**Atmospheric
Chemistry
and Physics
Discussions**

*Interactive comment on* "Observation operator for
the assimilation of aerosol type resolving satellite
measurements into a chemical transport model"
*by* M. Schroedter-Homscheidt et al.

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We again appreciate the helpful comments provided by the ACP reviewers and provide
a point-by-point reply to the reviewers' comments in this document.

Reviewer #1 : 1) Online page 13857, line 10: dust is usually not using databases for
emissions but instead takes modeled winds to define the emission rate

Answer:

This is certainly right. Dust mobilisation is usually modelled by using numerical weather
prediction wind fields together with source region maps describing both natural and

anthropogenic dust sources (e.g. Zender et al., JGR, 108, D14, 4416-4438). These
source region maps can be seen as a 'database' which 'shows deficiencies in spatial
resolution' (as discussed e.g. in Engelstaedter et al., Earth-Science-Reviews, 78, 1-2,
73-100, 2006). The second error source in modelling dust outbreaks are the wind fields
itself and the related parameterisation of dust generation. Emitted mass concentrations
in different size bins shows an uncertainty which is a result of incomplete knowledge
of region mineral dust characteristics in a certain source region (which is again part of
the source region map database).

We add a sentence for clarification purposes in the manuscript:

'Typically, databases show deficiencies in spatial and temporal resolution, quantitative
values and their evolution over time (Memmesheimer et al., 2004). Irregular episodic
events like fires or variable sources in transportation or vegetation can not be modelled
on this basis. Additionally, dust source region databases are typically not detailed
enough in terms of spatial resolution and mineral dust size distribution (Engelstaedter
et al., 2006). Together with uncertainties in the modelled wind and surface stress fields
this results in deficiencies in modelling dust outbreaks as another class of episodic
aerosol events.'

2) Online page 13860, line 25: what if "the uniqueness test" is not passed?

Answer:

Only pixels passing the uniqueness test are used in this study.

Other pixels can be generally used assuming an unknown aerosol type as described
e.g. in Holzer-Popp et al., ACP, 8, 7651-7672, 2008, but are useless in this study
focusing on an aerosol component wise assimilation approach.

A sentence for clarification has been added.

3) Online page 13862, line 21: the statement "not further described" does not quite
make sense to me.

Answer:

The anthropogenic primary fine mode aerosol class is not further described with respect to its chemical composition in the underlying emission data base (http://www.air.sk/tno/cepmeip). It is introduced as a mass balancing aerosol class to cope with the difference of known total particulate emissions and the soot-containing emissions.

We remove the 'not further described' wording in section 2.2 and discuss the issue of unknown chemical composition of primary particles only in section 3.2 when dealing with the question how to set refractive indices.

4) Online page 13863, line 4: why are the 1995 emission used? There has been many studies with updated emissions. Even over Europe, emissions have drastically changed since then.

Answer:

The study uses a EURAD model run for 2003 as we need the three-dimensional mass concentration fields of all internal EURAD model aerosol classes. The standard output of EURAD is only PM10. Therefore, this study can be done either by using this existing 2003 run or by creating a new model run for a more recent period. Due to computational restrictions and unavailability of necessary input data for other periods the latter option was not feasible.

On the other hand we can assume that aerosol emissions have not changed as dramatically as gas phase emissions, perhaps with the exception of anthropogenic secondary organic aerosols. The aerosol emission problem is only part of the deficiency of today's aerosol models to attain observed aerosol levels, as described in the paper.

5) Online page 13867, Equation (4): nothing on the right-hand side depends on "j". Please check all indices and correct.

Answer:

The index j represents the different components – this has been added in the 'for all j components' part of the equation.

6) Online page 13868, line 17: is it "adopted" or "adapted"?

Answer:

Adopted is correct.

7) Online page 13870, line 3: why is that assumption made? It seems to me unnecessary since the amount of aerosols above that level is probably quite small and contributes little to the AOD.

Answer:

Yes, the amount of aerosols is small above 6 km and therefore, the computation is stopped at 6 km. This statement is mentioned to clarify that we don't treat stratospheric aerosols in this model/study. This has been added also in the text.

