In contrast, the Deep Blue Aerosol Optical Depth 550 Land SDS, using the Deep Blue algorithm, is available only at a resolution of 10 km. There is no corresponding 3-km product. For this reason, the Optical Depth Land And Ocean SDS products for both 3-km and 10-km resolutions were used in this study to investigate if the higher-resolution product is better correlated with surface PM_{2.5} concentrations.

2.1.3. Meteorological data

In order to develop multivariate regression models to predict ground level fine particle concentration, some meteorological variables are needed. The meteorological data were obtained from National Center for Environmental Prediction (NCEP) Climate Forecast System Reanalysis (CFSR) web page (NCEP, 2016). NCEP provides high resolution (approximately 0.2°) data in global scale. Only temperature (T), u-component of wind, v-component of wind, relative humidity (RH), height of planetary boundary layer (HPBL) parameters from Version 2 data set were downloaded. U and V components of wind were used to calculate wind speed (WS).

2.1.4. Back trajectory data

To further improve regression models, long range transport of particulate matter in free troposphere (between 2000 and 10,000 m) must

Table	3
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Air quality monitoring stations in marmara region.

AQMS Name	StID	Latitude	Longitude	Elevation (m)	County	Area (km ²)	2015 Population	2015 Vehicles
Bursa Uludağ Uni MTHM	S08	40.22333	28.87139	289	Nilüfer	552	397,303	76631
Çanakkale Lapseki MTHM	S09	40.40306	26.77056	12	Lapseki	821	25,865	4805
Edirne Karaağaç MTHM	S10	41.65889	26.53722	36	İpsala	741	28,249	6896
Edirne Keşan MTHM	S11	40.85111	26.63528	111	Keşan	1098	81,054	18,283
İstanbul Kağıthane MTHM	S12	41.09222	28.97472	43	Kağıthane	15	437,942	167,397
İstanbul Silivri MTHM	S13	41.07306	28.25528	8	Silivri	858	165,084	75,117
İstanbul Ümraniye MTHM	S14	41.02417	29.09972	149	Ümraniye	46	688,347	205,430
Kocaeli Gölcük MTHM	S15	40.72583	29.79444	29	Gölcük	217	152,607	120,480
Kocaeli Kandıra MTHM	S16	41.13056	30.00639	48	Kandıra	840	48,937	2601
Sakarya Ozanlar MTHM	S17	40.79056	30.39667	26	Adapazarı	324	269,079	18,742
Tekirdağ Çerkezköy MTHM	S18	41.31833	27.98000	146	Çerkezköy	86	133,626	10,483
Yalova Altınova MTHM	S19	40.70056	29.50778	16	Altınova	113	24,140	29,342
Yalova Armutlu MTHM	S20	40.52917	28.78444	21	Armutlu	166	8492	4000 ^a

^a Assumed value due to lack of data.



Fig. 1. Geographic locations of PM2.5 measuring AQMS sites in Turkey (at the end of 2015).

be eliminated. The Saharan Desert emits half of the global dust emissions and these emissions are associated with medium and long range transport events (Michaelides et al., 2018). Furthermore, northern and western parts of the Turkey are under the influence of long range particulate transport from European countries (Kindap et al., 2006). Thus, PM transport from Saharan Desert and polluted portions of Europe should be determined by means of back trajectory modeling. In order to apply 5 days back trajectory analysis, global meteorological data are needed. Meteorological data were obtained from NCEP/NCAR (National Center for Atmospheric Research) Reanalysis Data Archive web site (NCEP/NCAR, 2016).

2.1.5. Temporal coverage

6 years $PM_{2.5}$ concentration data (2010–2015) were available for stations in Ankara, and 3 years $PM_{2.5}$ concentration data (2013–2015) were available for stations in Marmara Region. MODIS AOD image files were downloaded for a period of 6 years (2010–2015). CFSR Version 2 contains data starting from January 1, 2011. Therefore, meteorological data set covers the period of 2011–2015. To sum up, the temporal coverage of data used for Ankara stations are in the period of 2011 and 2015. Due to the lack of $PM_{2.5}$ measurements, the data of Marmara Region stations are only for the 2013–2015 period.

2.2. Data integration

Different data sets should be integrated both spatially and temporally for each site, so as to find a relationship between $PM_{2.5}$ and AOD. Hourly ground based $PM_{2.5}$ measurements require no further processing. However, AOD data requires some processing. MODIS AOD data uses a sinusoidal projection. In order to obtain an AOD value for certain latitude and longitude, hdf files must be converted to geotiff format. For this reason, HEG-Tool (HDF-EOS to GeoTIFF Conversion Tool) was used. HEG-Tool also allows user to make spatial subsets of a certain location in order to decrease processing time. In this study, the upper left corner of subset is 42N 26E and the lower right corner is 39.5 N 33.5 E. After converting hdf files to geotiff format, these files were processed to compute AOD data at the coordinates where air quality monitoring stations located. Date and time information are available in MODIS files to generate a corresponding AOD and surface PM dataset.

