ASSIMILATION OF SATELLITE-BASED AEROSOL MEASUREMENTS IN A CHEMICAL TRANSPORT MODEL USING AEROSOL COMPONENT INFORMATION

Dmytro Martynenko(1), Thomas Holzer-Popp(1), Marion Schroedter-Homscheidt(1)

(1)Deutsches Zentrum für Luft- und Raumfahrt (DLR) e.V., Deutsches Fernerkundungsdatenzentrum (DFD), Oberpfaffenhofen, D-82234 Wessling, Germany. Email: dmytro.martynenko@dlr.de

ABSTRACT

Aerosol monitoring is of growing interest in atmospheric physics and chemistry research area due to the impact of aerosol particle concentration on human health and the global climate. The key question of this paper is how the assimilation of satellite atmospheric aerosol observations improves the capability of a chemical transport model in reproducing the distribution of tropospheric particles. The study is carried out using the Model for Atmospheric Transport and Chemistry (MATCH).

Synergetic Aerosol Retrieval (SYNAER) observational and model MATCH data can be coupled by means of data assimilation. MetOp-SYNAER measurements are able to distinguish between different aerosol components such as water-soluble, soot, sea salt and long-range transported mineral aerosols. Therefore, a component-wise assimilation approach is under development. During the assimilation procedure, the final analysis is highly dependent on the specification of the relative weights to both model and satellite source of information through the error covariance matrices. Since observation and background error covariance matrices are not perfectly known, a large potential for improvements of the analyses is offered by methods allowing their constructing and tuning. In this study, the method proposed by Desroziers and Ivanov [4] is used to tune background and observational error statistics of the 3D-Var assimilation procedure.

1. INTRODUCTION

In this paper the information content of reflectance measurements in the wavelength bands used in SYNAER is investigated. The number of Degrees of Freedom of the Signal (DFS) and the separable aerosol components are quantified by applying an information content analysis to synthetic reflectance spectra for a large number of scenarios with various aerosol models, observation geometries and surface types. The information content theory after [10] was applied in an unusual way, namely to independently assess the information content of the existing retrieval method and discern the input of different aerosol types in the measurements. This point of view on the retrieval problem allows concluding some facts about capabilities and limitations of SYNAER to estimate aerosol composition. The results of the information content analysis are immediately applicable to the SYNAER algorithm, since the DFS analysis is applied to the synthetic reflectance data stored in the Look-Up Tables (LUT) of SYNAER. The results of the DFS analysis depend on the aerosol parameter ranges covered by the set of aerosol models considered. The basic assumption made in this study is that the aerosol models cover the natural variability of tropospheric aerosol. The number of DFS obtained is representative for the number of aerosol parameters that can be retrieved independently from reflectance measurements provided that the surface albedo spectrum is accurately known and the presence of clouds can be completely excluded or corrected, see [7].

Model based data assimilation aims to make use of all information sources: that is, those provided by measurements and models.

Both model based chemistry data assimilation and complex aerosol modelling in full-fledged air quality models are emerging issues of only recent years. As both disciplines are challenging in terms of development and computational demands, the attempt to combine state of the art chemistry data assimilation methods with state of the art aerosol modules together with advanced satellite retrieval method for extracting aerosol type information has not yet been made. Rather, all these lines of development evolved separately, and aerosol assimilation studies so far dedicated sophistication to either side.

For example in [3] the authors applied the MATCH model, in which sulphate, black carbon, organic carbon and mineral dust are predicted while sea salt aerosols are diagnosed. As assimilation scheme optimal interpolation is applied; the assimilation parameter is the aerosol optical depth (AOD) from NOAA AVHRR over ocean.

The second task of this paper is application of DFS analysis in the assimilation procedure for SYNAER observational data and model data from DLR/MATCH.