8) Online page 13870, line 13: could you provide an estimate and a reference for the SOA yields used?

Answer:

The reference Schell et al., 2001 has been given in section 2.2 and is repeated here as a clarification.

9) Online page 13870, line 19: "known with" is better than "known by"

Answer:

Has been corrected.

10) Online page 13872, line 23: what do you mean by "relevant"?

Answer:

'Relevant' means that it should not be neglected in this case. Has been reworded

towards 'should be assessed again in future once large particles in the mineral and/or sea salt components will be assimilated'.

11) Online page 13874, Equation (11): it looks like the indices on the right-hand side should be "i", not "l". By the way, those are somewhat difficult to differentiate. It might be easier to use "m" for example.

Answer:

The index should be "l" both for the left-hand and the right-hand side as it reflects the "l" wavelengths. No "i" is used in this equation. The error has been corrected.

12) Online page 13876, line 8: change "which is might be" to "which might be"

Answer:

Done.

13) Online page 13876, line 9-10: it seems to me that there should be studies (regional or global) available to substantiate the degree to which dust emissions will affect AOD over Europe. It would be nice to include some.

Answer:

We include a discussion on typical dust AOD values at the end of section 2.2 where we already discussed this issue: 'Tegen et al. (1994) report on a European seasonal mean modelled dust AOD based on the NASA-GISS model below 0.05 for the seasons September to November and December to February, while mean AOD increases in summer to values up to 0.1 for March to May and June to August. For sea salt Tegen et al. (1997) report an annual average AOD below 0.08 for Europe. Generally, it has to be noted that dust events have a typical duration of a few days, occur typically at 5-7 % of days in Europe and cause typical mean AOD values in dust cases of up to 0.25 as identified by AERONET and lidar measurements (e.g. Meloni et al., 2007; Papayannis et al., 2008). Individual dust outbreaks reach values between 0.2 and 0.5 in Italy and

Greece, while stations like Leipzig or Kühlungsborn in Germany observe values up to 0.27 and 0.13, respectively. A comparison against SYNAER observations in the study period shows an underestimation of the total aerosol optical depth between -0.01 and -0.1 in 25 % of 24747 coincidences over Europe, while an underestimation between -0.1 and -0.2 is found in 7 % of all cases and a larger underestimation is found in 3 % of all cases.'

14) Online page 13876, line 20: a 0.3 error will only get you so far to remove the 100% or so bias that the model has. Why so low? By the way, a systematic bias might be more easily removed by the use of a bias estimated such as Dee's papers Dee, D. P., and A. M. da Silva (1998), Data assimilation in the presence of forecast bias, Q. J. R. Meterol. Soc., 124, 269– 295. Dee, D. P., and R. Todling (2000), Data assimilation in the presence of forecast bias: The GEOS moisture analysis, Mon. Weather Rev., 128,3268– 3282.

Answer:

As we state in our conclusions a background bias handling scheme has to be developed in future. This should take the model changes into account which were implemented since the ASSET project which run from 2003 to 2006. Therefore, it was decided not to spend further effort in developing a bias handling scheme for the ASSET model version (which we had to take as the existing dataset with the fully resolved aerosol information in the existing output data set).

Also, it should be noted that model biases are variable in daytime and location and also depend on meteorological conditions. The general view is that models are too low, but evidently to a different degree. Both in situ and AERONET ground measurements are available with only a poor spatial coverage not sufficient for a sophisticated bias description. With ENVISAT or METOP overpasses the spatial data coverage is improved, but a bias correction includes always the risk of optimising only for late morning hours as the typical overpass time.

Finally, any bias correction scheme should be based on SYNAER observations with a reduced bias than they have been available for ERS-2. Such observations with a smaller bias are available from ENVISAT in the meanwhile (but this version of data was only made available after this study). The ENVISAT observations used in this study are also affected by a bias and seem therefore not suitable as the basis for a bias correction.

Therefore, we remain with this assumption without giving a deeper scientific motivation than our approach of taking a value for the background error significantly higher than the observations. We think that this is justified as the focus of this study is the development of the observation operator and a first test if the use of aerosol type resolving satellite observations is promising. For the future development a bias assessment/removal scheme based on a larger data set and also based e.g. on 'running bias estimation methods' as described in Dee's papers is foreseen.

