Chapter 15
Retrieval of Particulate Matter from MERIS Observations

Wolfgang von Hoyningen-Huene, Alexander Kokhanovsky, and John P. Burrows

Abstract Environmental control of pollution uses concentrations of particulate matter (PM) for evaluation of the pollution load. Retrievals of PM from satellite observations are supplementary information to ground-based national observation networks. A method of PM determination using retrievals of spectral aerosol optical thickness is described. The method has been applied to MERIS L1 data over Germany. PM retrievals from satellite observations have been compared with ground-based PM10 measurements of the Federal Environmental Agency, Umweltbundesamt (UBA).

Keywords: MERIS, PM10, BAER, AOT, aerosol

15.1 Introduction

The determination of particulate matter (PM) from space-borne aerosol observations in terms of spectral aerosol optical thickness is required to fill gaps between ground-based stations of the national air quality networks and to get information on PM for regions with no or poor access to ground-based network data. It is relevant information for environmental control.

The importance of control and observations of PM mass concentrations increases with the relevance of national and European regulations on various air pollution species. National ground-based observation networks of air pollutants deliver information at local stations. Since satellites give normally columnar observation of the whole atmosphere, and PM data are valid only for the atmospheric boundary layer, the satellite-derived data for columnar PM must be reprocessed to account for conditions at the ground (e.g., at 2 m height as observed by ground stations).

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Therefore, the retrieval of PM requires the integration of very different information: (a) aerosol optical thickness (AOT), (b) aerosol type and composition, (c) vertical profile and distribution of aerosol and (d) humidity.

The most approaches, exploring this task in the past, use empirical correlations between AOT and PM observations or simple linear relationships between number concentration and AOT. (Fraser 1974; Fraser et al. 1984; Kaufman and Fraser (1990); Gasso and Hegg 1997, 2003). Since this neglects the inherent physical relations between the AOT, the aerosol type (size distribution, main shape of particles and composition), vertical structure and ambient meteorological conditions, correlations of AOT and 'dry' PM data are relatively poor, (Uhlig and von Hoyningen-Huene 1993). The reason is, that while the ground-based aerosol sampling for PM concentrations are performed for 'dry' measurement conditions in the atmospheric surface layer, the AOT is a columnar aerosol parameter of the whole atmosphere, containing all ambient air influences. For this purpose, the boundary layer fraction of the aerosol must be separated and transformed into a 'dry' reference status. First estimations of columnar aerosol concentrations from satellite observations of AOT considering variations in effective radius (r_{eff}) are made by Kokhanovsky et al. (2006).

Al-Saadi et al. (2005) presented an integrated complex approach for the American air quality forecast.

The present contribution integrates spectral AOT retrievals using MERIS L1 data made with the Bremen AErosol Retrieval (BAER) approach (von Hoyningen-Huene et al. 2003) with the estimation of r_{eff}, number concentration and finally mass load within an atmospheric column. Estimates of planetary boundary layer (PBL) height and average relative humidity yield the transfer of these information into concentrations of PM10 within the PBL. The approach is demonstrated using a MERIS L1 scene over Germany.

15.2 Theory

The retrieval of particulate matter from satellite observation uses spectral properties of AOT, as derived by BAER for clear sky conditions. The retrieval of AOT provides the spectral behaviour of AOT for seven shortwave channels of the MERIS instrument, which are used for the determination of the spectral slope in terms of the Angström α-parameter. Angström α is obtained using AOT, retrieved from the seven MERIS channels with wavelength $\leq 0.665\,\mu m$. The BAER approach is described by von Hoyningen-Huene et al. (2003, 2006) and is used in different applications (Kokhanovsky et al. 2004; Lee et al. 2004, 2005). AOT for a certain reference wavelength, here MERIS channel 1 or 2 with 0.412 or $0.443\,\mu m$ is used, and the Angström α-parameter is the basis for the PM retrieval.

