Product User Manual

Surface PM2.5 concentrations from MODIS/SLSTR

Signatures

Action: Name	***Affiliation***	***Function***	***Date***	***Sign.***
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Document Change Log

Issue	***Rev.***	***Date***	***Section***	***Description of Change***
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SENTINEL-BASIERTE ATMOSPHÄRENPRODUKTE ZUR BEWERTUNG DES EINFLUSSES VON VERKEHRSEMISSIONEN AUF DIE LUFTQUALITÄT IN DEUTSCHLAND (S-VELD)

Problemstellung

Luftqualität spielt eine wichtige Rolle in der aktuellen Umweltdiskussion. Millionen Menschen leben heute in Regionen mit stark verschmutzter Luft. Hohe Schadstoffbelastungen sind für Atemwegs- und Herz-Kreislauf-Erkrankungen verantwortlich und führen zu erhöhten Sterblichkeitsraten. Zum Schutz der menschlichen Gesundheit gelten deshalb europaweit unter anderem Grenzwerte für Stickstoffdioxid (NO_2) und Feinstaub. Überschreitungen der Grenzwerte beider Komponenten finden sich derzeit vor allem an durch Verkehr hoch belasteten Standorten.

Projektziel

Das Projekt S-VELD hat zum Ziel, auf Grundlage neuester Sentinel-Satellitenmessungen von NO_2 und Feinstaub sowie Verkehrsdaten des BMVI, die verkehrsbedingten Schadstoffemissionen und deren Anteil an der Umweltbelastung in Deutschland besser zu quantifizieren.
Mit der Bereitstellung hochaufgelöster Karten zur Schadstoffbelastung und verbesserten Emissions-Daten soll das Potential der Copernicus Sentinel-Flotte für das Umwelt-Monitoring als Entscheidungshilfe für Behörden demonstriert und als wichtige zukünftige Datenquelle etabliert werden.

Durchführung

Aus Messungen der Sentinel-Satelliten werden bodennahe NO_2- und Feinstaubkonzentrationen für das Bundesgebiet und die angrenzenden Länder bestimmt und über einen Web Mapping-Datendienst zeitnah für die Endnutzer bereitgestellt. Diese Fernerkundungsdaten werden mit Emissions- und Ausbreitungs-Modellen kombiniert. Anhand räumlich und zeitlich detaillierter Daten zur Verkehrsbelastung der BASt unter Verwendung technologieabhängiger Emissionsfaktoren können dann wichtige Erkenntnisse über Emissionen des Kfz-Verkehrs gewonnen werden.

Verbundkoordinator

Deutsches Zentrum für Luft- und Raumfahrt e.V., Oberpfaffenhofen

Projektpartner

- Freie Universität Berlin, Institut für Meteorologie, Berlin
- IVU Umwelt GmbH, Freiburg
- TNO, Climate Air and Sustainability Unit, Utrecht, die Niederlande

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1 INTRODUCTION

1.1 Purpose and scope

The purpose of this document is to present the user manual of the surface PM2.5 concentration products derived from MODIS and SLSTR satellite AOD data sets. These products contain monthly mean surface PM2.5 concentrations for Germany and surrounding areas for the period from January 2018 to December 2019.

1.2 Product description

1.2.1 Surface PM2.5 concentrations (monthly)

The generation of the PM2.5 products is based on a semi-empirical method, taking in to account meteorological parameters and optical aerosol properties to derive ground-level PM2.5 concentrations from satellite-based column measurements of aerosol optical depth (AOD). The PM2.5 values were validated with in-situ station measurements of PM2.5 by performing a linear regression procedure (see 3.2). The product presented here is a combination of validated MODIS and SLSTR based PM2.5 concentrations. The data is available over a time period from January 2018 to December 2019.

The surface PM2.5 concentration products are organized into user-friendly and self-describing NetCDF-4 (Network Common Data Form) files.