We added a comment in the conclusion section: 'For a future operational application of the study results, a background bias correction scheme needs to be developed to ensure the BLUE. It could either be based on an assessment of a long-term dataset or on a continuous bias monitoring scheme as applied e.g. in Dee et al. (1998). It has to be noted that the settings of the background error covariance matrix in this study are preliminary allowing an assimilation experiment within the study and therefore, the assessment of the value of aerosol component distinguishing satellite observations in an assimilation scheme.'

Please refer also to our answer to comment 8 made by reviewer #2 dealing with the same point of setting background and observation covariance matrices.

15) Section 4.1: why is MODIS (or other AOD measurements from satellite) not used here?

Answer:

C8096

This paper deals with an observation operator for aerosol type resolving observations as provided by SYNAER/ENVISAT. MODIS only provides a distinction between fine and coarse mode aerosols, which is still under scientific discussion - Levy et al., ACPD, 2010 even 'recommend that users NOT use size products quantitatively' from MODIS Collection 5.

We add a sentence on 'MODIS based fine and coarse mode observations might be another option in the future, but are still under scientific discussion (Levy et al., 2010)' in our conclusions.

Reviewer #2 1) Online page 860: A formula would help understanding the least square fit.

Answer:

The formula has been added.

2) Online page 863, line 21: "Maritime and mineral aerosol components are not included in the EURAD version used for this study." There should be a discussion about this. This can have significant consequences on the simulations.

Answer:

Our understanding is that we have discussed this to some extent already in the paper (p. 13863 directly after this statement by comparing to total AOD ENVISAT measurements; p. 13876 assessment and interpretation of background error quantification including added reference to Breitkreuz et al., 2009; p 13881 on validation of dust outbreak situation).

We also added a section on typical findings in the literature on aerosol dust loads in the atmosphere in 2.2 (answering also to comment no. 13, reviewer #1; new text is given above).

3) Online page 868, line 22: "Observations are assumed to be uncorrelated to each

C8097

other". Why? This may be questionable because all observations are produced by the same instruments and the same algorithms.

Answer:

Kokhanovsky et al. (2007) showed a 1% agreement of the calibration among the EN-VISAT instruments SCIAMACHY and MERIS. Therefore, we assume that there is no gross calibration error affecting all observations. Generally, aerosol retrieval schemes are ill-posed causing that pixel to pixel error correlations are negligible compared to other retrieval assumptions applied in the surface reflectance estimation and the aerosol model. Therefore and having in mind that this is a first assimilation study, observations are assumed to be uncorrelated to each other resulting in diagonal covariance matrices. The text has been changed accordingly.

4) Online page 868, line 24: please give the formula.

Answer:

Following Weaver and Courtier (2001) we would need to copy large parts of their paper into this text to give understandable and complete formulas. They use a rewritten version of the cost function and its gradient providing a preconditioning by using B1/2 together with an operator-based representation of the background error covariance. The implementation chosen has been described in detail (over 2.5 pages) in Elbern et al., 2007. This paper has been added as a citation.

5) Online page 869, line 1: Why the correlation length (actually, decorrelation length) for AOD is taken as (de)correlation length for *errors* in AOD?

Answer:

We interpret the correlation length as derived by Anderson et al. as a measure of typical spatial AOD variability. We assume that the test of an influence radius in the assimilation scheme above this range is not necessary. Therefore, we restrict our tests to a range below this variability range. We find that setting the influence radius in the

error diffusion approach to 1.0 grid boxes results in optimum validation results.

The text has been reworded accordingly.

By the way, we corrected an error in the original manuscript in this section. 0.5 grid boxes have been applied in first assimilation tests using ERS SYNAER observations and a previous model resolution of 125km. This was mixed up with the 56 km grid box size EURAD version which has been used for all ENVISAT-based results shown in this paper.

6) Online page 872, line 20: this step seems to make the observation operator non linear. If so, it should be mentioned.