The PM retrieval requires an assessment of a size distribution model to convert spectral AOT into columnar aerosol volume, respectively mass. Kokhanovsky et al. (2006) used a mono-modal logarithmic size distribution, characterized by the r_{eff} and

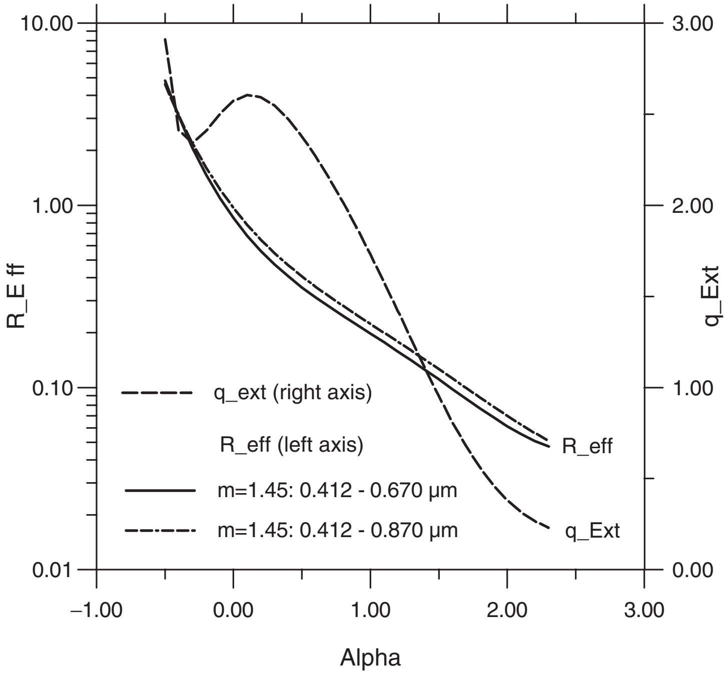

Fig. 15.1 Effective radius (r_{eff}) (black and blue curve) and extinction factor (red curve) as functions of Angström α-parameter

a fixed mode width σ = 0.8326. Mie theory is used to derive parameterisations for r_{eff} and extinction factor as a function of spectral slope of AOT $\delta_{\mathrm{Aer}}(\lambda)$, expressed by the Angström α-parameter: $r_{\mathrm{eff}}=f_1(\alpha)$, $q_{\mathrm{ext}}=f_2(\alpha)$. The relationships for $r_{\mathrm{eff}}=f_1(\alpha)$ and $q_{\mathrm{ext}}=f_2(\alpha)$ derived are presented in Fig. 15.1.

Both quantities give together with the AOT a columnar number concentration of aerosol:

$$n_{Aer} \approx 8 \cdot \delta_{Aer}(0.412\mu m)\frac{1}{\pi \cdot r_{eff}^2 \cdot q_{ext}} \tag{1}$$

at σ = 0.8326, which is an adequate mode width for PM10. Thus a dynamical link between the spectral AOT and columnar number concentrations is obtained.

The simple monomodal lognormal size distribution can be substituted later by a more complex bimodal model to distinguish between fine and coarse aerosol fraction. The selected monomodal size distribution fits to the size range, relevant for PM10.

An assessment of aerosol density ρ_{Aer} relates the columnar number concentration to an estimate of the columnar aerosol mass:

$$M_{Col} \approx \frac{\pi}{6}\rho_{Aer} \cdot n_{Aer} r_{eff}^3. \tag{2}$$

For the estimation of PM concentrations the columnar aerosol mass needs to be related to the planetary boundary layer (PBL) conditions. Under clear sky conditions about 90% of aerosol is within the PBL. The observed aerosol exists under ambient humidity conditions with the relative humidity (rh). Therefore, a correction for humidity effects is required, giving $r_{eff}(dry) = r_{eff}(rh)\, f(rh)$, where $f(rh)$ is given by Hänel (1984). Finally PM concentration can be estimated by

$$PM10 \approx a \frac{M_{Col}(r_{eff}(dry))}{h_{PBL}}. \qquad (3)$$

The parameter a gives the fraction of total aerosol, which is within the PBL and h_{PBL} characterizes the thickness of PBL. The approach is described in detail by Kokhanovsky et al. (2006) together with applications to the Sea-viewing Wide Field-of-view Sensor on the SeaStar spacecraft (SeaWiFS).

15.3 PM10 Retrieval from a Satellite: A Case Study

The retrieval of PM10 requires scenes with clear sky conditions only. Cloudy parts of the scenes need to be excluded by a rigorous cloud screening. For the purpose of PM10 retrieval, the MERIS L1 scene with reduced resolution ($1.2 \times 1.2\,km^2$), October 13, 2005, 09:45:11 UTC, over Central Europe is selected. It shows the most parts of Germany as cloud free, thus retrievals of PM10 should not be disturbed by cloud influences. The RGB image of the selected scene is presented in Fig. 15.2.