Traditionally data assimilation results from different retrieval and model platforms are heuristically validated by withholding a few observations from assimilation and use them for estimating improved analyses or forecasts. While these tests are helpful, no indication is given whether necessary (but not sufficient) conditions in defining covariances are fulfilled. To this end, the a

Proc. '19th ESA Symposium on European Rocket and Balloon Programmes and Related Research, Bad Reichenhall, Germany, 7–11 June 2009 (ESA SP-671, September 2009)

posteriori diagnosis tests compliances with necessary conditions, whether consistency between data and analysis results is attained after the assimilation procedure or not. In a paper [10] demonstrated an a posteriori verification of assimilation success, by statistical evaluation of differences between observations and analyses. The methodology has been further extended by [1], [2], [4], and [5]. Given the various different measurement devices, a special difficulty in assimilating optical thickness data and lumped in situ from different data sources is the quantification of the relative influence of each observation type on the assimilation result. In the case of the present work objectives especially the information values of the aerosol component resolved information from SYNAER can be estimated.

2. RETRIEVAL METHOD SYNAER

At the German Remote Sensing Data Center (DFD) the aerosol retrieval method SYNAER was developed [7] which delivers boundary layer aerosol optical depth and type over both land and ocean, the latter as percentage contribution of 9 representative components based on the OPAC (Optical Parameters of Aerosols and Clouds, [6]) dataset to AOD. The SYNAER method consists of two parts. In the first part the AVHRR radiometer data are used to retrieve aerosol optical depth and surface reflectance for a selected aerosol type. In the second part the spectrometer data are then used to select the most plausible aerosol type. As the estimation of the aerosol type is the most innovative part of SYNAER, a study provided an analysis of the information content of the second SYNAER part with regard to aerosol composition following [9]. Consequently, the focus of this analysis was on exploiting the spectrometer measurements explicitly using the results of the first retrieval step, namely aerosol optical depth at 0.55 µm and surface reflectance at 0.55, 0.67 and 0.87 µm for each aerosol mixture. In the analysis of the information content 9 basic components (water soluble, water insoluble with high and low hematite content, sea salt accumulation and coarse mode, anthropogenic soot, biogenic soot and mineral dust with high and low hematite content) were used to define a set of 40 mixtures (see Tab. 1), which was then applied to radiative transfer calculations of simulated GOME-2 spectra.

Table 1. Pre-defined external aerosol mixtures of the basic components which are used in SYNAER. Adapted from [7]. WA = watersoluble, IN = insoluble, SS = sea salt, SO = soot, MI = mineral dust

	Component contributions to aerosol optical depth (AOD) at 0.55 µm [%]				
Name	WA	IN	SS	SO	MI
Pure water-soluble	100				
Continental	95	5			
	90	10			
	85	15			
Maritime	30		70		
	30		70		
	15		85		
	15		85		
Polluted water-soluble	90			10	
	80			20	
Polluted Continental	80	10		10	
	70	10		20	
Polluted Maritime	40		50	10	
	30		50	20	
Desert Outbreak	25				75
	25				75
	25				75
Biomass Burning	85			15	
	70			30	
	55			45	

3. ANALYSIS OF INFORMATION CONTENT

The method used to examine and analyse the information content is the singular value decomposition (SVD). The following theoretical description is based on the inverse methods methodology of Clive D. Rodgers, [10]. SVD is a useful tool to identify the dominant parts of the observations. This allows identifying the number of parameters which can be retrieved from observations and analysing the separability of the variables retrieved. Generally, the number of observations does not equal the degrees of freedom because not all observations are independent.

For any remote measurement, the measured quantity, $\boldsymbol{y}$, is a vector-valued function $\boldsymbol{F}$ of the unknown state vector $\boldsymbol{x}$, and of a set of other parameters $\boldsymbol{b}$ excluded from the state vector, considering also the experimental error term $\boldsymbol{\varepsilon}$:

$$y = F(x,b) + \varepsilon \tag{1}$$

where $\boldsymbol{y} \in \boldsymbol{R}^{m}$ is the measurements vector of dimension $\boldsymbol{m}$, i.e. reflectances at m wavelengths; $\boldsymbol{x} \in \boldsymbol{R}^{n}$ is the state vector of dimension $\boldsymbol{n}$; $\boldsymbol{b}$ is the vector containing all the other parameters necessary to define the radiative transfer through the atmosphere to the spacecraft, $\boldsymbol{F}: \boldsymbol{R}^n \to \boldsymbol{R}^m$ is the forward model that describes the physics of the measurements that map from the state space to the measurements space and $\boldsymbol{\varepsilon} \in \boldsymbol{R}^m$ is the measurement error vector.