The first step to investigate the relation between $PM_{2.5}$ and AOD, is the development of a simple linear regression model. Nevertheless, as stated in literature (Guo et al., 2009; Kloog et al., 2015, 2014), AOD and $PM_{2.5}$ are not strongly correlated. In order to find a better relationship between AOD and $PM_{2.5}$, multivariate regression models are recently used with the addition of local meteorological parameters such as planetary boundary layer height, relative humidity, wind speed and surface temperature (Kloog et al., 2011; Sorek-hamer et al., 2015). These parameters were processed for the locations the air quality monitoring stations and added to the dataset.

Before the development of any regression model between AOD and PM_{2.5}, it is important to separate the particulate pollution in the boundary layer and free troposphere (Koukouli et al., 2010). Kumar et al. (2007) mentioned that good correlations are found between PM2.5 and AOD if particles are within the boundary layer. Li et al. (2011) stated that long range transport may influence both air quality and the performance of statistical models. In the presence of long range transport (dust or smoke), poor or no correlations were observed. Therefore, the dust transport from Saharan deserts and particulate transport from Europe in free troposphere were investigated. Floutsi et al. (2016) examined the aerosol characteristics on the Mediterranean Basin over 12 years (between 2002 and 2014) by using Aqua MODIS AOD and reported that the dust events are observed in Eastern Mediterranean generally in spring and sometimes in winter months. Several studies reported that air quality in Turkish cities is under the influence of long range transport of aerosols (Agacayak et al., 2015; Kabatas et al., 2014; Karaca et al., 2009; Kindap et al., 2006). In order to decide transported particulate matter days, backward trajectory analysis was performed. A GIS based software called TrajStat (Wang et al., 2009), which runs HYSPLIT (The Hybrid Single-Particle Lagrangian Integrated Trajectory) model, was used for trajectory analysis. 5-day back trajectories were

Average PM _{2.5} concei	ntrations (μg/1	n ³) for stations in A	Ankara.									
AQMS	2010 N. S. ^a	2010-2011 H. S.	2011 N. S.	2011-2012 H. S.	2012 N. S.	2012-2013 H. S.	2013 N. S.	2013-2014 H. S.	2014 N. S.	2014-2015 H. S.	2015 N. S.	2015–2016 H. S. ^b
Ankara Bahçelievler	23	44	27	22	19	29	19	24	10	20	12	28
Ankara Demetevler	31	54	42	20	17	37	32	46	20	35	11	27
Ankara Dikmen	19	36	26	24	30	27	22	39	20	33	18	21
Ankara Kayaş	38	64	25	32	29	40	21	37	28	26	12	32
Ankara Keçiören	23	47	23	27	20	32	20	36	20	23	7	12
Ankara Sıhhıye	44	64	39	40	33	36	29	40	24	30	19	17
Ankara Sincan	31	49	32	31	27	30	17	33	10	17	7	9
^a Starts on 15 May ^b Ends on 31 Dece	2010. mber 2015.											

fable 4

initiated at 12:00 UTC every day. 5 years (2011-2015) and 3 years (2013-2015) back trajectories are generated for stations located in Ankara and Marmara Region respectively. Then cluster analysis was applied to merge trajectories into clusters. Nine clusters were obtained. PM_{2.5} and AOD data pairs were removed if their trajectories clustered in the free troposphere (at 5000-7500 m) originated from Saharan Desert or PM polluted regions of Europe. The EMEP officially reported emission Data (http://www.ceip.at/ms/ceip home1/ceip home/webdab emepdatabase/gridded_data/) were used to determine the polluted areas of Europe. If the trajectories passed through EMEP high emission grid cell with a probability of 60% or higher, the AOD and PM data pairs were excluded in the analysis.

2.3. Model development

In order to develop regression models to presume PM25 concentrations JASP statistical software (JASP, 2018) were used. Several linear and non-linear models (Eqs. (1)-(4)) were applied to find a relationship between PM2 5 concentration and AOD from Terra and Aqua MODIS retrievals.

$$PM_{2.5} = \alpha + \beta_1 \cdot AOD \tag{1}$$

 $PM_{2.5} = \alpha + \beta_1 \cdot (AOD/HPBL) + \beta_2 \cdot (AOD/WS)$ (2)

 $\ln(PM_{2.5}) = \alpha + \beta_1 \cdot \ln(HPBL) + \beta_2 \cdot (RH) + \beta_3 \cdot \ln(AOD)$ (3)

$$\begin{split} \ln(PM_{2.5}) &= \alpha + \ \beta_1 \cdot \ln(HPBL) + \ \beta_2 \cdot \ln(T) + \ \beta_3 \cdot \ln(WS) + \ \beta_4 \cdot \ln(RH) \\ &+ \ \beta_5 \cdot \ln(AOD) \end{split} \tag{4}$$

where PM_{2.5} is hourly measured ground-based PM_{2.5} mass concentration (µg/m³), AOD is Aerosol Optical Depth at 550 nm (unitless) retrieved from either Terra or Aqua MODIS, HPBL is height of planetary boundary layer (m), T is surface temperature (K), RH is surface relative humidity (%), WS is surface wind speed (m/s), α is intercept and $\beta_1 - \beta_5$ are regression coefficients.