Over land surface, the spectral AOT has been retrieved by BAER for MERIS channels 1–7 (0.412–0.665 µm). Using these channels Angström α-parameter is determined. The AOT and Angström α-parameter of the scene above are presented in Figs. 15.3 and 15.4, respectively.

The most parts of the scene are suitable for a retrieval of PM10 concentrations. Unless a cloud screening is applied, some cloud disturbances, such as thin *Ci* or contrails, are still visible in the AOT results. Over Germany, AOT at 0.443 µm is ranging between 0.2 and 0.3. Pollution is clearly visible in northern Italy with values of AOT in the range 0.4–0.65. The Angström α-parameter over land surface ranges between −0.2 and 1.1. Clearly a change in aerosol type can be seen from west to east of the scene, with low values in the west and the highest values in the east. Over sea, Angström α-parameter has not been determined. Therefore, PM retrieval has been performed only over land.

The results of AOT retrieval over land have been used for the determination of the columnar size distribution parameters, columnar number concentration and columnar r_{eff}, using equations given above. The size distribution is the basis for the determination of PM10 concentrations.

Figure 15.5 gives the regional pattern of r_{eff}. Since the average relative humidity from ECMWF reanalysis for 1000 hPa is about 50%, a humidity correction

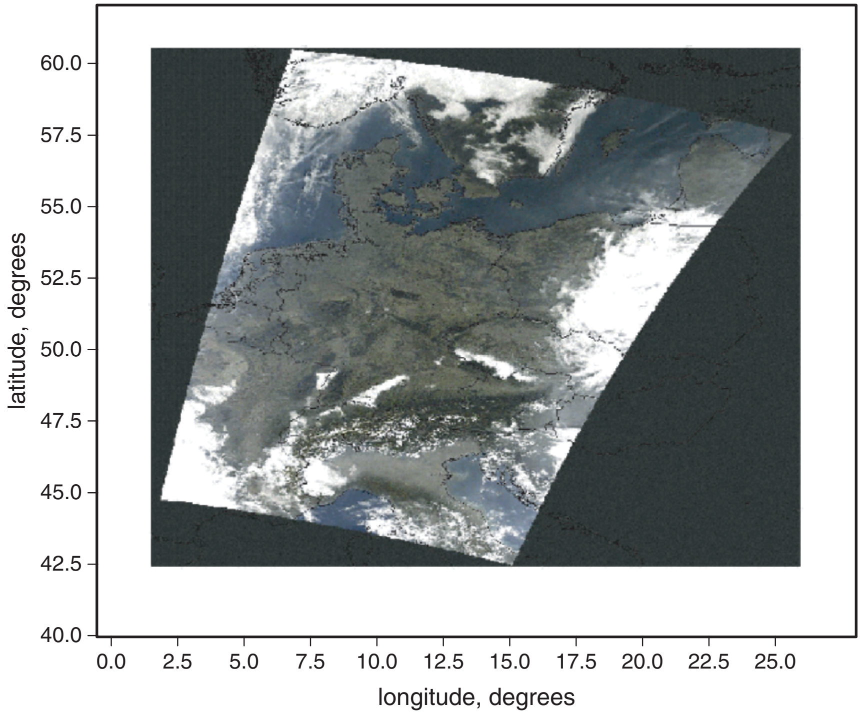

Fig. 15.2 RGB image of the MERIS RR scene of October 13, 2005 09:45:11 UTC over Central Europe

of r_{eff} was not required. Regional differences in humidity are therefore not considered.

One can see an increase of r_{eff} form east to north-west part of Germany, comparable with the change of Angström α-parameter. The region in the north-west, however, has relatively low AOT. The change of Angström α and r_{eff} seems to be connected with a change in aerosol type.

For the calculation of the PM10 concentration, according to Eq. 3, PBL height h_{PBL} and aerosol fraction a in the boundary layer are required.

We assumed a boundary layer height of 1 km. This is based on observations of Meteorological Observatory Lindenberg, giving PBL = 1.2 km at 10:00 UTC, and the PBL height of ECMWF. ECMWF PBL underestimates the values of Lindenberg by about 20%. Although regional differences in PBL height from ECMWF model predictions exist, for a first assessment we used a fixed h_{PBL} for the whole scene.

