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SYNAER Validation Report

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Executive Summary

This report summarizes the validation results of the synergetic aerosol retrieval SYNAER version 2.2 exploiting the combination of the sensors AATSR (Advanced Along Track Scanning Radiometer) and SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Cartography), both onboard the ENVISAT platform. SYNAER data have been processed for the period 2003 – 2009 covering the field of view of the geostationary satellite METEOSAT SECOND GENERATION, i.e. Europe, Africa, the Atlantic and parts of Southern America and Africa; for 2008 also a first global dataset has been produced. As primary validation dataset AERONET level 2 version 2.0 direct sun measurement data are used. Also an initial analysis of the SYNAER capabilities for estimating the aerosol type is made. This includes the assessment of multi-spectral AOD and uses also few coincidences with AERONET inversion products (fine and coarse mode AOD, Angstrom coefficient and single scattering albedo).

The validation shows for AOD550 with all stations where coincidences are found an overall correlation of 0.70, standard deviation of 0.12 and bias of -0.06 - in the light of the comparatively large SYNAER pixel size of 60x30 km^2 these results are reasonable. 67% of the SYNAER pixels are found to be within $AOD_{SYNAER} = \pm 0.1 \pm 0.20 * AOD_{AERONET}$

The AOD550 error analysis as function of several parameters, of different stations and spatial-temporal distance between the SYNAER and AERONET measurements reveals some issues, were further algorithm improvements can be made (predominantly surface reflectance parametrization).

Also multi-spectral AOD as well as fine / coarse mode AOD show similar correlation as AOD550. The assessment of Angstrom coefficient and single scattering albedo can only done for a very small number of coincidences with large AOD550 values to assure sufficient information content in both the AERONET inversion and SYNAER retrieval algorithms. These first results can not clearly proof the SYNAER capabilities, but show some potential – it is evident that the underlying inaccuracy of the AOD retrieval should first be improved.

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1. Introduction

1.1 SYNAER method and processing status

The synergetic aerosol retrieval method SYNAER (Holzer-Popp et al., 2002a) exploits the complementary information of a radiometer and a spectrometer onboard one satellite platform to extract aerosol optical depth (AOD) and speciation (as a choice from a representative set of pre-defined mixtures of water-soluble, soot, mineral dust, and sea salt components). SYNAER consists of two retrieval steps. In the first step the radiometer is used for accurate cloud screening, and subsequently to quantify the aerosol optical depth (AOD) at 550 nm and spectral surface brightness through a dark field technique for different pre-defined aerosol mixtures. In the second step the spectrometer is applied to choose the most plausible aerosol mixture through a least square fit of the measured spectrum with simulated spectra using the mixture-dependent values of AOD and surface brightness retrieved in the first step. This method was developed and a first case study evaluation against few (15) multi-spectral ground-based AERONET sun photometer observations was conducted with a sensor pair (ATSR-2 and GOME) onboard ERS-2 (Holzer-Popp, et al., 2002b). SYNAER was then transferred to similar sensors AATSR and SCIAMACHY onboard ENVISAT. While transferring to the new sensor pair significant improvements in the methodology were made based on a thorough evaluation of the methodology (Holzer-Popp, et al., 2008). In this paper also a brief assessment of atmospheric noise impact on comparisons of pixel and station measurements a validation against ground-based measurements established error bars for the SYNAER/ENVISAT method version 2.0 using 50 coincidences of spring / summer 2005 in Europe (and few in Africa): the standard deviation for 550 nm was found at 0.10, the bias near 0 and correlation at 0.80. Furthermore, a theoretical analysis of the information content with regard to aerosol composition (second retrieval step) was made which showed quantitatively the potential and limitations of this new capability provided by the SYNAER method with up to 3 degrees of freedom in the retrieval in addition to AOD and surface reflectance. A detailed algorithm description of the SYNAER method is provided in Holzer-Popp, et al., 2009.

In this report a larger SYNAER version 2.2 (with some minor fine tuning of the surface reflectance estimation module) dataset over 7 years (2003 – 2009) in Europe, Africa, the Atlantic and parts of South America is analysed.

1.2 Known issues and limitations of SYNAER

Already the analysis of first SYNAER results in Holzer-Popp et al. 2008 showed following limitations of the algorithm and dataset with ENVISAT measurements:

- The SYNAER pixel size of 60x30 km^2 means a clear limitation due to atmospheric noise with at least a fundamental scatter of 0.05 (depending on the continent analysed) as shown with AERONET variograms for Europe, Asia and the US. In addition, the SYNAER/ENVISAT sampling is restricted severely due to the scan modes of both sensors (AATSR 512 km swath width, SCIAMACHY alternating nadir-limb scanning), which means a repeat cycle of about 12 days at the equator. Assuming an average cloud cover of 50% (this may be much higher for a specific region or season) and taking the

SYNAER quality assurance into account (see third bullet point; overall reduction of pixel number is about 40%) at one location / measurement station a maximum of 6 coincidences per year can be expected if ground-based measurements are done every day. With improved radiative transfer tables (see bullet point 2) the exploitable pixel number should increase. To improve the overall sampling the SYNAER method is transferred to a similar sensor combination GOME-2 and AVHRR onboard METOP with a combined repeat cycle every 1-2 days (experimental algorithm exists, treatment of calibration issues and validation is ongoing).

- SYNAER uses a polynomial fit of second order instead of exact radiative transfer calculations. This leads to a bias of AOD550 for medium (slight overestimation) and high values (strong underestimation) as is shown in figure 1. Furthermore, different radiative transfer tables (with not exactly the same data points used for determining the fits) are used for the different retrieval steps (AATSR dark field inversion, AATSR surface albedo inversion, SCIAMACHY spectral fit) which introduces another inaccuracy. The exact size of these effects depends on geometric retrieval conditions as well as the aerosol amount and properties and other parameters (e.g. surface reflectance). It is thus difficult to estimate their integrated impact. Most likely, this inaccuracy is also the reason due to which almost no very high AOD values with mineral dust are found over the Atlantic ocean. In the next revision SYNAER will use fully consistent radiative transfer tables with finer mash and based on piece-wise linear fits to achieve lower inaccuracies.