Since HPBL and other meteorological variables together with MODIS AOD data could not be used to create a PM_{2.5} distribution map, some spatial parameter like AQMS elevation, population and area of a county, population density and number of vehicles were added to the regression equation. AQMS of Ankara were quite close to each other, thus the spatiotemporal model (Eq. (5)) was only applied for Marmara Region. In spatiotemporal modeling, both spatial and temporal predictors of PM_{2.5} can be included in the regression equation together with AOD data. Spatial predictors are topography data (digital elevation), land use data (land type, population density etc.), and particulate emissions related data (point, area and line sources) whereas temporal predictors are meteorological parameters, NDVI (Normalized difference vegetation index) and HPBL (He and Huang, 2018; Hu et al., 2017; Kloog et al., 2014; Zhai et al., 2018). In this study, all variables in Table 3 were added to the regression equation and the solution was computed using the backward method. The backward method repeatedly eliminates one independent variable from the regression equation if the p value of that variable is insignificant until it finds a significant model.

$$\begin{split} n(PM_{2.5}) &= \alpha + \beta_1 \cdot \ln(HPBL) + \beta_2 \cdot \ln(T) + \beta_3 \cdot \ln(WS) + \beta_4 \cdot \ln(RH) \\ &+ \beta_5 \cdot \ln(AOD) + \beta_6 \cdot HPBL + \beta_7 \cdot T + \beta_8 \cdot WS + \beta_9 \cdot RH \\ &+ \beta_{10} \cdot AOD + \beta_{11} \cdot E + \beta_{12} \cdot \ln(E) + \beta_{13} \cdot P + \beta_{14} \cdot \ln(P) + \beta_{15} \cdot A \\ &+ \beta_{16} \cdot \ln(A) + \beta_{17} \cdot PD + \beta_{18} \cdot \ln(PD) + \beta_{19} \cdot V + \beta_{20} \cdot \ln(V) \end{split}$$
(5)

where E is station elevation (m), P is the population of a county which contains AQMS in at the end of 2015, A is the area of a county (km²), PD is the population density, V is the daily average of sum of vehicles in state ways and highways, α is intercept and β_1 - β_{20} are regression coefficients.

1

Table 5

Average $PM_{2.5}$ concentrations ($\mu g/m^3$) for stations in Marmara Region.

AQMS	2012–2013 H. S. ^a	2013 N. S.	2013–2014 H. S.	2014 N. S.	2014–2015 H. S.	2015 N. S.	2015–2016 H. S. ^b
Bursa Uludağ Uni MTHM	27	22	35	21	31	27	33
Çanakkale Lapseki MTHM	18	18	21	18	20	15	17
Edirne Karaağaç MTHM	17	16	29	18	24	17	34
Edirne Keşan MTHM	53	26	77	30	81	28	104
İstanbul Kağıthane MTHM	34	25	45	22	38	20	41
İstanbul Silivri MTHM	22	17	28	14	24	15	24
İstanbul Ümraniye MTHM	37	26	39	23	34	19	31
Kocaeli Gölcük MTHM	27	17	35	16	27	14	25
Kocaeli Kandıra MTHM	15	12	22	12	18	10	22
Sakarya Ozanlar MTHM	36	23	62	23	46	21	51
Tekirdağ Çerkezköy MTHM	30	21	34	19	31	15	33
Yalova Altınova MTHM	29	20	31	22	26	19	25
Yalova Armutlu MTHM	21	19	23	19	21	18	18

^a Starts on 1 March 2013.

^b Ends on 31 December 2015.

2.4. Model validation

The performances of regression models were determined by statistical measures like the Pearson correlation coefficient (R) (Equation (6)) and root mean squared error (RMSE) (Equation (7)) (Sathe et al., 2019).

$$R = \frac{\sum (C_p - \bar{C}_p)(C_o - \bar{C}_o)}{\sqrt{\sum (C_p - \bar{C}_p)^2 \sum (C_o - \bar{C}_{p_0})^2}}$$
(6)

$$RMSE = \sqrt{\frac{2}{n} \frac{C_{P} - C_{0}}{n}}$$
(7)

where, Cp and Co are the predicted and observed $PM_{2.5}$ concentrations respectively and n is the number of observations.

3. Results and discussion

3.1. Analysis of PM_{2.5} measurements

Tables 4 and 5 list the heating season (H. S.) and non-heating season (N. S.) averages of PM2.5 concentrations measured in Ankara and Marmara Region respectively. Valid and missing data rates of PM_{2.5} measurements were provided in Supplement 1. Since PM related air pollution problem is more important in winter season in Turkey, only the heating season $PM_{2.5}$ concentrations are included in regression analysis. The heating season starts on 15th October and ends on 14th May (212 days/year). Most of the stations in Ankara exceeded the European Union (EU) $PM_{2.5}$ standard value (25 µg/m³). This was expected due to the location and atmospheric conditions of Ankara. Ankara is located in the valley, and in winter season inversion event occurs frequently. None of the stations in Ankara met the threshold value in 2010-2011 heating season. As seen from Table 4, there was a slight decrease in fine particulate matter concentrations over years. 4 stations met the EU standard at the end of 2015 in Ankara. In Marmara Region, Çanakkale Lapseki, Kocaeli Kandıra and Yalova Armutlu stations have met the EU standard for PM2.5 pollutant for 2013-2015 period. Among all stations, higher concentrations were recorded at Edirne Keşan and Sakarya Ozanlar stations. Edirne Keşan was the most problematic place with poor air quality due to domestic heating especially in winter season. Main reasons of air pollution in Keşan are topographical structure of city and poor quality of fuels (Özşahin et al., 2016). It is clear from Tables 4 and 5 that particulate matter pollution generally occurs and poses a threat for public health in the heating season.

