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Background error statistics for aerosols

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Abstract

As part of the European initiative for Global Monitoring for Environment and Security (GMES), the Global and regional Earth-system Monitoring using Satellite and in-situ data (GEMS) project has been funded to provide forecasts and analysis of atmospheric constituents such as aerosols, and greenhouse and reactive gases. In this context, the development of an aerosol analysis system based on four–dimensional variational (4D–Var) assimilation was started in March 2005 at the European Centre for Medium–Range Weather Forecasts (ECMWF). Among the main building blocks of the system, an error background covariance matrix for aerosol mixing ratio was built based on background statistics constructed from aerosol forecasts. These statistics were generated from the differences between the 48h and 24h forecasts of aerosol mixing ratios for sea–salt, desert dust and continental particulate, using the NMC method. This method has been widely used by many Numerical Weather Prediction Centres to build background error statistics for state variables. This is the first time, to our knowledge, that it is applied to a novel variable such as aerosol mixing ratio, in the context of a global model. Aerosol assimilation systems have been successfully run with either observationally–derived or model–prescribed error covariance matrices with pre–assigned correlation lengths. In this study, the aerosol vertical and horizontal structures of these error correlations as derived with the aid of a state-of-the-art model are investigated and discussed in depth. Successively these error correlations are modelled through a spectral/wavelet approach and used to construct a background error covariance matrix. Application of this background matrix in the context of a single observation 4D–Var experiment produced successful preliminary analyses of total aerosol mixing ratio.

1. Introduction

Monitoring of atmospheric aerosol has recently been acknowledged as a fundamental component of environmental monitoring due to the role that aerosols play in regional air quality and the related implications for human health. Knowledge of aerosol characteristics has also been proven important for the correct interpretation of satellite data commonly used in atmospheric, land and ocean applications. Moreover, it has been recently shown that a correct description of aerosols can improve weather forecasts on a global scale by reducing errors in precipitation and wind (Rodwell, 2005). Regional–scale impact has also been shown in the improved description of the low–level East–African jet and the African monsoon thanks to a better desert dust climatology (Tompkins et al., 2005). Aerosols have also been under the spotlight of climate research for a number of years due to their impact on the radiative balance and their interaction with other radiatively/dynamically active components of the Earth's system such as clouds (Haywood and Boucher, 2000). Much uncertainty still remains on their net radiative effect and research is ongoing to quantify aerosol properties and their impact on weather and climate using advanced models and new observations from in situ and spaceborne instruments (Kaufman et al., 2002).

As part of this scientific effort, the European Union funded GEMS (Global and regional Earth-system Monitoring using Satellite and in-situ data) to create a new European operational system for global monitoring of atmospheric chemistry and dynamics and to produce improved medium–range and short–range air–chemistry forecasts, through improved exploitation of satellite and in–situ data. The project is in its second year, and the building blocks for a forecast and analysis system which would include atmospheric constituents are already in place. The premises for these systems are the operational ECMWF Integrated Forecasting System (IFS) and the incremental 4D-Var system, extended to include new prognostic variables for the atmospheric tracers (i.e. gases and aerosols). In this paper, we will focus mainly on the developments in the aerosol analysis system, in particular on an essential component of the analysis: the background error matrix. We will also briefly present the changes to the IFS for the implementation of aerosol forecasts, instrumental to the creation of the background statistics presented here.

The problem of defining appropriate background statistics is central to any data assimilation technique, and many authors recognize the importance of a correct definition of these statistics (Fisher, 2003; Rabier et al., 1998). At the core of the variational assimilation is the minimisation of a cost function defined as the sum of the quadratic distance between the observations and their model counterpart, and of the background term, weighted by their respective error covariance matrices. In the variational context, it is primarily the background error covariance matrix that determines how information from observations is spread to nearby model grid–points and levels. However, there are many challenges in defining background statistics, especially for variables which are newly introduced into a specific analysis system. Most commonly, a number of assumptions have to be made.

Specifically for aerosols, successful analyses have been obtained using the four–dimensional variational technique (4D–Var) (Fonteyn et al., 2000; Errera and Fonteyn, 2001), Kalman filter (Weaver et al., 2005) and Optimal Interpolation (Collins et al., 2001) . In these studies, the background statistics were prescribed either by using *ad hoc* diagonal matrices without accounting for horizontal and vertical background error correlations as in Weaver et al. (2005) or by assigning a vertical and horizontal correlation length in observation space as in Collins et al. (2001). Fonteyn et al. (2000) derived the surface aerosol background and its error covariance by interpolating observations, and included temporal correlations. However, they concluded that this temporal variability was not large enough due to poor data coverage. Moreover they found that the aerosol field from the transport model exhibited a larger variability than the background which was more representative of a climatological average. While all these methods are a viable solution to test the feasibility and the value of an aerosol analysis, for an operational system there is the need to provide error statistics that are representative of the short-term error forecasts which are the used as “background” in the variational assimilation. An overview of methods to diagnose background error statistics for application in Numerical Weather Prediction (NWP) is provided in Fisher (2003). The main approaches are either based on innovation statistics, i.e. observations minus model differences at observation locations, or on model fields generated on the model grid and whose statistics are assumed to be similar to those of the background error. An example of the first category of approaches is the (Hollingsworth and Lönnberg, 1986) method which consists in assuming that the observations are uncorrelated and in plotting the innovation statistics as a function of the distance between pairs of observations. While this allows the relative contribution of background and observation errors to the variance of the innovations to be estimated, it requires a high–density, good quality observing network, which might not be available globally. Moreover the method provides estimates for observed variables rather than model variables which makes it unusable for variables related to radiance observations such as aerosols. Of the second category of approaches, those based on model fields, the most used is the Parrish and Derber (1992) method (also known as NMC method). This method consists in taking the differences between forecasts of different length that verify at the same time, and assumes that this represents a good sample for the background error. The pairs of forecasts typically used are 48 and 24 hours, to minimise the chance of erroneously incorporating aspects of the diurnal cycle into the background errors and to reduce the risk of spurious “spin–up” effects. The main advantage is that the forecasts required to calculate the statistics are readily available, even for new prognostic model variables, provided those are prognostic variables. For this reason it was chosen in this study to build the background statistics for the aerosol variables recently introduced in the ECMWF model as part of the forecasting component of the GEMS project (Morcrette et al., 2005/6). This is the first attempt, to our knowledge, to create background error statistics from a forecast model and from those a background covariance matrix for aerosol mixing ratio.