- A quality assurance module has been introduced to screen for retrieved pixels with large probability for high AOD errors. This module analyses the difference in AOD due to non separable aerosol types as well as the quality of the retrieval spectral fit and the underlying retrieval conditions. Table 1 summarizes the selection criteria which should be applied to SYNAER v2.2 data (all parameters are contained in the HDF product files) to select “good” pixels. Overall, the application of these selection criteria reduces the number of SYNAER pixels to about 40%.

selection criterium	**value / range**	**comment**
observing zenith angle	< 19.5°	Avoid SCIAMACHY pixels at edge not fully covered by AATSR swath
relative azimuth	5° < … < 175°	
spectral fit error	< 0.0085	approximately equal to 3-4% relative error of TOA reflectances
intrinsic aerosol-type induced AOD error	0.05	
retrieved ocean surface albedo	< 3.5	
retrieved land surface albedo	< 25	

Tab. 1.: Quality assurance: post-processing selection criteria for “good” SYNAER pixels

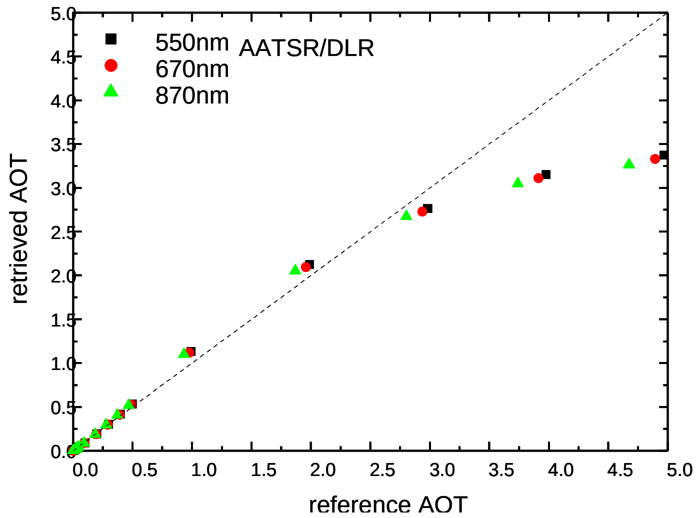

Fig. 1.: Comparison of example top of atmosphere reflectances for maritime aerosol calculated with an exact radiative transfer code (reference AOT) and the second order polynomial fit used in the SYNAER retrieval (courtesy of A. Kokhanovsky).

1.3 Validation data used

For the inter-comparison AERONET sun photometer measurements of the best quality (automatic and manual cloud screening) are used (level 2, version 2.0). Most validation results exploit the direct sun observations of multi-spectral aerosol optical depth (AOD). To assess the capabilities for aerosol type estimation, also an initial attempt to exploit the AERONET inversion product was made. However, the number of measurement taken is substantially smaller and for aerosol properties a restriction to cases with large AOD550 was taken to assure sufficient information content of both inversion algorithms. Thus only a low number of coincidences could be analysed, which provide no clear picture, yet.

To take into account the SYNAER limitations and known issues, coincidences of multi-spectral AOD were only used, after SYNAER selection criteria were applied and when the distance of the AERONET station from the SYNAER pixel centre was not larger than 0.5° $\sqrt{(\Delta lat^2+\Delta lon^2)}$ and the temporal difference was not larger than 30 minutes. An assessment of the impact of different settings (up to 2 hours time difference and 2° spatial distance) was made and is discussed in section 2. Also, temporal averaging of the AERONET measurements over 0.5, 1 and 2 hours was tested to be consistent with the spatial smoothing through the large pixel size – however such a pre-processing of AERONET measurements had no impact on the results.

2. Validation of AOD550

2.1 AOD550 validation results

Validation of AOD550 was conducted with all data of the period 2003 – 2009 as plotted in the scatter plot in figure 2 and the histogram in figure 3. These were then broken down per season and per year as listed in table 2. A total of 2509 coincidences from 166 stations (many of these not operating all years) were found within ±30 min and ±0.5°. After application of the SYNAER quality assurance (see selection criteria in table 1) 839, i.e. about 40% of these remained and were exploited. The 3D histogram plot in figure 2 shows a reasonable agreement (given the pixel size) but also shows a clear underestimation of low AOD values and a large scatter of medium AOD values. Table 2 shows the statistical characteristics of the whole dataset and their breakdown to different data years and seasons. It can be seen that no season or particular data year has any outstanding validation results. For 2008 also part of the SYNAER orbits over the whole globe were processed – here the standard deviation is larger which requires further investigation.