For monthly data, the logical file name convention is:
MODIS_SLSTR_PM25_CONC_MONTH_YYYYMM.nc
The meaning of the different subset of character string is given below:

- YYYY (4 digits) is the year of the processed products
- MM (2 digits, 01-12) is the month of the year of the processed products

The attributes for the monthly files are listed in the following table:

Table 1-1: List of attributes of monthly data with typical values and a short description.

Global Attributes	typical values	Description
process_time	YYYY-MM-DD HH:mm:ss	date and time when this file was created
Conventions	CF-1.7	Climate and Forecast convention for variable names, units and dates
license	CC-BY-NC 4.0	official licence for data usage
Composite_type	month	Type of aggregation
institution	DLR Deutsches Zentrum für Luft- und Raumfahrt	institute the creator of the data belongs to

creator_name	Jana Handschuh	Name of the person responsible for the data
creator_email	jana.handschuh@dlr.de	contact address
description	Merged PM2.5 product from MODIS and SLSTR	short description of the file content
baseProduct	Level 3 S-VELD	Basis of this data product
baseProductVersion	v 1.0	version of the underlying data
productAlgorithmVersion	v 1.0	Version of this data product
project	SVELD	Project name
sensor	MODIS, SLSTR	sensor names
platform	Aqua, Sentinel-3a	Satellites
geospatial_lat_min	45.7416	minimum latitude (degree)
geospatial_lat_max	56.3915	maximum latitude (degree)
geospatial_y_resolution	500 m	Resolution in y dimension (m)
geospatial_y_units	meter north	unit in y dimension
geospatial_long_min	0.2396	minimum longitude (degree)
geospatial_long_max	17.9294	maximum longitude (degree)
geospatial_x_resolution	500 m	Resolution in x dimension (m)
geospatial_x_units	meter east	unit in x dimension
grid_mapping_name	transverse_mercator	Name of the gridtype
_CoordinateTransformType	Projection	
_CoordinateAxisType	GeoX GeoY	

Each monthly surface PM2.5 concentration product is produced on a long/lat grid at a spatial resolution 0.01° and regridded to a regular 0.5km×0.5km X/Y grid (UTM projection) using bilinear interpolation. The grid attributes of the projection are given in Table 1-2, the dimensions of the X/Y grid are given in Table 1-3.

Table 1-2: List of grid attributes of monthly data with typical values and a short description.

Grid attributes	typicale values	Description
grid_mapping_name	transverse_mercator	name of the gridtype
semi_major_axis	6378137.0	semi major axis of spheroid (semi distance from earth center to equator)
semi_minor_axis	6356752.0	semi minor axis of spheroid (semi distance from earth center to pole)
inverse_flattening	298.257	flattening of spheroid
latitude_of_projection_origin	0.0	origin of y coordinate
longitude_of_central_median	9.0	longitude of the central meridian on grid, origin of x coordinate
scale_factor_at_central_median	0.9996	scale factor applied for central meridian

Grid attributes	typicale values	Description
false_easting	500000.0	misalignment of eastern coordinates
false_northing	0.0	misalignment of northern coordinates
spatial_ref	PROJCS["ETRS89 / UTM zone 32N",GEOGCS["ETRS89",DATUM["European_Terrestrial_Reference_System_1989",SPHEROID["GRS 1980",…]…]…]…]	description of coordinate reference system

Table 1-3: Overview of the dimension in the data file.

Dimension name	Unit	Size	Description
Y	meter north	2320	500 m resolution in y direction
X	meter east	2200	500 m resolution in x direction
Time	months since YYYY-MM-01 00:00:00	1 (unlimited)	start and end date of monthly product

2 INSTRUMENTS AND AOD RETRIEVALS

The surface PM2.5 concentration data it based on satellite AOD data from two different satellites and sensors. The instruments and AOD retrieval methods are briefly described below. For more detailed information please consider the given references.