Aerosol fraction within the PBL is estimated from backscatter LIDAR at Lindenberg. From the vertical profile, one can conclude that 90% of the aerosol expressed by the AOT is within the PBL. This aerosol fraction is used for the whole scene. With these assumptions PM10 concentration has been derived. Figure 15.6 presents the cloud screened PM10 concentration of the scene.

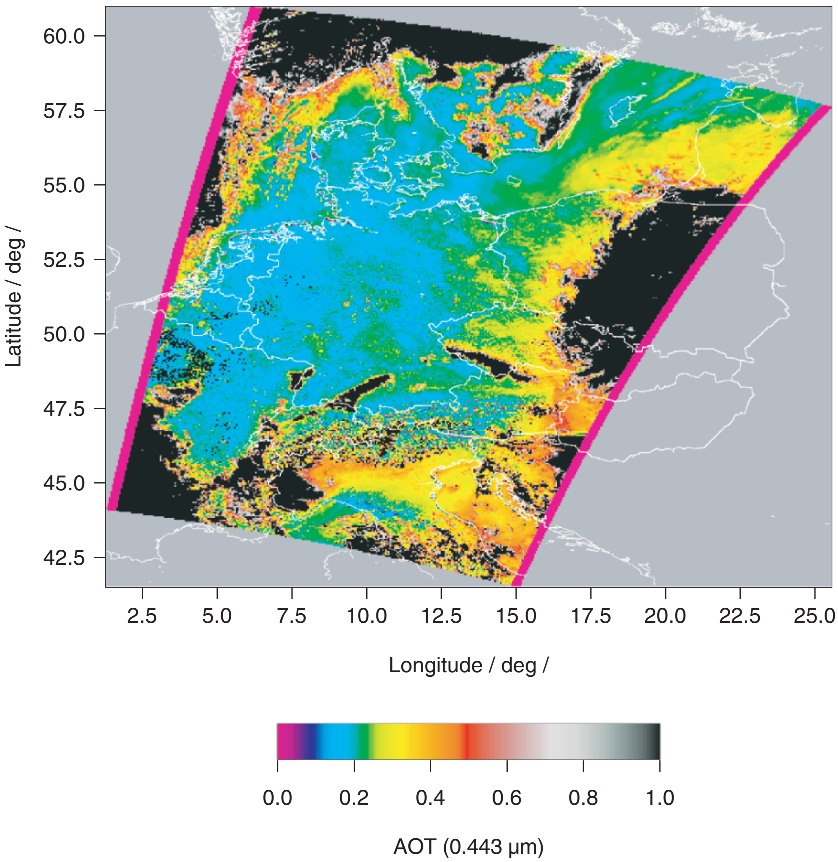

Fig. 15.3 Aerosol optical thickness for MERIS channel 2 (0.443 µm) of the scene of October 13, 2005. Black parts of the scene are excluded because of cloud or snow

15.4 Cloud Screening

The first application of the method showed multiple disturbances by various effects, mainly caused by an insufficient cloud screening. Locally, single very high, partly unrealistic, PM10 concentrations are obtained. For these spots no indication of clouds in the RGB data and in cloud mask products for MERIS could be found. However, the unrealistic high spots occurred in regions close to cloud fields. Thus the cloud screening applied before has not been effective enough for the task of PM retrieval.

The cloud screening applied in BAER determines clouds from radiance boarders for different spectral channels. This removes thick clouds of significant cloud