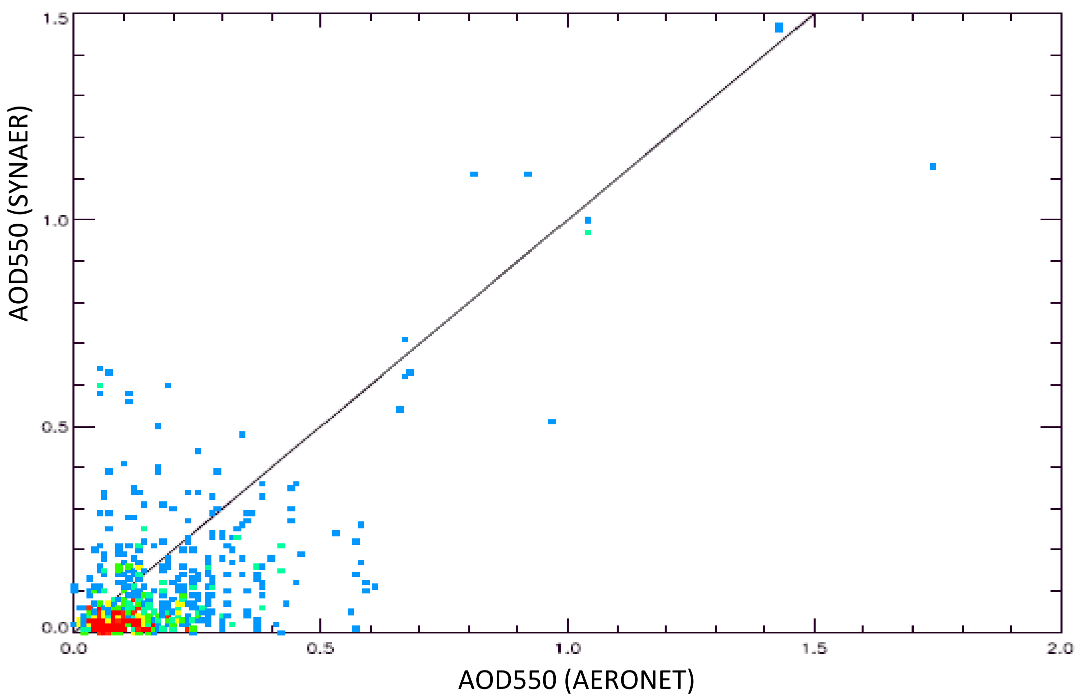

Fig. 2.: 3D histogram of overall SYNAER AOD550 validation against AERONET

Table 2 also shows the breakdown of validation statistics to pixels over land, ocean and coastal sites. It becomes evident that the standard deviation is lowest over ocean and highest over land. Figure 3 shows the overall histogram of AOD550 differences with clear negative bias and rather symmetrical distribution but also some large outliers.

period	correlation	mean bias	standard deviation
all years /seasons	0.70	-0.056	0.119
spring / all years	0.51	-0.06	0.125
summer / all years	0.77	-0.05	0.099
autumn / all years	0.43	-0.07	0.095
winter / all years	0.79	-0.06	0.120
land / all years	0.68	-0.054	0.140
ocean / all years	0.58	-0.061	0.075
coast / all years	0.76	-0.073	0.094
2003 / all seasons	0.56	-0.08	0.136
2004 / all seasons	0.49	-0.05	0.085
2005 / all seasons	0.71	-0.04	0.083
2006 / all seasons	0.52	-0.08	0.145
2007 / all seasons	0.25	-0.05	0.110
2008 / all seasons	0.82	-0.04	0.137
2009 / all seasons	0.87	-0.10	0.087
2008 / global	0.77	-0.05	0.159

Tab. 2.: Overall validation statistics for AOD550 with 839 coincidences within ±30 min and ±0.5°.

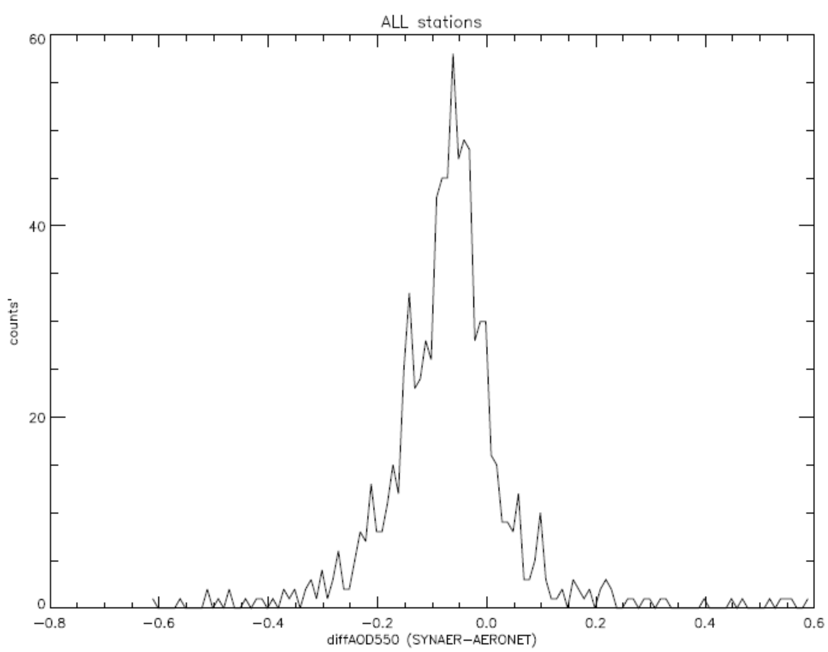

Fig. 3.: Histogram of overall SYNAER AOD550 validation against AERONET

maximum time difference [±minutes]	maximum spatial distance [±°]	number of coincidences	mean bias	standard deviation
30	2.0	12230	-0.064	0.154
	1.0	3265	-0.061	0.136
	0.5	839	-0.056	0.119
	0.3	322	-0.058	0.112
	0.2	142	-0.053	0.099
	0.1	41	-0.062	0.088
120	0.5	987	-0.058	0.132
60		919	-0.060	0.131
30		839	-0.056	0.119
15		716	-0.056	0.114
10		658	-0.056	0.115
5		449	-0.058	0.119
120	2	14714	-0.066	0.157
5	0.1	21	-0.070	0.094

Tab. 3.: AOD550 validation statistics as function of the spatial / temporal window allowed around the SYNAER pixel centre point

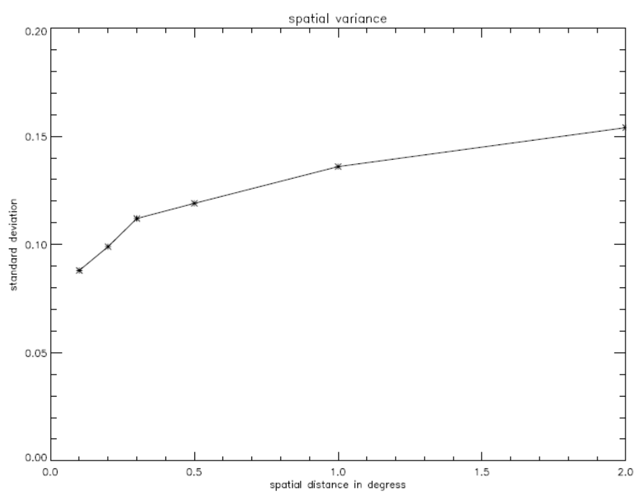

Fig. 4.: Dependence of AOD550 standard deviation to spatial distance

Table 3 and figure 4 discuss the effect of spatial and temporal difference between the SYNAER pixel centre and the AERONET measurements. The mean bias and remains almost stable at -0.06. For the standard deviation it is clearly evident that for the large SYNAER pixels the temporal distance should be not larger than ±30 minutes (but below no significant difference is seen), whereas the spatial difference shows a dependence converging to a value 0.08 at distance 0. In this ultimate value of the standard deviation still the “miss-integration” error due to the large SYNAER pixel size against the AERONET point measurements is contained.