3.2. MODIS AOD retrieval data availability

Ground measured $\text{PM}_{2.5}$ data were correlated with 4 different

MODIS derived aerosol products: Aqua 3 and 10 km resolution AOD, Terra 3 and 10 km resolution AOD. To analyze 6 years MODIS AOD data in the study area, a total of 8288 (4144 \times 2) MODIS image files were download from Goddard Space Flight Center website for Aqua 3 and 10 km aerosol data products. 7806 (3903 \times 2) MODIS images were downloaded for Terra 3 and 10 km aerosol data products. More than 95 GB of data were analyzed. The number of valid and missing retrievals, and missing data rates for each station grid cell and each aerosol product were shown in Supplement 2. It is seen from Supplement 2 that on the average Terra 3-km aerosol product has lower missing data rates (in other words more retrievals) in Ankara. For most of the Ankara station pixels, AOD retrievals from Terra satellite have more valid data than Aqua satellite. It may result from cloud formation in the afternoon. Such difference was not found for stations in Marmara Region. The retrieval rates of Terra and Aqua 10-km aerosol products were better than that of 3-km aerosol products in Marmara Region. Much lower retrieval rates were found in urban areas like İstanbul Kağıthane, İstanbul Ümraniye and Kocaeli Gölcük. There were more successful retrievals for rural areas such as Bursa Uludağ University. Çanakkale Lapseki, Edirne Karaağaç, Edirne Keşan, Kocaeli Kandıra and Sakarya Ozanlar. The explanation is that the Dark Target algorithm performs better in vegetative areas (generally rural areas). Its performance is worse in bright surfaces like deserts, urban areas and shorelines as compared to the Deep Blue algorithm (Martin, 2008; Sorekhamer et al., 2015). In this study, as seen from Supplement 2 that 10 km aerosol products had more data points than 3 km aerosol products for Terra and Aqua. The highest retrieval rate was observed at Edirne Karaağaç with 28% AOD retrievals for Terra 10-km aerosol product while the lowest retrieval rate was seen at Kocaeli Gölcük with 1% for both Aqua and Terra 3-km resolutions.

Successfully retrieving AOD data is not easy. As stated in the literature (Gupta and Christopher, 2008; Remer et al., 2013), the pixel must be cloud, ice and snow free. Favorable surface conditions (low reflectance) are required for AOD retrieval. Moreover, some meteorological conditions increase the chance of successful retrievals such as deep boundary layers, low RH, low wind speed, and high air temperature (Liu et al., 2009). Gupta and Christopher (2008) found the availability of MODIS AOD of 47% for their 7 years study in Southeastern United States. On the other hand, Emili et al. (2010) found this value to be 17% in the European Alpine region in 2008 (at least one observation either from Terra or Aqua).

3.3. Back trajectory modeling results

Cluster analysis was applied to the backward trajectory results to determine the cases of long range transport of particulate pollution. Fig. 2 shows an example result of clusters coming to one of the AQMS



Fig. 2. Cluster analysis of HYSPLIT model for the period of 2013 and 2015 heating seasons at Bursa Uludağ University MTHM station.

(Bursa Uludağ University MHTM) station between 2013 and 2015 (only in heating seasons). Cluster 1 is originated from south east of United Kingdom. That region is classified as a high $PM_{2.5}$ emitting region according to the EMEP map. Cluster 4 carries Saharan dust to the location of interest. $M_{2.5}$ measurements that fall into the long range transport days were removed from our dataset. Removing long-range transport effected data provided generally better correlations but reduced the number of observations. As an example, the number of observations and R values of Equation (4) before and after back-trajectory analysis are provided in Supplement 3. As a result of back-trajectory analysis for Eq. (4), R values increased in 37 cases, decreased in 23 cases and remained the same in 8 cases.

3.4. AOD - PM_{2.5} regression analysis results

First of all, the regression equations for each AQMS station were developed separately. It should be noted that dealing with only heating season data (or eliminating the summer season data) reduced the size of our dataset (n). Since most of the successful satellite retrievals were on the summer season when the sky was clear and no snow covered on ground. Moreover, removing long range particulate transport in free troposphere again reduced the size of dataset. Lastly, some of the AOD retrievals were not used due to lack of ground based $PM_{2.5}$ measurement on that day. Therefore, at some sites there weren't enough AOD and $PM_{2.5}$ data pairs (n < 25) to develop a regression model. The largest data size was 100 data points at Ankara Sincan station for Terra 3 km resolution. Since AOD data show spatial differentiation, regression models were developed for each site and for each MODIS aerosol products.