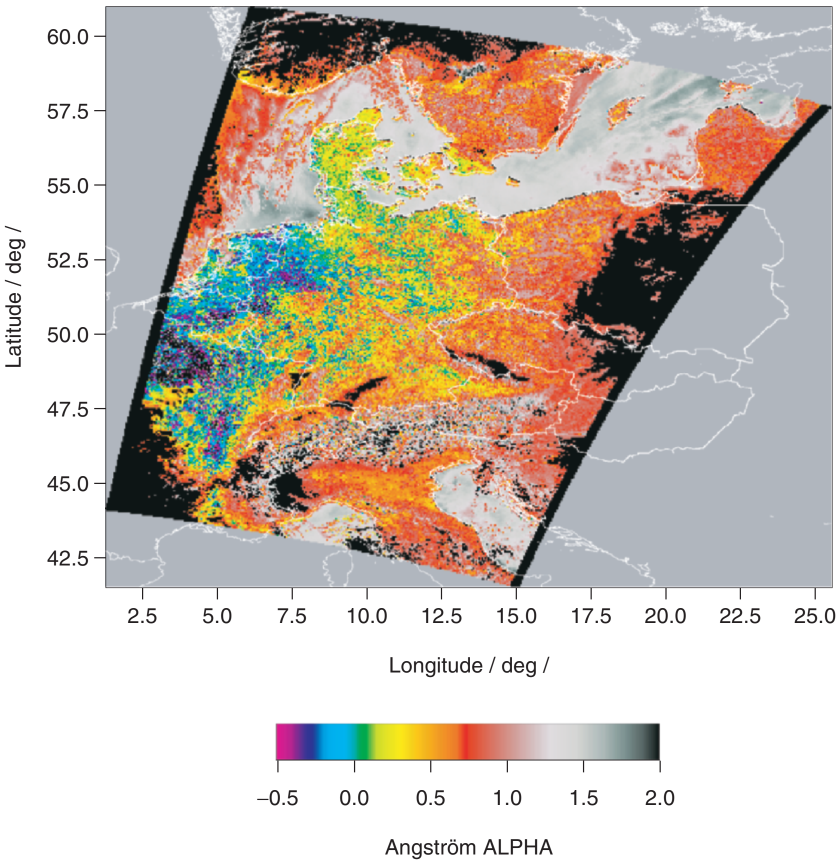

Fig. 15.4 Angström α-parameter

fractions within the scene (>10%). Thin cirrus or sub-pixel clouds with low cloud fractions will not be recognized well by these radiance boarders.

A cloud disturbance results in lowering Angström α significantly and increasing the r_{eff}. This can be caused by both aerosol and cloud disturbances. Assuming that aerosols are more homogeneous distributed than convective clouds, a high standard deviation within a sub-mask of 5 × 5 pixels, indicates for cloud disturbance in this area.

For the purpose of cloud screening we calculated average PM_{Av} and standard deviation σ within a moving 5 × 5 pixel matrix and removed all PM10 results, if the ratio $R = \sigma/PM_{Av} < 0.04$. Thus regions of high PM10 variability will be excluded to avoid cloud disturbance in PM10 retrievals. All unrealistically high PM10 concentrations disappeared.

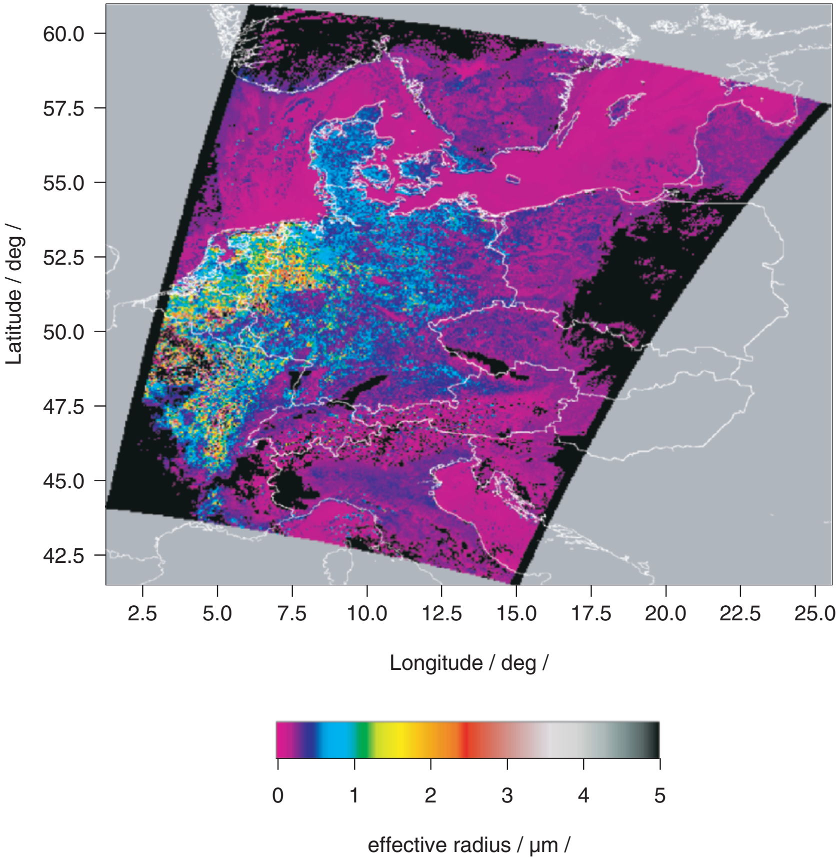

Fig. 15.5 Effective radius

Now three different criteria for the cloud screening are used:

1. The top-of-atmosphere MERIS reflectance ρ_{TOA} for three shortwave channels is spectrally neutral and larger than 0.2.
2. The ratio $\rho_{TOA}(0.412\,\mu m)/\rho_{TOA}(0.443\,\mu m)$ is smaller than 1.07. This indicates reduced Rayleigh- and aerosol scattering and, therefore, a contribution of elevated clouds.
3. The standard deviation of PM within a moving 5×5 pixel mask is lesser than 4%.

All criteria together enable an effective cloud screening for the purpose of PM retrieval. Thus, effects of small sub-pixel clouds with a cloud fraction <0.1, cirrus and contrails could be reduced significantly. A real cloud free scene is a pixel fulfilling all three criteria. All other pixels are rejected from the PM10 retrieval and are masked in the figures with black colour.

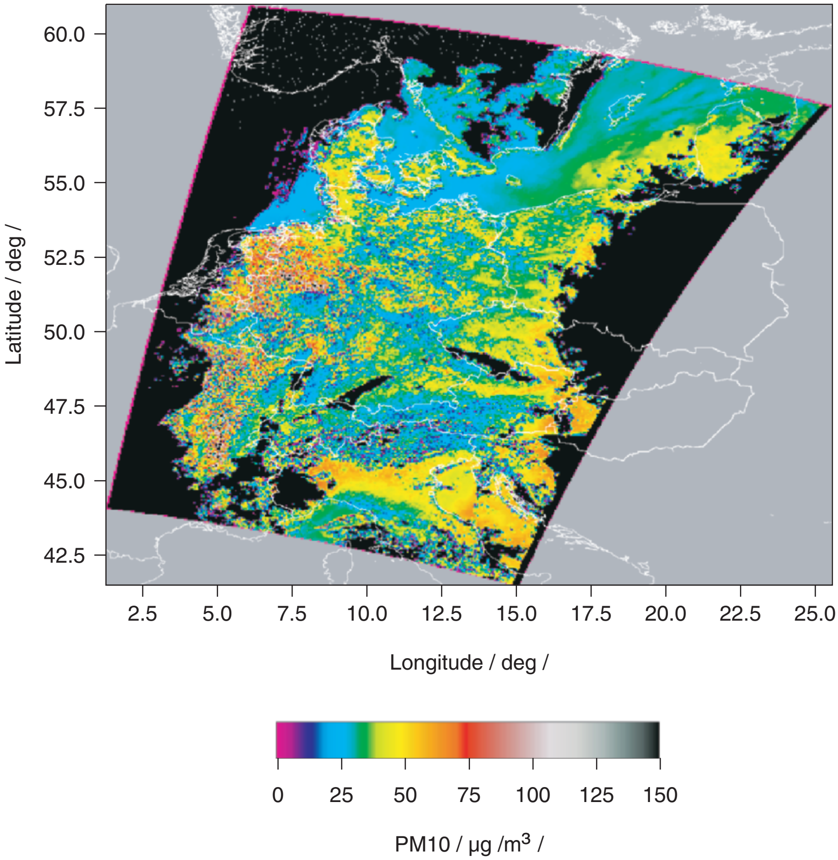

Fig. 15.6 Retrieval of PM10 concentration for the scene of October 13, 2005

15.5 Discussion and Validation of Results

After the additional rigorous cloud screening, the regional pattern of PM10 concentrations over central Europe is obtained for the MERIS RR scene of October 13, 2005. In the vicinity of thick clouds, still effects of thin-high clouds, like cirrus and contrails remain. These clouds do not have a high spatial variability like convection events at the PBL.