The validation discussed so far contains all AERONET stations and all coincidences, which were found. No selection of stations or validation coincidences in terms of representativity for the 60x30 km^2 SYNAER pixel is made. A look into individual stations is presented in figures 5 and 6 and table 4.

Figure 5 shows typical examples of station validation results. This reveals stations with low bias (Belsk), high bias (Palencia), large scatter (Evora), and overall good correlation of low or higher AOD (Hamburg, Ilorin, Dakar) in different climate zones.

Table 4 summarizes the statistical validation characteristics of all stations with at least 10 measurements. The numbers of coincidences for one station range up to 24 (which is about 50% of the maximum total number of 42 coincidences at 1 station measuring completely over all 7 years). The table shows that large variability of the validation results between stations. Apart from SYNAER inherent errors potential other reasons for weak results are lacking station representativity (e.g. near mountains, coast or cities), low mean AOD values, and high surface reflectance. This needs further analysis and together with the findings of this report will define further algorithm improvements.

Figure 6 shows the spatial distribution of validation characteristics at the various AERONET stations. It again shows good and bad, which needs further analysis.

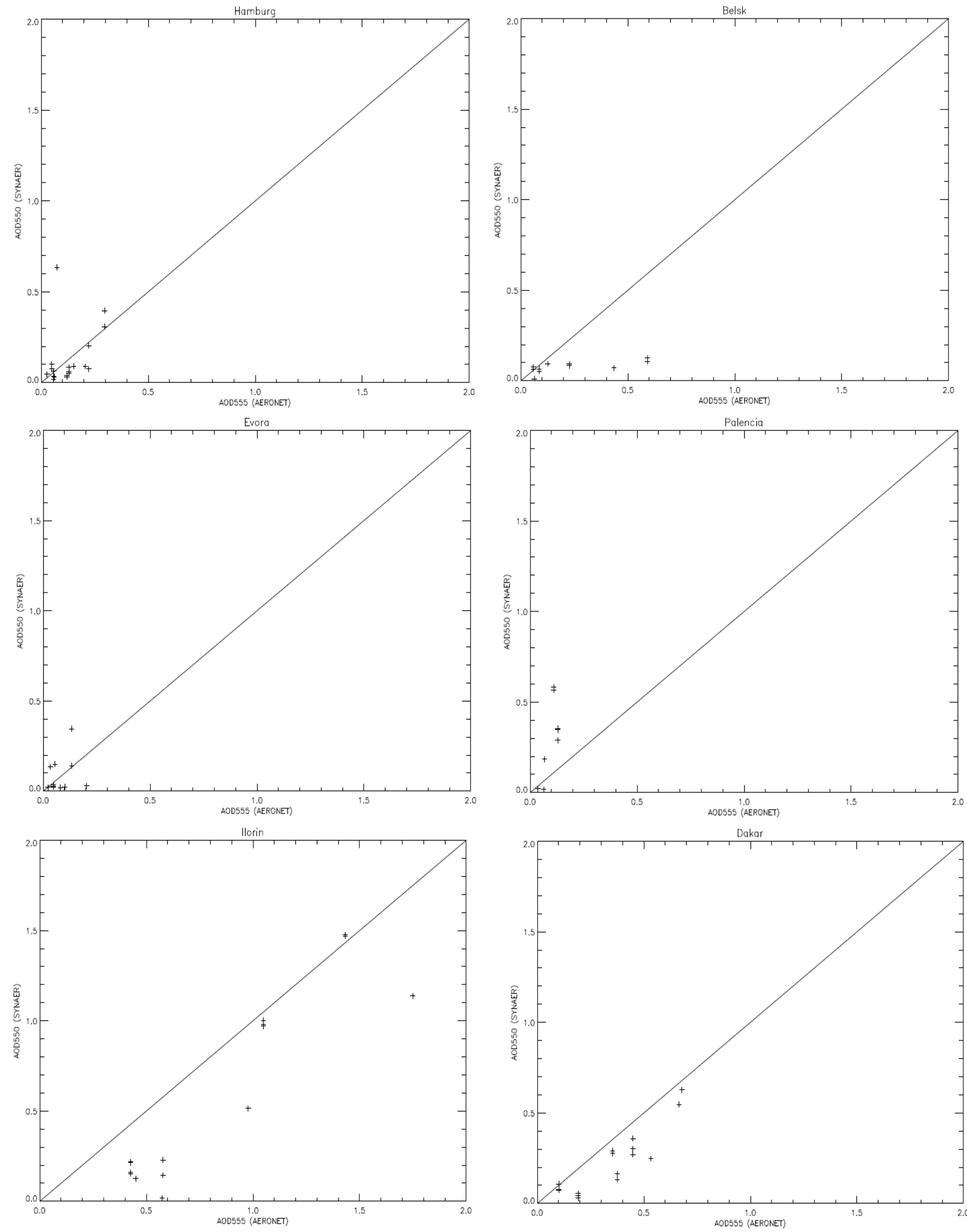

Fig. 5.: validation of AOD550 for typical AERONET station examples (from top left to bottom right): Hamburg, Belsk, Evora, Palencia, Ilorin, Dakar