Firstly, the simple linear regression model was tried (Equation (1)). There wasn't any strong correlation between $PM_{2.5}$ and AOD data at any of the stations. Correlations at all the sites were weak except the İstanbul Silivri MTHM Station that showed a moderate correlation. At the İstanbul Silivri MTHM Station, the highest value of correlation

coefficient (R) was 0.605 (n = 67) for Aqua 10 km resolution aerosol product. Table 6 summarizes this linear model and the best regression models obtained by using Equations (2)–(4). The linear model was able to explain 36% of the data variance ($R^2 = 0.36$). It has a slope of 79.9 and an intercept of 8.13 (p < 0.001, RMSE = $10.677 \,\mu g/m^3$). Guo et al. (2009) found slopes of their regression equations as $37 \,\mu g/m^3$ of $PM_{2.5}$ and 57 µg/m³ of $PM_{2.5}$ when AOD is corrected for RH. They also summarized the regression slopes of several studies and stated that this value changes from 19 to $125 \,\mu\text{g/m}^3$ of PM_{2.5} in literature. Xin et al. (2014)found an empirical relationship of $PM_{2.5} = 100.10 \cdot AOD + 12.13$ (R² = 0.57) for daily measurements of PM_{2.5} over Northern China. They also stated that the slopes and intercepts of linear regression equations change significantly for different seasons. Xie et al. (2015) reported that their linear model has R² value of 0.47. You et al. (2016) found the linear model with R = 0.28 $(R^2 = 0.08)$ between MODIS AOD and PM_{2.5}. Another study tried to use simple linear regression model between PM₁₀ and MODIS AOD and reported the R as 0.49 ($R^2 = 0.24$) (Li et al., 2011). The correlation between MODIS derived AOD and ground measured PM_{2.5} is generally weak to moderate. However, finding a strong correlation is possible with the help of improved retrieval algorithms. Wang et al., 2013a,b found $R^2 = 0.75$ for their linear model between AOD and PM_{2.5}. It can be concluded that simple linear regression was unsuccessful to explain the relation between particulate matter and AOD only. In literature, researchers generally use simple linear models to demonstrate their non-linear or mixed models perform better than linear models (Li et al., 2011; You et al., 2016).

In order to achieve better correlations, meteorological parameters were included in the regression models. In Equation (2), planetary boundary layer height and wind speed parameters were added to the model together with AOD. This time regression model gave somewhat improved results. There were 2 strong correlation sites, one of them was at Ankara Demetevler Station with R = 0.850 (n = 25) for Terra 10 km product. This model described 70% of ground level PM_{2.5} variance.

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Summaries of best regression models obtained for single monitoring site.

Model	Station	MODIS AOD Product	Model Summary
1	İstanbul Silivri MTHM	MYD04_L2	n = 67, R = 0.605, R ² = 0.36, RMSE = 10.677 μ g/m ³ (p < 0.001)
2	Ankara Demetevler	MOD04_L2	Coefficients: constant = 8.128 (p < 0.001), AOD = 79.905 (p = 0.002) n = 66, R = 0.850, Adj. R ² = 0.70, RMSE = $23.518 \mu g/m^3$ (p < 0.001) Coefficients: constant = 33.572 (p < 0.001), AOD/HPBL = 67657.330 (p < 0.001), AOD/WS = -167.484
3	Edirne Keşan MTHM	MOD04_L2	(p < 0.001) n = 60, R = 0.751, Adj. R ² = 0.54, RMSE = 0.481 µg/m ³ (p < 0.001) Coefficients: constant = 9.310 (p < 0.001), RH = 0.008 (p = 0.079), ln (HPBL) = -0.810 (p < 0.001), ln
4	Edirne Keşan MTHM	MYD04_3K	$\begin{aligned} &(AOD) = 0.122 \ (p = 0.163) \\ &n = 37, R = 0.790, Adj, R^2 = 0.62, RMSE = 0.336 \ \mu g/m^3 \ (p < 0.001) \\ &Coefficients: constant = 96.295 \ (p = 0.003), ln \ (HPBL) = -0.519 \ (p = 0.003), ln \ (RH) = -0.363 \ (p = 0.284), \\ &ln(T) = -15.359 \ (p = 0.002), ln \ (WS) = -0.120 \ (p = 0.245), ln \ (AOD) = 0.144 \ (p = 0.030) \\ &n = 37, R = 0.781, Adj, R^2 = 0.61, RMSE = 0.337 \ \mu g/m^3 \ (p < 0.001) \\ &Coefficients: constant = 82 \ 769 \ (n = 0.001) \ ln \ (HPBL) = -0.415 \ (n = 0.003), ln(T) = -13 \ 350 \ (n = 0.003), ln(T) \\ &= -10.003 \ ln(T) $
			$(WS) = -0.173 (p = 0.060), \ln (AOD) = 0.133 (p = 0.041)$

Although the correlation coefficients were significant, the root mean square error (RMSE) value of this equation was calculated as $23.5 \,\mu g/m^3$, much higher than that of using Equation (1). Another strong correlation was found at Ankara Keçiören Station for Aqua 10 km product (R = 0.851, n = 26). 9 moderate correlations were also found (3 for Terra 10 km, 2 for terra 3 km, 2 for Aqua 10 km and 2 for Aqua 3 km).