Answer:

Yes, observations with a large disagreement in their size distribution versus the current model state introduce the risk of violating the linear approximation. Therefore, we point out that this effect has to be assessed for each assimilation exercise. We propose a pre-processing and quality control step to exclude observations affected by this situation.

We added two comments about the potential of violating the linear approximation and the need for pre-processing and quality control schemes in a later operational scheme in the text.

7) Online page 873, line 4: the statement is too optimistic. I suggest to reword. If I understand correctly, 18% of AODs have an error greater than 50% of the target average error. This is not negligible. The error may be neglected in the present study, nonetheless it should not be qualified as negligible.

Answer:

Certainly this effect is not negligible and we don't intend to give this impression. Therefore, it has been evaluated and we state in the previous section and also in the conclu-

sions that this effect should certainly be taken into account as soon as large particles will be assimilated. It should be included in an appropriate pre-processing and quality control step in later operations. This comment has been added to the manuscript text. Nevertheless, we feel still confident that within the objectives of our study this can be neglected.

8) Online page 875, line 13: if 0.12 is the RMSE, it cannot be the diagonal of the matrix R. R is a variance and the RMSE can be identified to the standard deviation (if there is no bias).

Answer:

Sections 3.3.1 and 3.3.2 deal with quantification of observation errors mainly. In the concluding part of each section we falsely described a standard deviation as a variance. This has been reworded by adding a $(\ldots)^2$ to both the value of 0.12 discussed in section 3.3.1 and to the value of 0.3 discussed in section 3.3.2.

Rewiever:

In addition, the authors should comment why they use the RMSE with AERONET data, without discounting the error in AERONET measurements. Likely, they assume that the error in AERONET is negligible compared to that of SYNAER, which is supported by earlier considerations but should be written explicitly in this paragraph.

Answer:

Yes, a sentence has been added: 'Additionally, it is assumed that the error in AERONET is negligible compared to the bias found for SYNAER.'

Reviewer:

Finally, there should be a discussion about the bias. In their data assimilation approach, observations should be unbiased. But here, the bias does not seem negligible at all. The bias is -0.08, which is comparable to the standard deviation of 0.1, and it is 30%

of the mean before the quality control. I understand it is difficult to apply rigorously the chosen data assimilation procedure, and I think it is acceptable here. However this issue should be explicitly noted. Future work should remove the bias in some preprocessing stage or more powerful assimilation schemes should be used. There is just a discussion later for the background. The observation part should be mentioned as well.

Answer:

We included a discussion of the observation part already in the conclusion section of the original manuscript. But for clarification we follow the reviewer's advice and report about this already in section 3.3.1:

'Compared to the 0.1 target accuracy of nowadays satellite retrieval scheme the bias is rather small and therefore neglected here even if it is close to the standard deviation found. It should be noted that a recent validation of SYNAER version 2.2 observations has shown a reduced bias of -0.01 (instead of -0.08 for the SYNAER version 1.8 used in this study) and an improved standard deviation of 0.08 (Holzer-Popp et al., 2008).'

9) Online page 877, line 3: what does "coincidences" mean? This is not a lot of observations, compared to the 2268 "coincidences" mentioned earlier. How are the 189 coincidences found? Explanations are needed. Every time an observation is available, an analyzed field can be computed. One the one hand, an AERONET observation may be far from the locations observed by the satellite. In this case, the analysis is essentially the same as the background. On the other hand, how the corrections are spatially distributed in space is important. Thus one should not compare only in the grid cells where there is a SYNAER observation.

Answer:

189 coincidences are found if a non-zero analysis increment is taken as criterion to identify AERONET measurements in the vicinity of an ENVISAT observation. Spatially

distributed corrections have to be analysed in principle, but due to the sparse orbit pattern of ENVISAT this is only meaningful for a future (and foreseen) use of METOP. In this study, it has been found that the impact of assimilation is diluted by many grid boxes without any influence of any observation in its vicinity. Assessing spatial distributions based on ENVISAT observations would merely result in a mapping of satellite tracks than of physically meaningful spatial patterns.