station / number	correlation	mean bias	standard deviation
La Laguna / 13	0.98	-0.049	0.106
Ilorin / 15	0.92	-0.267	0.206
Dakar / 17	0.90	-0.125	0.080
Erdemli / 11	0.89	-0.111	0.098
Moldova / 17	0.87	-0.031	0.074
Munich / 14	0.83	-0.050	0.048
Cabo da Roca / 15	0.76	-0.055	0.064
Rome / 20	0.73	-0.040	0.055
Saada / 16	0.73	-0.090	0.070
Belsk / 13	0.70	-0.051	0.178
Venise / 21	0.66	-0.144	0.116
Fort Crete / 10	0.55	-0.056	0.038
Dunkerque / 10	0.55	-0.016	0.127
Trovavere / 20	0.48	-0.053	0.107
Thessaloniki / 10	0.46	-0.123	0.128
Moscow / 22	0.42	-0.08	0.069
Hamburg / 24	0.41	-0.029	0.133
Sao Paolo / 10	0.37	-0.107	0.053
Lecce / 15	0.35	-0.060	0.051
Blida / 10	0.33	0.013	0.042
Ascension / 13	0.31	-0.178	0.107
Evora / 13	0.30	-0.022	0.094
Villefranche / 16	0.26	-0.078	0.042
Carpentras / 19	0.24	-0.049	0.132
Avignon / 21	0.19	-0.067	0.073
Skukuza / 18	0.16	-0.031	0.109
Mongu / 18	0.13	0.016	0.097
Arenosillo / 13	0.03	-0.038	0.159
Minsk / 20	-0.03	-0.036	0.125
Barcelona / 14	-0.10	-0.019	0.043
Izana / 13	-0.11	-0.021	0.034
Paris / 13	-0.18	-0.136	0.165
Cape Verde / 20	-0.40	-0.057	0.042

Tab. 4.: validation statistics for AERONET stations with at least 10 coincidences

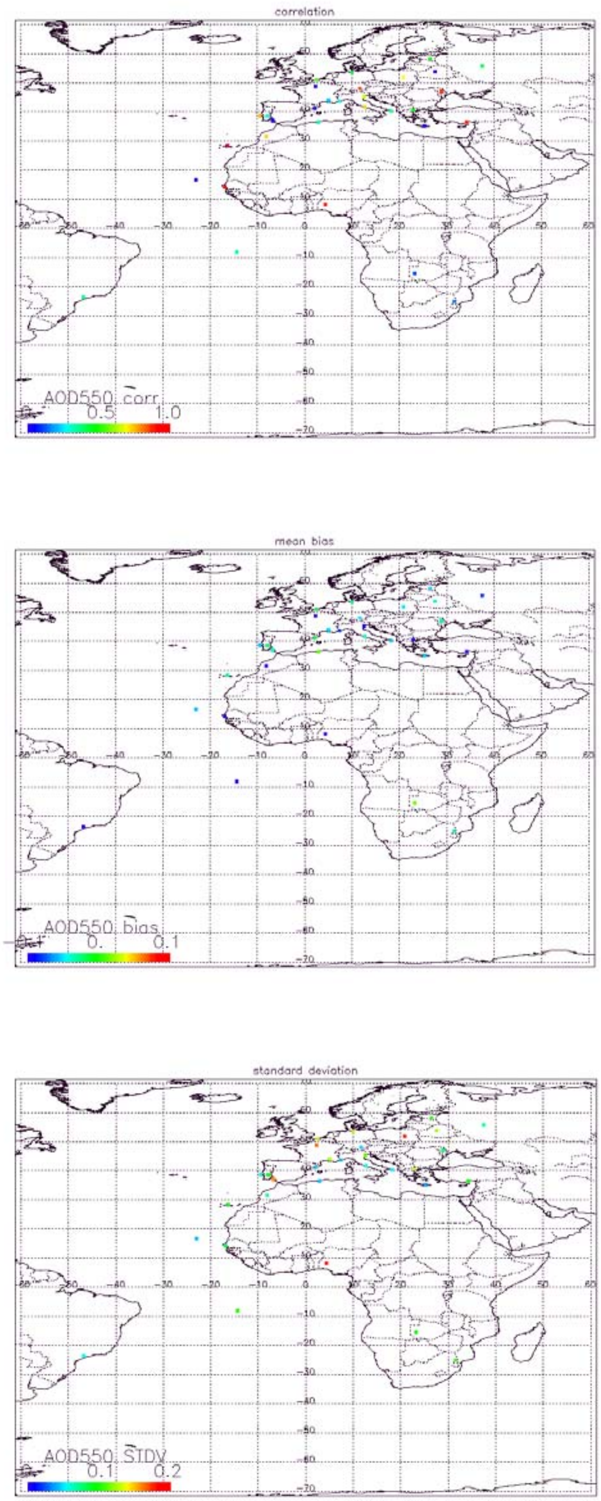

Fig. 6.: validation results of AOD550 for AERONET stations with at least 10 coincidences (from top to bottom): correlation, mean bias, standard deviation