The measurement vector for this theoretical analysis of the SYNAER retrieval consists of simulated spectra at 10 (m = 10) wavelengths for 40 (n = 40) different aerosol mixtures for a given surface type. The state vector consists of 40 elements corresponding to the different aerosol mixtures from the 9 basic components. For the purpose of information content and error analysis it is necessary to linearize the forward model around some reference state $\boldsymbol{x_0}$:

$$y - F(x_0) = \frac{\partial F}{\partial x}(x - x_0) + \varepsilon = K \cdot (x - x_0) + \varepsilon \qquad (2)$$

where $\boldsymbol{K}$ is the weighting function matrix of dimension $\boldsymbol{m} \times \boldsymbol{n}$. Each element of $\boldsymbol{K}$ is the partial derivative of a forward model element with respect to a state vector element:

$$k_{ij} = \frac{\partial F(x)_i}{\partial x_j}; \forall i = 1..m, \forall j = 1..n \qquad (3)$$

The act of measurement maps the state space into the measurement space according to the Forward Model. Conversely, a given measurement could be the result of a mapping from anywhere in the state space. It is necessary to have some prior information about the state, which can be used to constrain the solution.

The information content can be condensed into the Degrees of Freedom for Signal (DFS). DFS can be interpreted as the number of independent linear combinations of the state vector that can be independently retrieved from the measurements. It is given by:

$$DFS = \sum \frac{\lambda_i^2}{1 + \lambda_i^2} \qquad (4)$$

where $\boldsymbol{\lambda_i}$ are the singular values of $\boldsymbol{(S_\varepsilon)^{-1/2} K (S_a)^{1/2}}$.
$\boldsymbol{S_\varepsilon}$ and $\boldsymbol{S_a}$ correspond to measurement covariance and a priori covariance matrices.
DFS as a function of AOD is given at Fig. 1. With the growing of AOD, the growth of the DFS values is relative fast. This means that SYNAER retrieval algorithm should show adoptable results also for the small values of AOD. Already at AOD = 0.2 the curve on Fig. 1 shows the saturation at about DFS = 4. The offset of the additional 2 DFS at the beginning on this and following figures supposed to correspond to the different choice of surface type and AOD. Degrees of freedom also depend on such parameters as sun elevation angle and surface type. Fig. 2 describes DFS dependency from sun elevation angle and AOD. The nonmonotone growth of DFS regarding to sun elevation angle is supposed to be due to phase function. The blue points on Fig. 2 correspond to the DFS values from Fig. 1.

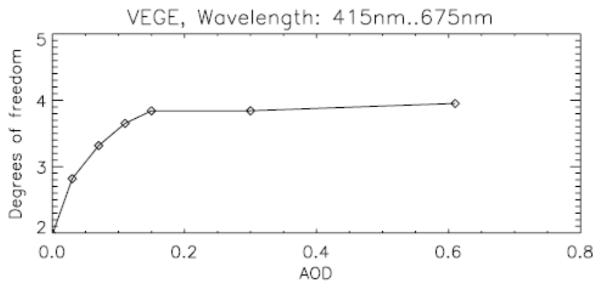

Figure 1. Degrees of freedom as function of aerosol optical depth for solar zenith angle 42.5° and surface type “vegetation”.

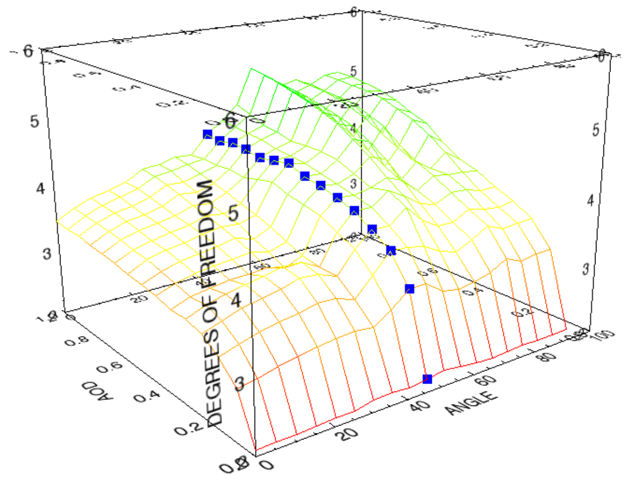

Figure 2. Degrees of freedom as function of aerosol optical depth and solar zenith angle for surface type “vegetation”. The blue dots indicate the line of Figure 1.