2.1 MODIS (Aqua)

The Moderate Resolution Imaging Spectroradiometer (MODIS) has been in operation onboard the NASA satellite Aqua since 2002, providing retrieval products of the AOD and other aerosol and cloud parameters. With a swath width of 2330km in nadir it samples the full earth surface in 1-2 days, overpassing Germany and central Europe at 13:30 local solar time. MODIS measures Top-of-Atmosphere (TOA) reflectances in 36 spectral bands covering wavelengths from the ultraviolet to the infrared (0.42-15µm) with a spatial resolution of 250m to 1km, depending on band.

The used AOD product is part of the Collection 6.1 - MYD04_3K data set, containing AOD data at 550nm wavelength in a spatial resolution of 3km, derived with the “Dark Target” Algorithm over land and ocean. The data set was downloaded from the LAADS DAAC archive provided by NASA (https://ladsweb.modaps.eosdis.nasa.gov/archive/allData/61/MYD04_3K/). Detailed descriptions of the dataset and the aerosol retrieval algorithm can be found in Levy et al., 2013, Remer et al., 2013 and Munchak et al, 2013.

The Dark Target algorithm for aerosol retrieval is based on the concept, that aerosols tend to be light in the visible wavelength range compared to the underlying dark surface (dark target). The spectral contrast can be used to derive information on physical properties of the aerosols arranged in the atmospheric column. For the 0.55 µm (550nm) AOD retrieval in 3km resolution calibrated and geolocated TOA reflectances of the 0.47 and 0.66 wavelength bands (Level 1b products) are used, which are grouped to boxes with 9x9 500m pixels. The 2.21µm band is used to determine surface brightness and to identify unsuitable pixels for the algorithm. Additionally, cloudy pixels are identified and eliminated using a cloud mask and data on ozone profile and water vapor are considered to correct for atmospheric gas absorption. For the algorithm over land (ocean) another pixel selection process eliminates the darkest 20% (50%) and brightest 50% (50%) of the pixels. The reflectance values of the remaining valid pixels are averaged and used for the final aerosol retrieval. The AOD at

0.55µm is determined using look-up tables (LUTs). These consist of calculations of radiation transport models and represent the atmospheric optical properties under different aerosol conditions. By comparing the measured reflectances with the values of the LUTs, conclusions can be drawn about the state of the atmosphere and representative values of the AOD at 0.55 µm can be determined for each retrieval box.

2.2 SLSTR (Sentinel-3a)

The Sea and Land Surface Radiometers (SLSTR) is operating on board of the Copernicus satellite Sentinel-3a since 2017. SLSTR is a "dual-view" radiometer which measures reflectances in seven spectral bands from 0.55-10.85µm wavelength range in two viewing directions, downwards (nadir) and backwards ("along-track"). With a swath width of 1400 km (740 km) in the nadir (along-track), SLSTR needs around 2-3 days for global coverage overpassing Germany at around 10:30 am local time.

The AOD product used for the project was determined and provided by Swansea University (SU) and has a spatial resolution of 10km. Similar to the MODIS algorithm, the SU algorithm uses measured TOA reflectances to derive AOD at 550nm. The measurements with a resolution of 500m are grouped to "Super-Pixels" and invalid pixels (clouds, snow/ice, etc.) are removed before the retrieval. The pixel selection is performed separately for both viewing directions. However, in order for a pixel to be included in the super pixel, it must be valid for both viewing directions. If more than 50% of the pixels are valid, the super pixel is used for aerosol retrieval. The super pixels represent surface section specific TOA reflectances (averaged over all valid pixels) for the respective viewing direction. The advantage of the two viewing directions is that one does not have to assume a certain surface brightness for the retrieval, as with the MODIS Dark Target algorithm. By taking measurements at two different angles, the ground reflectivity and the AOD can be determined at the same time. Similar to the MODIS retrieval, LUTs for various aerosol models and atmospheric conditions serve as method to determine the final 550nm AOD values. A more detailed description of the SLSTR aerosol retrieval performed by SU can be found in the technical documentation from North & Heckel, 2020.