2.2 Sensitivity analysis

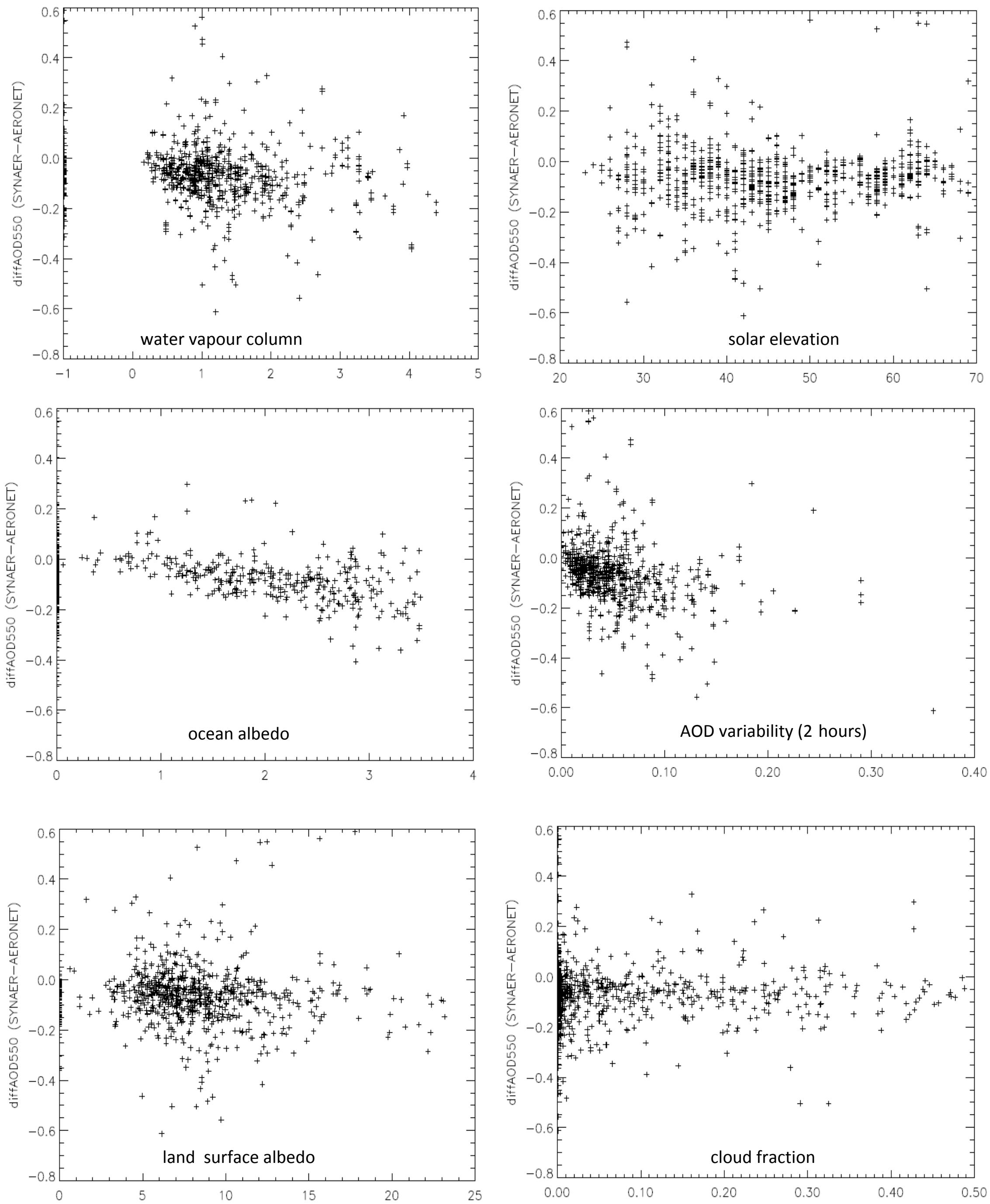

Fig. 7.: Sensitivity to retrieval parameters (from top left to bottom right): water vapour content ($g \cdot cm^{-2}$) solar elevation angle (°), ocean albedo at 670 nm, AOD variability over 2 hours (maximum – minimum in AERONET measurements), land surface albedo at 670 nm, cloud fraction

Figure 7 shows the analysis of sensitivities in AOD error with potential key parameters. It is clearly visible that water vapour content (AERONET) and solar elevation angle have no impact on the AOD550 error. Also the AOD variability (AERONET) within 2 hours before and after the satellite overpass and the cloud fraction within the SYNAER pixel (upto 50%) do not influence the AOD550 errors.

The surface albedo retrieved in SYNAER (which is based on a parametrization using NDVI and reflectance at 1.6 micron over land and another parametrization using 670/550 nm ratio over ocean) shows interesting features. There is a linear relation between ocean albedo and AOD550 error and a comparatively small scatter, whereas the scatter over land is much higher. Here 2 elements for improvement can be seen in the surface reflectance parametrizations used in SYNAER.

Further parameters were analysed (not shown) and exhibited no correlation at all. These included the observation zenith angle, the relative azimuth angle and scatter angle, the Angstrom coefficient (AERONET), the month of the year, the aerosol type estimate (SYNAER), the surface type selected in the SYNAER retrieval and the surface elevation of the AERONET station.

3. Initial validation of aerosol type information

3.1 Multi-spectral AOD

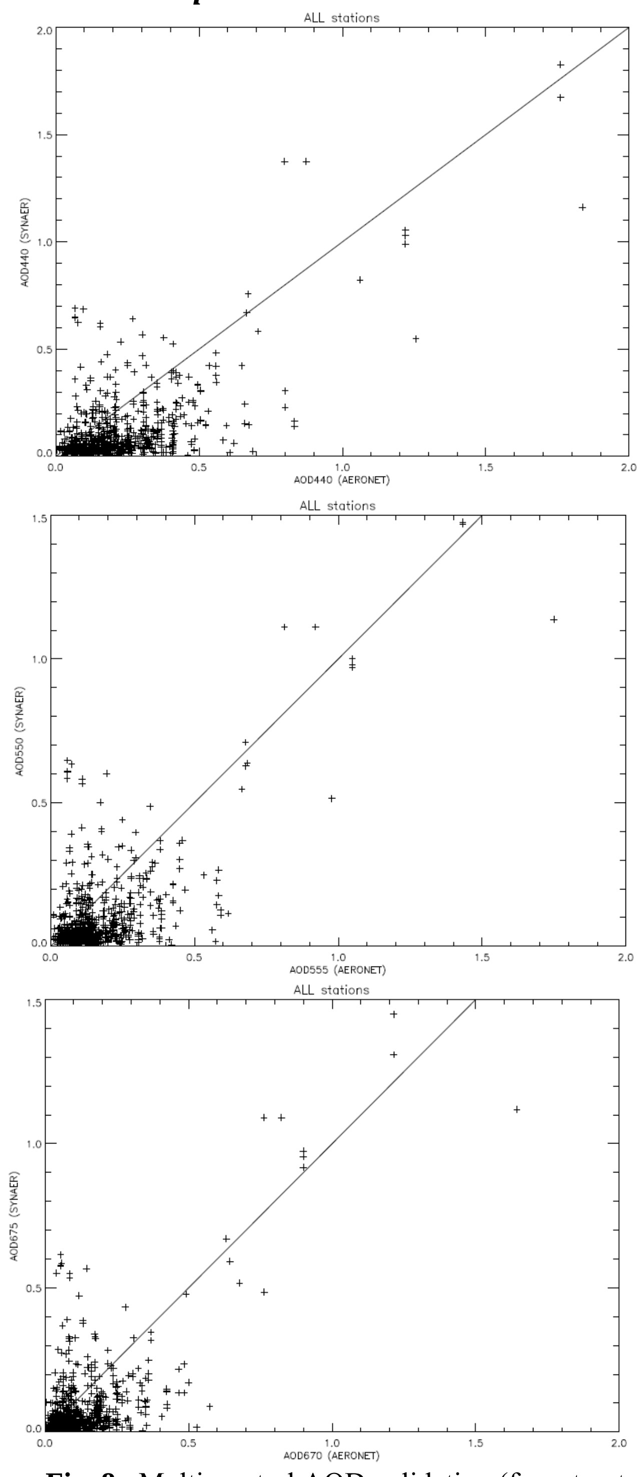

Fig. 8.: Multispectral AOD validation (from top to bottom) at 440, 550 and 670 nm