4. MODEL FOR ATMOSPHERIC TRANSPORT AND CHEMISTRY (MATCH)

The DLR/MATCH [11] is a three-dimensional global transport model predicting an external aerosol mixture containing sulphate, black and organic carbon and mineral aerosols. Sea salt aerosols are treated only in the diagnosis mode without any transport. Nitrate aerosols are not taken into account. DLR/MATCH is an offline model using NCEP operational or reanalysis meteorological fields as meteorological driver every 6 hours, but not at each time step like an online model. The model can be operated in a 0.7, 1.4 or 1.9 deg

resolution and includes parameterizations of all major physical processes, i.e. convection, large scale precipitation, shallow convection, gravity wave drag, radiation with diurnal cycle and interaction with clouds, boundary layer physics, an interactive surface hydrology and vertical and horizontal diffusion processes.
A two years lasting period of MATCH modelling was performed at the German Remote Sensing Data Centre (DFD), department for Climate and Atmospheric Products at the German Aerospace Centre (DLR). Part of this dataset states the main database for the investigations presented in section 5.

5. ASSIMILATION OF SATELLITE–BASED AEROSOL MEASUREMNTS FROM SYNAER IN MATCH

The method of 3Dvar is based on minimising a cost function J(x), that weights the measurements against the model background. It is set up in the following manner:

$$J(x) = J_0 + J_B = \frac{1}{2}\left[(x_b - x)^T B^{-1}(x_b - x)\right] + \\ + \frac{1}{2}(y - H(x_0))^T R^{-1}(y - H(x_0)) \quad (5)$$

x: current model state; $\mathbf{x_b}$: background state; **B**: background error covariance matrix; y: measurement; **H**: observation forward operator; **M**: model operator; **R**: Observation error covariance matrix.

Equation (5) is the full cost function for 3Dvar. In 3Dvar **N** equals 0 and a model operator is not needed, since assimilation is preformed for a fix point in time. In the case of SYNAER data assimilation into DLR/MATCH 3DVAR procedure is considered.
The cost function is then minimised by iterative application of a Newton - minimisation -algorithm, the LBFGS (Limited memory Broyden-Fletcher-Goldfarb-Shanno). Finally, the analysis (the result of assimilation) delivers the estimate of the state of the aerosol load of the atmosphere at a certain point in time.
A special focus must be set on the derivation or generation of the **B** and **R** – background and observation error covariance matrices. These matrices are the most critical part of the cost function, in generation as well as in application.
Following [4] the tuning of these matrices can be applied:

$$B^t = s_b^t \cdot B^{t-1} \qquad R^t = s_o^t \cdot R^{t-1} \quad (6)$$

where:

$$s_o^t = \frac{2E(J_o^{\min})^t}{\dim(I_N) - Tr\left(\frac{\partial Hx}{\partial y}\right)^t} \quad (7)$$

$$s_b^t = \frac{2E(J_b^{\min})^t}{Tr\left(\frac{\partial Hx}{\partial y}\right)^t} \quad (8)$$

here: **E( )** – mathematical expectation, **x**: current model state; **y**: current satellite measurement state; **H**: observation forward operator; $\mathbf{I_N}$ – identity matrix of dimension **N**. **t** – assimilation iteration number.