Neglecting these effects, the regional pattern of PM10 concentration shows high pollution in northern Italy. Surprisingly, increased pollution can be seen in north-west Germany, where AOT was relatively low. The increased pollution is due to larger effective radii and is confirmed by the ground-measurements of PM10 too. The pattern of PM10 concentration, derived from MERIS observations, follows the

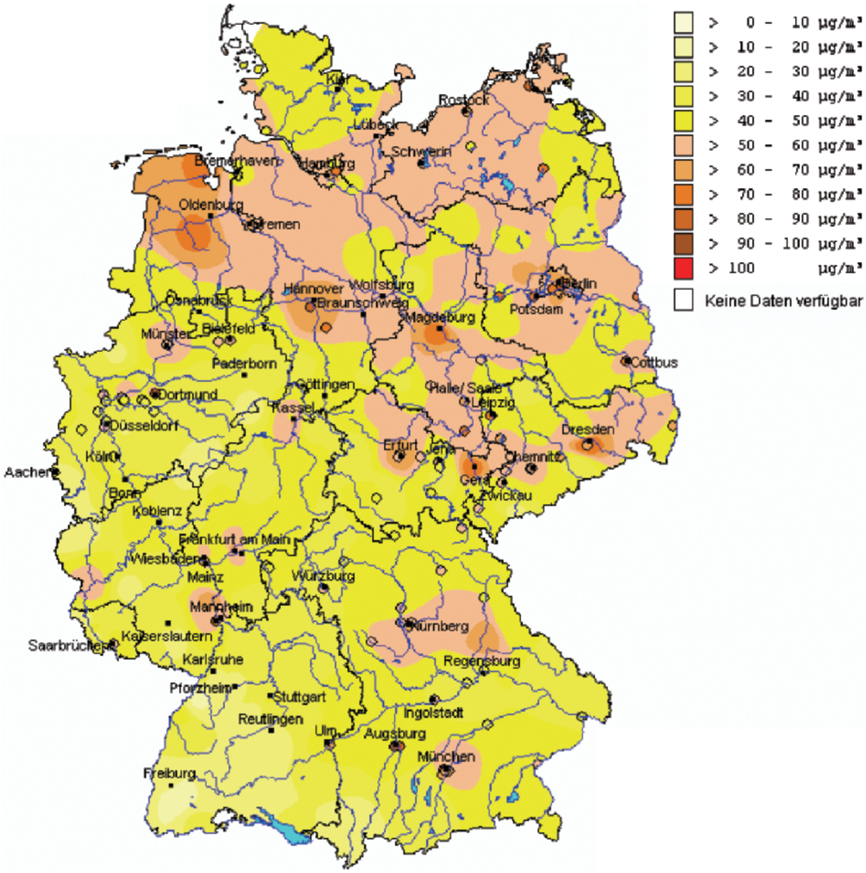

Fig. 15.7 Average daily PM10 concentration over Germany for October 13, 2005, published by Umweltbundesamt, http//www.uba.de

general PM10 distribution obtained from ground based measurements (see Fig. 15.7), with high values in north-west Germany and low values in south-west. AOT and PM10 are nearly uncorrelated over Germany. The correlation coefficient between the AOT (0.443 µm) and retrieved PM10 for the investigated scene is 0.02. An exception is the pollution in northern Italy, where increased AOT is connected with increased PM10 concentrations. Therefore, a monochromatic AOT alone do not display the pollution pattern.

The consideration of the spectral properties of AOT and the retrieval of the r_{eff} gives PM10 values comparable with ground based data as it is presented in Fig. 15.8.

Cloud-screened PM10 retrievals have been used for comparisons with ground-based PM10 measurements of the overflight time of ENVISAT. Ground-based PM10 measurements are obtained within the measurement networks of the 16