We added a general comment at the beginning of section 4:

'Due to the low repetition frequency of ENVISAT (12 days with cloud-free conditions and less due to clouds) and the restricted number of available observations an overall impact of the assimilation can hardly been seen. Assessing spatial impact distributions based on ENVISAT observations would result merely in a mapping of satellite tracks than resulting in physically meaningful spatial patterns. It has to be noted that a future METOP assimilation will rely on a significantly larger number of observations. Therefore, further validation is performed only in the vicinity of existing SYNAER observations which might cause any positive or negative impact. Only grid boxes with non-zero analysis increment are taken into account. Non-zero analysis increment grid boxes occur due to a finite number of diffusion time steps. This criterion excludes situations where background and observations agree fully, but this occurs only in 0.04 % of all cases. This is also justified as these cases would not contribute to any impact on the assimilation result.'

And another comment has been added in the conclusions section:

'Due to the sparse data availability of ENVISAT all comparisons are made only in the vicinity of observations, which is classified by an analysis increment above zero.'

10) Online page 877, line 11: how is it possible that the analysis increment is zero? Is there some clipping in the values of B?

Answer:

C8102

The background error covariance matrix is modelled with a diffusion approach describing the spatial distribution of the observation's influence. Following Weaver and Courtier (2001) and Elbern et al. (2007) a length scale L of the diffusion equals $(2\kappa T)1/2$ with $\kappa \geq 0.2$ and T being the diffusion time. By setting L as external parameter the diffusion time is defined implicitely. During each diffusion iteration step the diffusion operator acts only on neighbouring pixels and after T time steps the diffusion stops. Areas outside the influence radius of an observation are changed only slightly following a Gaussian shape. Having a discrete number of diffusion time steps, this results in grid points where the analysis increment is zero. In the paper we introduced a sentence: 'Non-zero analysis increment grid boxes occur due to a finite number of diffusion time steps.'

Minor remarks

1) Online page 857, line 12: replace "methodologies" with "methods" or "methodology".

Answer:

Done both in section 1 and 4.1.

2) Online page 857, line 26: there are 6 references to papers of the second author and 6 references to the work of the rest of the community. Although the second author did a good job in the field, I think his contribution is far from deserving half the citations for such a generic topic (assimilation in chemical transport modeling).

Answer:

Has been reduced to the most relevant three papers.

3) Online page 859, line 25: what does "internal" mean?

Answer:

The study relies on the availability of three-dimensional mass concentration fields of all EURAD model aerosol classes, while the standard output of the operational EURAD

C8103

model version provides only PM10. As the mass concentration fields are not part of they standard output, we called them 'internal' model variables. This has been replaced by the complete explanation.

4) Online page 862, line 18: replace "km" with "kilometers".

Answer:

Done by writing 'grid size down to 1 km'.

5) Online page 863, line 26: it is not clear what "in the meanwhile" means.

Answer:

The EURAD model version used in this study originates from the ASSET project (2003-2006). Since then further model improvements have been implemented. A clarification has been included in the 'study setup' section.

6) Online page 869, line 3: "approximately the SYNAER pixel size" in one direction, and half the size in the other direction.

Answer:

Changed – see comment 5.

7) Online page 871, line 18: "speciese"

Answer:

Done.

8) Online page 872, line 7: replace "methodology" with "method"

Answer:

Done.

9) Online page 873, line 15: I suggest to replace "a negligible low probability" with "a

negligible probability".

Answer:

Yes.

10) Online page 874, line 14: the second sum in the inequality depends on l, not on i.

Answer:

Yes, has been corrected.

11) Online page 875, line 17: why referring to "coincidences"? The model is available all time and everywhere in the domain. Only AERONET is limiting here.

Answer:

A coincidence is meant as a model grid box containing an AERONET measurement within 9 and 11 UTC. In case of several AERONET measurements within this time period, the closest measurement has been chosen. Depending on AERONET availability there are EURAD model grid boxes without any ground measurement. The text has been extended to describe the temporal selection window further.

12) Online page 879, line 1: what does "impact" refer to?

Answer:

Impact is understood as an improvement in statistical measures – the text has been reworded.

13) Online page 879, line 21: replace "und" with "and".

Answer:

We have searched for this error in the whole manuscript and corrected it.