Having tried linear models, it is focused on developing non-linear models. Emili et al. (2010) suggested a non-linear relation between AOD and PM. Planetary boundary layer height, relative humidity and AOD were included as separate variables in the model. Equation (3) provided better results. Using the regression equation in non-linear form sharply reduced the RMSE of the model. In total, it was found 4 strong correlation sites. For Terra 10 km resolution R values were 0.751 (n = 60) and 0.735 (n = 47) at the stations located in Edirne Keşan and İstanbul Ümraniye, respectively. The regression equation obtained at Edirne Keşan is given in Table 6. Model was able to describe 54% of ground level PM2.5 variance. Using the non-linear model reduced the RMSE value to less than 1. The coefficients for AOD and RH have positive signs which mean they have a positive association with PM2.5 concentration. HPBL showed a negative association with PM2.5 concentration since it has a negative sign. When the height of planetary boundary layer increases, particulate matter becomes more diluted because of large vertical mixing, therefore ground-level concentration reduces (Liu et al., 2007; You et al., 2016). The results of this study are similar to the literature. Positive AOD and negative HPBL terms were found in another study (Emili et al., 2010). The regression model was statistically significant (p < 0.001); on the other hand, this was not true for coefficients (Table 6). Moreover, R = 0.727 (n = 38) was obtained by using Terra 3 km aerosol product at the İstanbul Ümraniye station; we found R = 0.702 (n = 38) at the Yalova Armutlu station.

In model 4, AOD, planetary boundary layer height, relative humidity, surface temperature and surface wind speed were included in regression equation. A non-linear model with the aid of more meteorological dependent variables gave much better correlations. There were total 17 strong correlations between PM2.5 and AOD. 7 strong correlations were obtained for Terra 10 km resolution at the following AQMS stations: Ankara Demetevler, Ankara Sincan, Bursa Uludağ Uni MTHM, Edirne Keşan MTHM, İstanbul Silivri MTHM, İstanbul Ümraniye MTHM, Kocaeli Gölcük MTHM. There were 4 strong correlations for Aqua 10 km resolution at Ankara Kayaş, Ankara Keçiören, Bursa Uludağ Uni MTHM and Edirne Keşan MTHM stations. 3 strong correlations were observed for 3 km resolution Terra products (Ankara Sihhiye, Edirne Keşan MTHM and İstanbul Ümraniye MTHM stations) and 2 strong correlations for 3 km resolution Aqua products (Edirne Keşan MTHM and Yalova Armutlu MTHM). According to our results, it can be concluded that 10 km resolution aerosol product worked better than 3 km resolution aerosol products. Similarly, AOD data obtained from Terra satellite worked better than that of Aqua satellite. At Edirne Keşan, it was found that for all 4 aerosol products, there were strong correlations: R = 0.834 (n = 60, Terra 10 km), R = 0.823 (n = 23, Terra 3 km), R = 0.744 (n = 50, Aqua 10 km) and R = 0.790 (n = 37, Aqua 3 km). In other words, both satellites at two different resolutions were successful in predicting particulate matter concentration in Edirne Kesan, which has serious air quality problems in recent years. In Table 6, the best regression equation obtained for Model 4 is given for Aqua 3 km product at Edirne Keşan. The model was statistically significant, but p values of some of coefficients were not below 0.05. Therefore, the backward method was applied to solve the regression equation, which eliminated one or more variables until it found the significant regression model. Most of the time, the RH term was dropped out from the model since it failed from t-test as discussed by Emili et al. (2010). On the other hand, Kumar et al. (2007) reported that RH showed strong association with PM2.5 in Delhi Metropolitan area. After that, the new model including AOD, HPBL, T and WS predictors is given in Table 6. This new model can explain 61% of ground level PM2.5 variance. The AOD term had positive sign, which represent

positive association with $PM_{2.5}$ concentration. On the other hand, all meteorological parameters showed negative association with $PM_{2.5}$ concentration. When the temperature decreases, people use more fuels for heating, and therefore more PM is emitted to the atmosphere. Low $PM_{2.5}$ is measured at higher temperatures due to less need of fuels for domestic heating. In windy conditions, higher wind speeds create more dilution of particulates; therefore, $PM_{2.5}$ concentration decreases (Hu et al., 2014; Liu et al., 2007; You et al., 2016).

In multivariate models, more strong correlations were found using AOD products from Terra satellite as compared to Aqua satellite. Terra measurements are in the morning at 10:30 local time whereas Aqua is an afternoon satellite. During the day, the mixing height tends to be lower in the morning and becomes higher in the afternoon. Consequently, ground based PM2.5 levels were higher in the morning and lower in the afternoon. A recent study in China revealed that half of the maximum PM2.5 cases occured in the morning, whereas only 5% maximum occurred in the afternoon (Guo et al., 2017). Therefore, Terra MODIS AOD correlated with ground based PM2.5 measurements better than Aqua MODIS AOD since the emission contributed AOD fraction was higher in the morning. Moreover, in this study, 10 km MODIS AOD products gave better correlations as compared to 3 km MODIS AOD products. The difference between these products is well discussed by Remer et al. (2013). They stated that 3 km and 10 km products are exactly same apart from the choice of reflectance pixels. Therefore, 3 km products may have a high-bias noise over bright and urban areas. Remer et al. (2013) also concluded that 3 km resolution MODIS AOD product is less accurate and less robust than 10 km resolution MODIS AOD products. Similarly, He et al. (2017) compared both MODIS 3 km and 10 km aerosol optical depths with ground based AERONET measurements over China. They stated that 3 km resolution product performed worse than 10 km product especially in bright surfaces like Beijing. In our study, strong correlations were found for 3 km Aqua at Yalova Armutlu, which is a rural place without strong surface reflectance. On the other hand, better correlations were found by using 10 km products at stations located in highly urbanized cities like Ankara, İstanbul, Bursa and Edirne for Equations (3) and (4).