3. SURFACE PM2.5 CONCENTRATION ESTIMATION

3.1 Input data

3.1.1 Satellite data

For the retrieval of PM2.5 surface concentrations the above described AOD data sets from MODIS and SLSTR were used. Both data sets are provided in orbit wise files. In order to pair up the satellite data with other data sets (meteorology), the AOD data was first gridded onto a regular lon/lat grid with 0.01° spatial resolution. Values of grid boxes which were covered more than once a day, were thereby averaged to daily values. The daily data sets were then corrected for outliers using an Inter Quartile Range (IQR) Method.

3.1.2 Ambient Air Quality Monitoring Station Data

Ambient PM2.5 concentrations data from in-situ measurement stations for Germany and Europe are provided by the European Environment Agency (EEA) and can be downloaded per year and country at https://discomap.eea.europa.eu/map/fme/AirQualityExport.htm. For our purposes we used PM2.5 measurements of the *E2a* data sets (hourly values) for the year 2018 and the region from 46°N to 56°N and 2°E to 16°E. This region comprises in total 350 stations in Germany (175), Poland (3), Czech Republic (32), Austria (24), Switzerland (1), France (54), Belgium (35), Luxembourg (4) and the Netherlands (24). Because of the irregular number of measurements per day and the fact, that not all stations provide measurements between 10:30 and 13:30 (satellite overpasses), we used daily mean values to increase the number of collocations for statistical analysis, thus improving the sampling base for the linear regression procedure described below.

3.1.3 Meteorological Data

Meteorological data for Europe is provided by the European Centre for Medium-Range Weather Forecasts (ECMWF). We used the *Atmospheric Model high resolution 10-day forecast (Set I - HRES)* data set with 0.1° resolution for daily information on Boundary Layer Height (BLH) and Relative Humidity (RH) for the greater Germany region. The downloaded data sets include daily values for a single timestep (12am, matching the mean overpass time of the satellites) interpolated to a grid with 0.01x0.01° latitude-longitude spatial resolution.

3.2 Surface PM2.5 Concentration Retrieval

The method to derive surface concentrations of PM2.5 from AOD data is based on a semi-empirical approach, which describes the physical relationship between aerosol optical and meteorological parameters. The relationship between PM2.5 and AOD can be written as follows (Koelemeijer et al., 2006; Di Nicolantonio et al., 2009):

$$PM_{2.5} = \tau \frac{4\,\rho\,r_{eff}}{3\,H\,f(RH)\,Q_{ext,dry}}$$

Where τ is the satellite-derived AOD, ρ the particle density, r_{eff} the effective radius of aerosol particles, $Q_{ext,\,dry}$ the Mie-extinction efficiency at dry conditions, H the boundary layer height and RH the relative humidity. It is assumed that aerosol particles are mainly concentrated in the planetary boundary layer (PBL) and are therein well mixed with height. That makes the planetary boundary layer height (H) the key parameter to derive ground-level PM2.5 concentrations from columnar AOD. Moreover, it's important to consider relative humidity, as it affects the water uptake process of aerosols and can cause changes in the aerosol size distribution, chemical composition and particle extinction properties. The function $f(RH)Q_{ext,dry}$ takes this so-called hygroscopic growth effect into account by describing the dependency of light extinction on relative humidity. The optical parameters r_{eff} and $Q_{ext,\,dry}$ strongly depend on aerosol optical properties and thus on aerosol type. The target region is assumed to be dominated by only one aerosol type (urban industrial – weakly/non- absorbing), that's why constant values for both of these parameters were used.