As a first step of assessing the aerosol type estimation in SYNAER multi-spectral AOD results at 440, 550 and 670 nm from the AERONET direct sun measurements are analysed. Results of this analysis are shown in figure 8 and table 5. Overall, the statistics indicate to similar quality of all spectral bands (in relation to growing mean values at shorter wavelengths) with equal features (negative bias mostly at low values, scatter highest at medium values, few reasonable high values).

wavelength	correlation	mean bias	standard deviation
440 nm	0.66	-0.089	0.148
550 nm	0.70	-0.056	0.119
670 nm	0.69	-0.047	0.108

Tab. 5.: validation statistics for multi-spectral AOD

3.2 Fine and coarse mode AOD

As second step of aerosol type retrieval evaluation, a first look into AERONET inversion products was made. This dataset contains significantly less measurements than the direct sun dataset (149 coincidences with SYNAER are found with the same spatial/temporal filtering criteria). Interestingly, the smaller sample does also have slightly different validation characteristics for AOD550 than the sample from the direct sun measurements discussed in section 2 - this indicates at the limitations due to the sampling. In SYNAER an initial estimation of the fine and coarse mode AOD is defined by putting 100% of each basic component either into the fine mode fraction (water-soluble, soot) or the coarse mode fraction (mineral dust, sea salt) – this is evidently only a first approach which needs further refinement. In this inversion dataset the fine and coarse mode AOD values are separated which are shown in figure 9 and table 6. Statistical characteristics are similar for fine and coarse mode as for AOD550. However, in the cases found the coarse mode AOD is comparatively small (< 0.25 in AERONET).

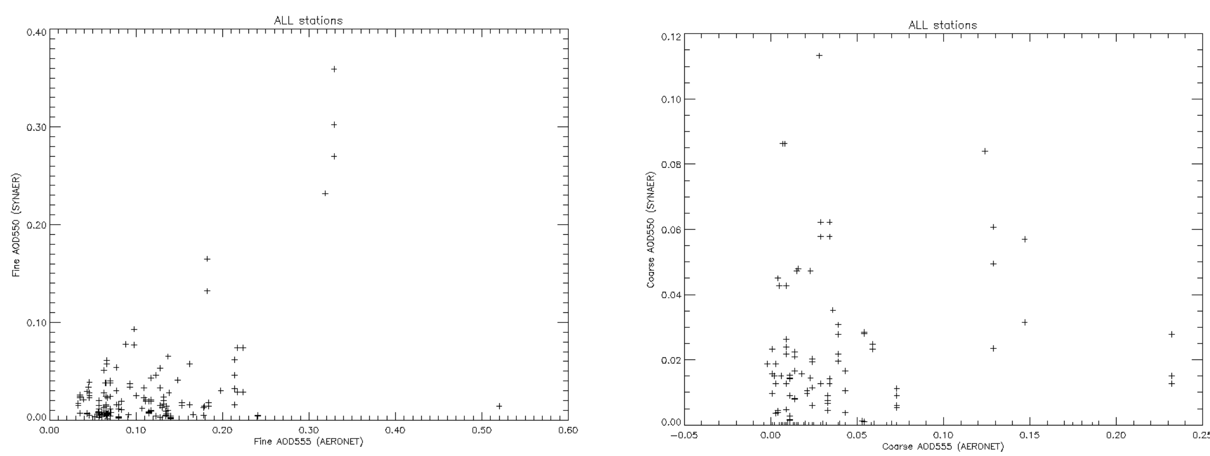

Fig. 9.: AOD validation of fine and coarse mode

mode	correlation	mean bias	standard deviation
total	0.63	-0.094	0.074
fine	0.89	-0.081	0.062
coarse	0.52	-0.025	0.051

Tab. 6.: validation statistics for fine and coarse mode AOD (coincidences with AERONET inversion products within ±0.5° and ±30 min geolocation)

3.3 Retrieved aerosol parameters

A final step to assess the estimated SYNAER aerosol type was the analysis of Angstrom coefficient (which is difficult to represent bi-modal aerosol distributions as used in SYNAER) and single scattering albedo. Here the number of coincidences vanishes almost due to also frequent lack of measurements in the AERONET dataset. Furthermore, the information content for these parameters in both AERONET and SYNAER is low for low AOD values. Therefore – for a first assessment – the analysis was restricted to high AOD values. Figure 10 and table 7 show the results for the Angstrom coefficient, which indicate a potential for the separation of small and large particles with high and low Angstrom coefficient, respectively.