Some results of assimilation with such a tuning technique are given in Fig. 3. Based on [4] newly adapted background and observation error covariance matrices were used to characterize the relative weighting of data and model in this case study. The first column in the image consists of SYNAER-MetOp aerosol optical depth values at 550 nm for two major aerosol components mineral dust in upper figure and sea salt in the lower figure. The respective DLR/MATCH model output with 1.9°-horizontal resolution for these components with data assimilation of SYNAER data is shown in column 2. A slight increase of sea salt aerosol optical depth values is monitored, whereas mineral dust shows regional decrease and increase by the available SYNAER dataset at this date. Using the bright surface type information of the considered satellite pixels assimilation input is computed with the help of enhanced error covariance matrix correction from Section 5 and shows only slight increase (in the case of sea salt) and decrease (in the case of mineral dust) for aerosol optical thickness values.

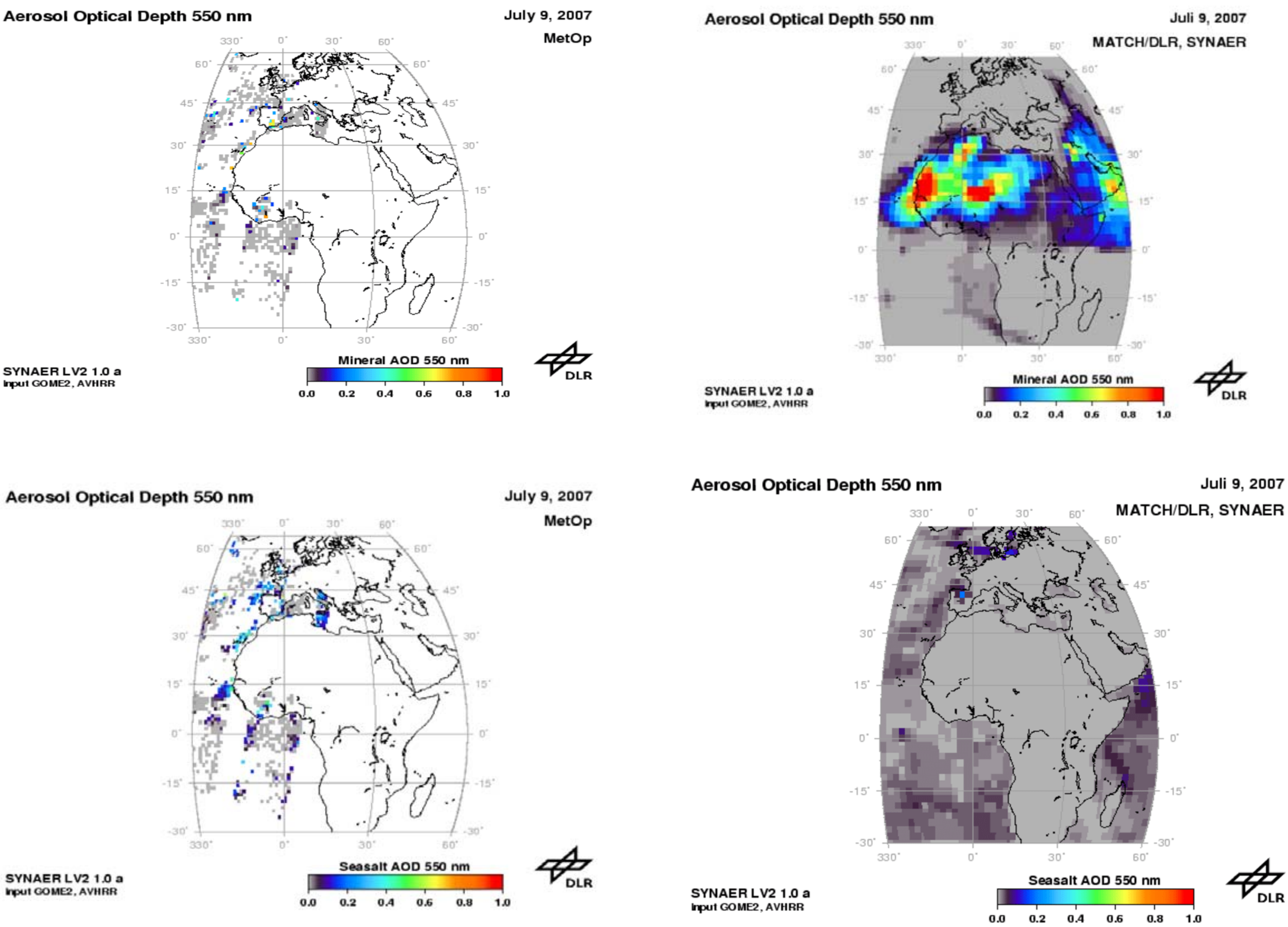

Figure 3. An aerosol retrieval method SYNAER applied to MetOp instruments AVHRR/GOME-2 was combined with a chemical transport model MATCH/DLR with the help of an advanced data assimilation procedure.