Up to now, only site specific correlations were on the focus. On the other hand, the ultimate goal of remote sensing studies in air pollution is to generate air pollution distribution maps. Therefore, ground based PM_{2.5} measurements of all sites were analyzed using regression models by using MODIS derived AOD and other meteorological parameters. In contrast to the results presented previously, all of the regression equations gave weak correlations. This makes it very difficult to create a PM_{2.5} distribution map. The reason of weak correlations can be explained by complex meteorological structure of the Marmara region. As indicated earlier in this paper, 3 different types of climate patterns are observed in this region. A recent study showed that Turkey has 16 subprecipitation regime regions and 15 sub-climate regime regions (Sahin and Kerem Cigizoglu, 2012). There are 3 sub-climate and 3 sub-precipitation patterns in the Marmara region. Therefore, separation of the study area into several sub regions is necessary. Kahya et al. (2017) performed hierarchical cluster analysis of PM_{2.5} measuring stations in the Marmara region. They found 5 clusters for PM_{2.5} monitoring stations. İstanbul Ümraniye, İstanbul Kağıthane and Tekirdağ Cerkezköy form first cluster. Bursa, Kocaeli Gölcük and Yalova Altınova are fall into second cluster. Yalova Armutlu, Çanakkale Lapseki, Edirne Karaağaç, İstanbul Silivri and Kocaeli Kandıra belong to third cluster. Lastly, Edirne Keşan and Sakarya Ozanlar fall into two different clusters alone. So these clusters were used in regression analysis to find better correlation between MODIS derived AOD and ground based measured PM_{2.5}. Since clusters 4 and 5 contain only one station, no analysis were performed for them. Equation (4) was the most successful model among the four regression models. Therefore, only Equation (4) was used in regression analysis. For the first cluster sites, 4 different MODIS AOD products gave moderate correlations ranging from R = 0.507 to R = 0.641. Air quality monitoring stations (İstanbul Ümraniye, İstanbul

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The best regression equations obtained for cluster 2 cities.

Model	MODIS AOD Product	Model Summary
4	MYD04_3K	n = 30, R = 0.725, Adj. $R^2 = 0.426$, RMSE = 0.414 µg/m ³ (p = 0.002) Coefficients: constant = -51.183 (p = 0.205), ln (HPBL) = -0.598 (p = 0.004), ln (RH) = -0.007 (p = 0.986), ln(T) = 10.422 (p = 0.141), ln (WS) = -0.219 (p = 0.058), ln (AOD) = 0.197 (p = 0.107) n = 30, R = 0.725, Adj. $R^2 = 0.449$, RMSE = 0.406 µg/m ³ (p < 0.001)
4	MOD04_L2	Coefficients: constant = -51.545 (p = 0.127), in (HPBL) = -0.598 (p = 0.003), in(1) = 10.481 (p = 0.084), in (wS) = -0.219 (p = 0.050), in (AOD) = 0.197 (p = 0.087) n = 74, R = 0.706, Adj. R ² = 0.461, RMSE = 0.515 µg/m ³ (p < 0.001) Coefficients: constant = -12.794 (p = 0.677), in (HPBL) = -0.463 (p < 0.001), in (RH) = -0.624 (p = 0.057), in(T) = 3.963 (p = 0.457), in (WS) = -0.363 (p = 0.005), in (AOD) = 0.229 (p = 0.015) n = 74, R = 0.703, Adj. R ² = 0.465, RMSE = $0.513 µg/m3$ (p < 0.001) Coefficients: constant = 10.069 (p < 0.001), in (HPBL) = -0.421 (p < 0.001), in (RH) = -0.794 (p < 0.001), in (WS) = -0.371 (p = 0.004), in (AOD) = 0.228 (p = 0.010)

Kağıthane and Tekirdağ Çerkezköy) of cluster 1 are located in the same sub climate and sub precipitation zones. As a result, similar correlations were obtained for 4 different aerosol products in this cluster. For the second cluster, two strong correlations were found for Aqua 3 km and Terra 10 km aerosol products, R = 0.725 and R = 0.706 respectively. A moderate correlation (R = 0.585) was obtained for Aqua 10 km; whereas, the correlation was a weak for Terra 3 km resolution data. Although the locations of monitoring sites in cluster 2 are closer, they fall into two different sub climate and two different sub precipitation zones. The complexity of meteorological conditions resulted in a wider range of correlations. Finally, all correlations were weak for cluster 3 except a moderate correlation (R = 0.509) for Terra 10 km aerosol product. Monitoring stations in cluster 3 were geographically far from each other as compared to the other clusters. That is the main reason that the regression model gave weak correlation results. Table 7 shows the best regression models obtained by using Equation (4) for cluster 2 sites.