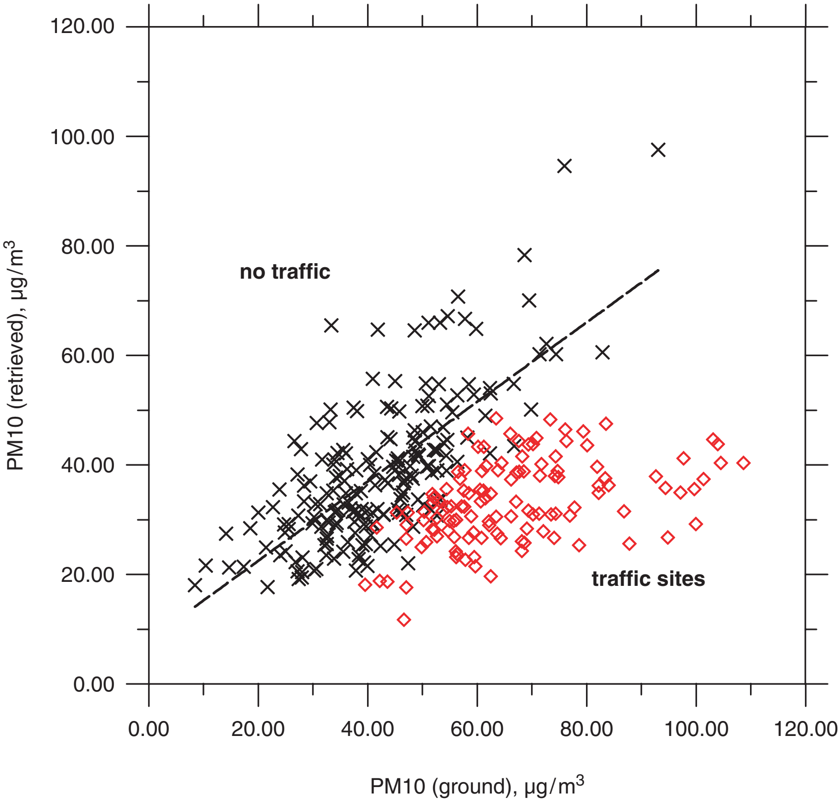

Fig. 15.8 Comparison of cloud-screened retrievals of PM10 from MERIS scene of October 13, 2005 and ground-based measurements of PM10 concentrations for the MERIS overflight time, provided by the German Federal Environmental Agency (Umweltbundesamt). For the traffic sites, no correlation between satellite derived and ground data is found

German federal countries, provided by the Federal Environmental Agency (Umweltbundesamt-UBA) of Germany. The results of the comparison are presented in Fig. 15.8.

Associating all cloud screened data to ground stations of the networks, on a first view it seems, that the retrieval from satellite observations does not reflect really PM10 from ground. (see all points [crosses + open circles] in Fig. 15.8). The reasons need a deeper analysis of the character of the ground stations.

A large number of them, mostly with high PM10 concentrations, are operating in urban areas and measure the pollution of traffic along main road connections. The MERIS RR data, however, give an average estimation for this parameter on a scale of 1.2 × 1.2 km, mostly above the urban canopy layer. This could explain why the satellite observations will underestimate these conditions. Comparisons with stations, affected strongly by urban traffic are indicated in Fig. 15.8 with open circles. This part of station gives no correlation with the PM10 concentrations, derived from satellite observations.

If one removes all stations affected strongly by urban traffic, one obtains a scatter plot, which gives a better correlation with ground data (crosses in Fig. 15.8). We performed a linear fit of PM10 derived using satellite measurements with those on the ground: PM (satellite) = 0.725 PM10 (ground) + 7.98 with a correlation coefficient of 0.71. The average standard deviation is 11 $\mu g/m^3$. Considering the fact, that the regional variability of the meteorological conditions is treated for the whole scene as constant, the scattering of the data is in an acceptable range. Further improvements can be expected, if the real regional meteorological conditions (rh and h_{PBL}) will be taken into account. The data shows, that the retrieved PM10 concentrations give the average pollution by particulate matter on the larger scale of the MERIS satellite pixel and not local peaks.

15.6 Conclusions

For real clear sky scenes, aerosol size distribution parameters, like r_{eff} and number concentration of a simple mono-modal lognormal distribution, is retrieved from spectral AOT measurements. On this basis, PM10 concentrations are obtained.

The cloud-screened PM10 concentration can give the general regional distribution of aerosol pollution.

For the derivation of PM information, the following are important:

1. Spectral AOT should be retrieved with several spectral channels (to obtain the spectral slope of AOT from measurements). For a retrieval over land, instruments are required, like MERIS, which operate with several spectral channels below the red edge wavelength of green vegetation. The retrieval approach needs to consider the whole available spectral information.
2. Improved cloud screening for especially sub-pixel cloud effects is required. Sub-pixel clouds bias the results on PM significantly. Sub-pixel cloud screening for this purpose is not a solved problem so far.
3. The presented results are promising, although regional meteorological influences are not considered in detail. This needs an integration of regional meteorological information, like rh and h_{PBL}.
4. The information seems to be limited by the spatial resolution of the satellite instrument. Thus MERIS RR data do not provide locally high pollution peaks in urban areas. For this purpose, investigations with higher spatial resolutions, like MERIS FR, will be required.

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