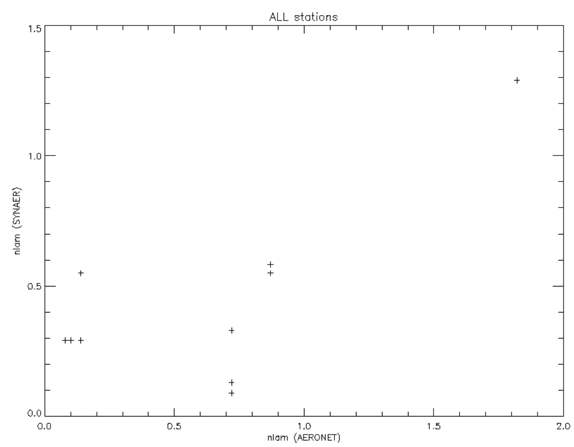

Fig. 10.: Validation of Angstrom coefficient (coincidences with AERONET inversion products within ±0.5° and ±30 min geolocation and for AOD > 0.4 and ΔAOD < 0.2)

number	correlation	mean bias	standard deviation
10	0.71	-0.18	0.36

Tab. 7.: validation statistics for Angstrom coefficient (coincidences with AERONET inversion products within ±0.5° and ±30 min geolocation and for AOD > 0.4 and ΔAOD < 0.2)

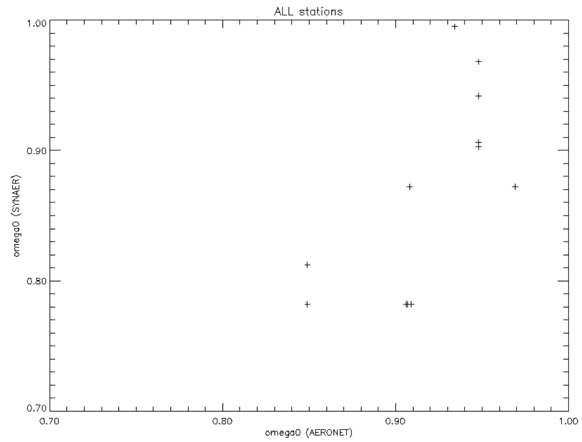

Fig. 11.: aerosol parameter validation of single scattering albedo (coincidences with AERONET inversion products within ±2° and ±120 min geolocation and for AOD > 0.6 and ΔAOD < 0.2)

number	correlation	mean bias	standard deviation
17	0.65	-0.042	0.052

Tab. 8.: validation statistics for single scattering albedo (coincidences with AERONET inversion products within ±2° and ±120 min geolocation and for AOD > 0.6 and ΔAOD < 0.2)

For the single scattering albedo it was necessary to increase the spatial / temporal sampling to ±2° and ±120 min in order to obtain any coincidences at all – this is assumed as possible since the variation of the aerosol type is expected with lower frequencies as AOD variations. Figure 11 and table 8 present the results. Again, the analysis indicates the potential to separate low and high absorbing aerosols but shows also the large scatter.

4. Conclusions

The validation shows for AOD550 an overall correlation of 0.70, a standard deviation of 0.12 and a clear negative bias of -0.06 - in the light of the comparatively large SYNAER pixel size of 60x30 km^2 these results are reasonable . The AOD550 analysis as function of several parameters, of different stations (including critical ones in terms of representativity) and spatial-temporal distance between the SYNAER and AERONET measurements reveals some issues, were further algorithm improvements can be made.

The analysis provided in this report gives the first systematic validation of SYNAER over all seasons and climate zones and several years. Compared to the first and partial validation in Holzer-Popp et al., 2008 a slight decrease in the assessed accuracy is found, but also more detailed insight.

The analysis of 839 coincidences in this report shows that **67% of the pixels** fall within

$$AOD550_{SYNAER} = \pm 0.1 \pm 0.20 * AOD550_{AERONET}$$

The distribution of AOD550 values in the coincidences between SYNAER and AERONET shows a high percentage of low AOD values as expected – there are relatively few pixels with high AOD which is maybe too pronounced – this could be due to problems for larger AOD induced by the polynomial second order fit in radiative transfer or by the underestimated sensitivity of reflectance at 1.6 micron and NDVI especially for large particles.

With regard to the aerosol type estimation in SYNAER multi-spectral AOD as well as fine and coarse mode AOD show similar correlation as AOD550. A first attempt for direct validation of aerosol properties (Angstrom coefficient, single scattering albedo) is made here. This assessment of Angstrom coefficient and single scattering albedo as well as fine / coarse mode AOD is made using AERONET inversion products. It should be noted that the retrieval of these derived parameters depends critically on the underlying AOD550 errors. Therefore, their analysis is initially only done for large AOD550 values and limited AOD errors (ΔAOD < 0.2) to assure sufficient information content in the AERONET inversion and SYNAER retrieval algorithms. First results can not clearly proof the SYNAER capabilities, but show some potential, which should be extended with improved AOD retrieval.

SYNAER is sensitive to the aerosol type through the spectral gradient in the SCIAMACHY measurements at 10 wavelengths from 405 to 670 nm (size mode) and due to the non-linear integration of different pixel sizes with AATSR and SCIAMACHY over heterogeneous surface albedo, i.e. land (absorption). This sensitivity is limited to high AOD and spoiled by significant AOD error. By using pre-defined aerosol types (with linked optical properties) a non-continuous parameter space is tested. On the other hand less variation of aerosol type is expected in space and time which means somewhat less critical sampling aspects. Further work is needed to identify reliable conditions for aerosol properties retrieval with SYNAER. To this end the surface reflectance and elevation heterogeneity within the SCIAMACHY pixel will be stored in future SYNAER version products.

Within MACC no further SYNAER algorithm improvement is planned. The focus will be on producing a multi-annual dataset. For this purpose the current scientific processing system will be improved (increased throughput) and further global processing and validation will be done. SYNAER production within MACC will benefit from further algorithm analysis and upgrades, which are foreseen within the ESA Climate Change Initiative project for aerosols (led by DLR; SYNAER included) – this project is currently in negotiation which are planned to be finalized by 24 June 2010. Within this project also an in-depth analysis of the modules (cloud screening, surface treatment, aerosol model) in different aerosol retrieval algorithms will be done, which will provide further insight into the assumptions made and approaches used in SYNAER.

Evidently, steps to improve SYNAER accuracy are still needed and should be feasible. Among these are improved parametrizations of ocean and land surface albedo (which may include also more sophisticated treatment of bi-directionality as for now only one fixed BRDF for forest is used for all dark fields in SYNAER) and upgrading pre-tabulated radiative transfer calculations. With such improvements AOD550 accuracy should be increased as well as errors in the selection of aerosols types. Also the number of coincidences should increase with better spectral fitting and less need for quality filtering criteria. Another aspect could be a specific increase in high AOD cases (where currently the radiative transfer second order polynomial leads to significant fit errors).

5. Acknowledgements

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6. References

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