6. CONCLUSIONS

A theoretical analysis of the information content with regard to aerosol composition of the methodology was conducted to understand the capabilities of using retrieval algorithm and to assess the limitations of this approach. The results of the DFS-analysis can be used in assimilation procedure in order to enhance the error covariance matrices. Techniques to evaluate the quantification of the impact of the observations, known as DFS, have been implemented for the DLR/MATCH-SYNAER data assimilation system. The balloon flights can be conducted at different latitudes and seasons in order to allow validating the products for a manifold of different retrieval conditions. For the future validation and advancement of the retrieval procedure by balloon-borne measurements in troposphere can be potentially considered.

7. REFERENCES

1. Chapnik B., Desroziers G., Rabier F. and Talagrand O.. (2004): Properties and first applications of an error statistic tuning method in variationnal assimilation. *Quart. J. Roy. Meteor. Soc*., 130, no. 601, pp. 2253-2275

2. Chapnik B., Desroziers G., Rabier F. and Talagrand O.. (2005): Diagnosis and tuning of observational error statistics in a quasi operational data assimilation setting. *Quart. J. Roy. Meteor. Soc.*

3. Collins, W. D., Rasch, P. J., Eaton, B. E., Khattatov, B. V., Lamarque, J.-F., and Zender, C. S. (2001). imulating aerosols using a chemical transport model with assimilation of satellite aerosol retrievals: Methodology for INDOEX. *Journal of Geophysical Research*, 106, No. D7:7313{7336.

4. Desroziers G., Ivanov. S. (2001), Diagnosis and adaptive tuning of information error parameters in a variational assimilation. *Quart. J. Roy. Meteor. Soc.*, 127, 1433-1452.

5. Desroziers, G. , Berre, L., Chapnik, B., Poli, P. , (2005): Diagnosis of observation, background, and analysis error statistics in observation space. *Quart. J. Roy. Meteorol. Soc.*

6. Hess, M., Koepke, P. , and Schult, I. (1998): Optical properties of aerosols and clouds: The software package OPAC, *Bull. Am. Meteorol. Soc.*, 79(5), 831–844.

7. Holzer-Popp, T., Schroedter, M., and Gesell, G. (2002a): Retrieving aerosol optical depth and type in the boundary layer over land and ocean from simultaneous GOME spectrometer and ATSR-2 radiometer measurements, 1, Method description, *J. Geophys. Res.*, 107(D21), AAC16-1–AAC16-17.

8. Holzer-Popp, T., Schroedter, M., and Gesell, G. (2002b): Retrieving aerosol optical depth and type in the boundary layer over land and ocean from simultaneous GOME spectrometer and ATSR-2 radiometer measurements, 2, Case study application and validation, *J. Geophys. Res.*, 107(D24), AAC10-1–AAC10-8.

9. Holzer-Popp T., Schroedter-Homscheidt, M., Breitkreuz, H., Klüser, L., Martynenko, D. (2008): Improvements of synergetic aerosol retrieval for ENVISAT, *Atmospheric Chemistry and Physics*, 7651-7672.

10. Rodgers, C. D. (2000), *Inverse methods for atmospheric sounding*, Theory and Practice,World Scientific Publishing Company, London, UK, ISBN 981-02-2740-X.

11. M. Schroedter-Homscheidt, A. Hartmann (2009): Standardisierung der Energieertragsprognose für solarthermische Kraftwerke (SESK), Report AP 7300.

12. Talagrand. O. (1999): A posteriori verification of analysis and assimilation algorithms. *In Proceedings of the ECMWF Workshop on Diagnosis of Data Assimilation Systems*, pages 17--28, Reading, November 1999.