To correct the PM2.5 estimates for bias and scaling errors in comparison to in-situ ground measurements, a linear regression approach was applied. Regression parameters (slope and intercept) from linear regression between in-situ and satellite-derived PM2.5 concentrations were used as correction factors and integrated to Equation (1) as follows:

$$PM2.5 = A_{i,j} * PM + B_{i,j}$$

Factor A stands for the slope and factor B for the intercept parameter of linear regression. Due to spatially and temporally varying aerosol conditions the linear regression procedure was performed for each station (i) and month (j). After an outlier correction, the received monthly station wise correction parameters were interpolated to a 0.01°x0.01° grid using an inverse distance weighting approach and solved as correction fields for the recalculation of ground-level PM2.5 concentrations.

Daily corrected surface PM2.5 concentrations were produced this way using the two different AOD data sets from MODIS and SLSTR. These two data sets were than combined by averaging the daily values per grid cell. Based on these combined daily values, the monthly mean surface PM2.5 concentrations were calculated.

3.3 Uncertainties of the PM2.5 estimates

The quality of the monthly surface PM2.5 estimates strongly depend on the number of measurements incorporated in average determination. The more measurements are taken in to account, the better and more representative are the estimates per grid box. Furthermore, the determination of the correction parameters is based on a statistical approach and is highly affected by the sample size. Thus, also the quality of the correction parameters has an important influence on the reliability of the PM2.5 estimates and depends on the number of satellite measurements. Due to weather conditions, most important the cloudiness, the number of measurements can be very limited for some days/periods. Especially for the winter period only few satellite measurements exist, leading to higher uncertainties in the PM2.5 estimates compared to other months. To roughly assess the data quality Table 3-1 gives the total and mean number of measurements for each month in 2018 and 2019 for the combined MODIS/SLSTR PM2.5 product and additionally the coverage of the target region in percent.

Table 3-1: Total number of measurements the mean number of measurements per grid cell and the coverage in % for the surface PM2.5 product per month.

	Number of measurements				Coverage	
month	**mean**		**total**		**%**	
	2018	**2019**	**2018**	**2019**	**2018**	**2019**
January	0.25	0.23	202095	169281	18.41	15.50
Feburary	1.67	5.22	667724	938081	61.14	85.90
March	1.77	3.81	775620	946419	71.02	86.66
April	3.54	9.86	973406	1019950	89.13	93.39
May	3.61	2.62	990564	952629	90.70	87.23
June	6.19	13.49	1052236	1079246	96.35	98.82
July	10.73	8.51	1076238	1079405	98.55	98.84
August	8.59	7.76	1078579	1080526	98.76	98.94
September	6.75	6.03	1080549	1082012	98.94	99.08
October	9.68	3.85	1074761	987738	98.41	90.44
November	1.91	0.27	851655	256569	77.98	23.49
December	0.07	0.17	55865	153494	5.11	14.05

Another point, that should be considered for the interpretation of the presented PM2.5 data, is the overestimation of PM2.5 concentrations in coastal regions. This issue is mainly originated in the difficulty to distinguish between land and ocean from satellite. As mentioned above, the aerosol retrieval is performed separately for land and water surface. Sometimes it's difficult to do an exact differentiation in the tideland of North Sea. That's why it happens that the wrong algorithm is performed for coastal pixels, leading to inexact AOD values. Moreover, the planetary boundary layer height is very low over ocean leading to very high and potentially overestimated PM2.5 concentrations in the coastal area according to the Equation (1). Also, the assumption of a constant aerosol type has to be seen critical for the coastal region, as the proportion of sea salt is much higher in these areas compared to the inland.

4. MONTHLY MEAN SURFACE PM2.5 DOWNLOAD DATA

4.1 Parameters for monthly surface PM2.5 product

The monthly surface PM2.5 concentration combined from MODIS and SLSTR retrievals is given for each grid cell in the netCDF files. The temporal resolution of the product is monthly (calendar). The data grid covers Germany and surrounding countries in UTM coordinates with resolution of 0.5kmx0.5km. A list of variables included in the netCDF files is given in Table 4-1. As an example, the monthly surface PM2.5 concentration (parameter mass_concentration_of_pm2p5_ambient_aerosol_particles_in_air) for June 2018 is shown in Fig. 4.1 as map plot.