AOD, HPBL and other meteorological variables did not provide sufficient correlations for creating a PM_{2.5} distribution map. Therefore, some spatial parameters like AQMS elevation, population and area of a county, population density and number of vehicles were added to the spatiotemporal model (Equation (5)) to create a distribution map. All of the AOD data (obtained from both Aqua and Terra satellites with both 3-km and 10-km resolutions) for all stations in Marmara Region were included in the model. Therefore, the size of dataset (n) was 1634. The descriptive statistics of PM2.5, AOD, HPBL, RH, TEMP and WIND were listed in Table 8. Other spatial parameters were previously listed in Table 3. Table 9 showed the model summary after backward method solution of Eq. (5). A moderate correlation was obtained with R = 0.593. This model could explain nearly 35% of variance in $PM_{2.5}$ concentrations (RMSE = $0.576 \,\mu g/m^3$, p < 0.001). Only the p value of AOD terms was not below 0.05, but the backward method did not drop this term from the solution. Fig. 3 shows the scatter plots between measured and spatiotemporally predicted ln (PM2 5) concentrations. Inverse Distance Weighted (IDW) interpolation method was used for distribution maps. As a result, PM_{2.5} distribution maps were created

Table 8

Descriptive statistics of PM2.5, AOD, HPBL, RH, TEMP and WIND for the spatiotemporal model (n = 1634).

	ΡΜ _{2.5} (µg/m ³)	AOD	HPBL (m)	RH (%)	TEMP (K)	WIND (m/s)
Mean	31.3	0.174	914.9	56.81	289.2	3.537
Median	25.0	0.141	796.5	56.50	289.0	3.127
Std. Deviation	26.9	0.125	574.7	13.79	5.3	2.129
Minimum	1.0	0.001	23.0	21.80	271.5	0.028
Maximum	340.0	1.010	3226.0	100.00	305.3	13.060
25th percentile	15.0	0.086	445.8	46.58	285.2	1.958
50th percentile	25.0	0.141	796.5	56.50	289.0	3.127
75th percentile	39.0	0.230	1285.0	66.30	292.4	4.647

Table 9

Spatiotemporal model summary for Marmara Region (n = 1634, R = 0.593, Adj. $R^2 = 0.346$, RMSE = 0.576 µg/m³ (p < 0.001)).

Model predictors	Coefficient	p value
Model predictors constant AOD In (AOD) HPBL WS E In(E) P A PD	Coefficient - 1.750 - 0.373 0.194 - 4.056e-4 - 0.055 - 0.006 0.544 9.787e-7 - 1.548e-4 2.454e-5	$\begin{array}{c} p \text{ value} \\ p < 0.001 \\ p = 0.093 \\ p < 0.001 \\ p < 0.001 \\ p < 0.001 \\ p < 0.001 \\ p < 0.001 \\ p < 0.001 \\ p < 0.001 \\ p = 0.046 \\ p < 0.001 \end{array}$
ln (PD) V ln(V)	- 0.158 - 1.190e-5 0.567	p < 0.001 p < 0.001 p < 0.001 p < 0.001



Fig. 3. Scatter plot of measured and spatiotemporally predicted ln (PM_{2.5}) concentrations.

successfully. Average PM_{2.5} distribution maps in heating seasons (a: 2012-2013, b: 2013-2014, c: 2014-2015 and d: 2015-2016) were given in Fig. 4. Maps showed similar distribution patterns over the years. According to the Fig. 4, PM_{2.5} pollution levels were above EU threshold in Edirne Keşan, Sakarya Ozanlar, Yalova Altınova and central parts of İstanbul Province.



Fig. 4. Average PM_{2.5} distribution maps in heating seasons a: 2012–2013, b: 2013–2014, c: 2014–2015 and d: 2015–2016.

4. Conclusions

In Turkey, there were some studies related with PM2.5 pollutant. However, they were site specific. Only one study used remote sensing data with a linear correlation analysis. To our knowledge, this is the first comprehensive study which used MODIS derived AOD data to explain the ground measured concentrations of PM_{2.5} over Turkey. This study was performed for the period of 2011-2015 at the Ankara stations and the period of 2013-2015 at Marmara stations. In this study, the retrieval availability of MODIS 10 km resolution aerosol product was better than 3 km aerosol products. After eliminating long range PM transport cases, four regression models were developed to predict ground level concentrations of PM2.5 for the heating season. All regression equations were evaluated separately for four different types of aerosol products and at all sites. The correlation coefficients of the simple linear regression model between $PM_{2.5}$ and AOD were weak at all stations except one moderate correlation site. In order to obtain better results, HPBL and some meteorological parameters were added into the models, and nonlinear models were developed. Inclusion of meteorological parameters except relative humidity improved the model performance significantly. Non-linear models had much lower RMSE values as compared to that of linear models. In our study, the MODIS derived AOD data from Terra satellite worked better than that of Aqua satellite since the emission contributed AOD fraction was higher in the morning. Moreover, 10 km resolution products (MOD04_L2 and MYD04_L2) gave better correlations than 3 km resolution products (MOD04_3K and MYD04_3K). All aerosol products were successful at the Edirne Kesan station, which suffers from serious particulate pollution. Observing air quality via remote sensing is especially important in countries like Turkey which has a limited number of air quality monitoring stations. With the aid of spatiotemporal model that used remotely sensed AOD data, PM2.5 distribution maps were created for the first time for Turkey. Therefore, it can be concluded that MODIS AOD data can be used as a useful tool to infer PM_{2.5} concentrations when coupled with meteorological and spatial information.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apr.2019.05.005.

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