Table 4-1: Variable list of monthly surface PM2.5 products.

Variable name	Unit	Size	Description
y	meter north	2320	Y coordinate of the center of the gridded data
x	meter east	2200	X coordinate of the center of the gridded data
time	month since YYYY-MM-01	1 (unlimited)	start and end date of the monthly averaged data
latitude	degree north	2320×2200	Latitude of the center of the gridded data
longitude	degree east	2320×2200	Longitude of the center of the gridded data
mass_concentration_of_pm2p5_ambient_aerosol_particles_in_air	µg m^{-3}	2320×2200	averaged surface PM2.5 concentration

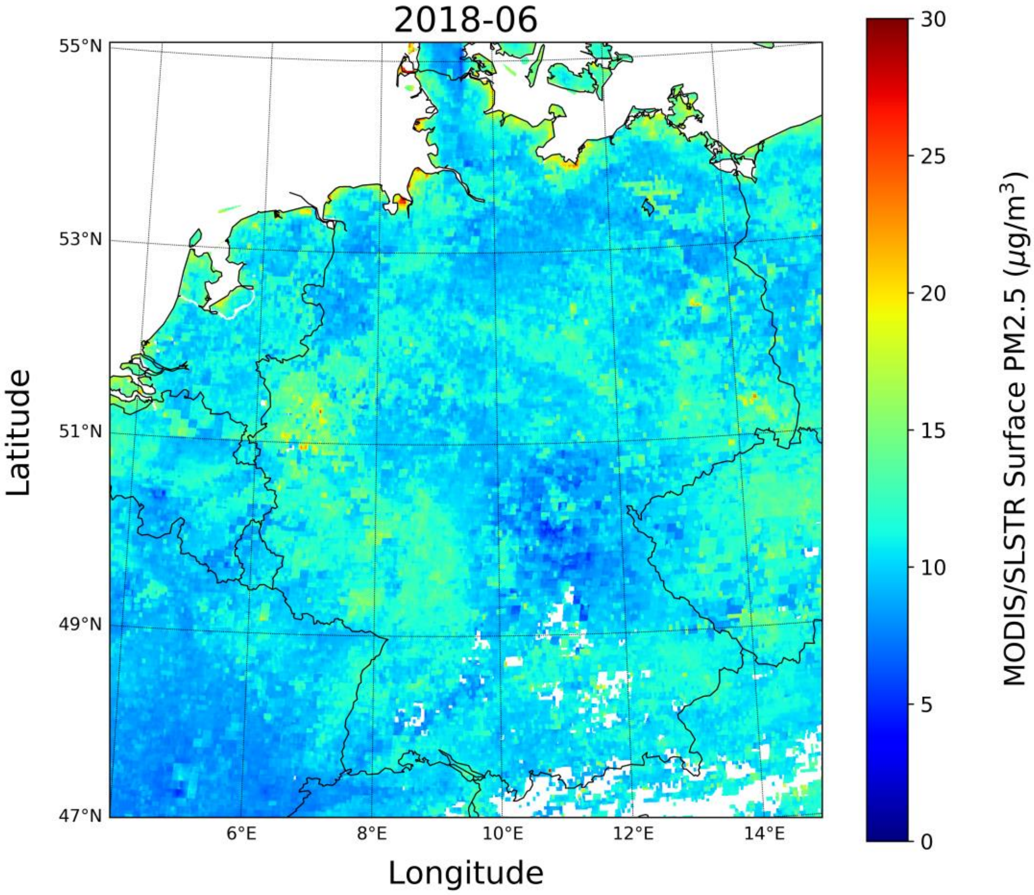

Figure 4.1: Spatial distribution of averaged surface PM2.5 concentration derived from MODIS and SLSTR AOD measurements in June 2018.

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