Section **2.** presents an overview of the aerosol model adapted to the ECMWF Integrated Forecasting System (IFS). The experiment set–up is introduced in section a., while the general methodology and results for the background error statistics for aerosol mixing ratio, obtained using the the Parrish and Derber approach, are presented in section **3.**. A “pre-operational” background error covariance matrix for aerosol is then constructed (section **4.**) and used in a single observation experiment performed using the ECMWF incremental 4D–Var system to show the applicability of these statistics for the assimilation of aerosol observations (section **5.**).

Potential improvements and future perspectives are discussed in section 6., along with a summary of the main findings.

2. Prognostic aerosols for a global weather forecasting model

The aerosol component of the GEMS project consists mainly of four tasks: (i) the definition of aerosol emission sources; (ii) the modelling of aerosol transport and physical processes using the ECMWF IFS; (iii) the assimilation of aerosol–related observations using the ECMWF 4D–Var, extended to include new control variables; and (iv) the verification and validation of the aerosol forecasts and analysis. Task (ii) has involved the introduction of new prognostic variables (i.e. aerosol mixing ratios) in the ECMWF model and the definition of aerosol–specific physical parameterisations (Morcrette et al., 2005/6). The physical package for aerosols was taken from the Laboratoire d'Optique Atmospherique (LOA) /Laboratoire de Météorologie Dynamique (LMD) model of Boucher et al. (2002) and Reddy et al. (2005). It includes sources for sea salt and desert dust and a representation of sedimentation, and wet and dry deposition processes. Wet and dry deposition schemes were adapted directly from the LMD model (also known as LMDz model) whereas the sedimentation follows recent developments by Tompkins (2005). All aerosol species are treated as tracers in the ECMWF vertical diffusion and convection schemes and are advected by the semi-lagrangian scheme, consistently with all other dynamical fields. In the current model configuration, a bin representation is used to treat various aerosol species and improved emission sources have been implemented (Morcrette et al., *op. cit*). However, at the time of this study these developments were still under way, and it was decided to build the background error statistics by initialising the aerosol variables from the revised aerosol climatology by Tegen et al. (1997) used in the radiation scheme. This climatology has been shown to improve the ECMWF model performance in the analysis of the African Easterly Jet (Tompkins et al., 2005) and in the representation of tropical precipitation, global 925–hPa winds and 500–hPa geopotential (Rodwell, 2005). The model configuration used in this study is described in more detail below.

a. Model configuration

Six months of 5–day forecasts were run at T_L159 resolution (approximately 1.1 degrees) with 60 vertical levels. Prognostic aerosol tracers included sea salt, desert dust and continental particulate, initialised from the aerosol optical depth climatology by Tegen et al. (1997). The vertical distribution of the optical properties for the different aerosol species was specified according to Hess et al. (1998). The extinction profile was transformed back into mixing ratio and the aerosols were then let evolve as passive tracers subject to horizontal and vertical advection, vertical diffusion and transport through convection. Sedimentation and dry/wet deposition of aerosol were not activated. The main feature of the IFS relevant to the aerosols were changes to handle convective transport of passive tracers, including fixes to ensure positivity of the fields, and a new boundary layer scheme based on a combination of diffusive mixing and mass flux transport. Both these changes ensured a better vertical distribution of the aerosol tracers in the mixed boundary layer as well as in the free troposphere. A summary of these recent changes to the physical parameterizations is reported in (Tompkins et al., 2004) along with a validation of all new schemes.

The aerosol forecasts starting from the analysis at 1200 UTC were run for January–March 2001 and July–September 2001. For forecasts verifying at the same time, the differences mainly arise from having been initialized from different analyses. Since there are no direct observations related to aerosols in the current model configuration and considering that we are not perturbing the emissions, the main source of differences consists in the wind field that the tracers are subject to. At each analysis new wind–related observations are ingested in the assimilation system, which in turn provides a different initial condition for the winds. This fact together with the uncertainties inherent to the transport model itself, creates the conditions for the forecast differences observed in the aerosol fields. The ECMWF model has a good degree of skill in representing wind fields (Cavaleri and Bertotti, 2003) and hence we believe that these differences can represent a good proxy for short–term forecast errors in transport–related aerosol processes, and they can be used to build background error statistics.

A detailed analysis of the background error vertical and horizontal correlations derived from these forecasts is shown for January 2001 only. However, the global background matrix used in the single observation 4D–Var experiments was constructed using six months of forecast differences.

Figure 1 shows examples of sea salt and desert dust global distributions at 1000 hPa from a 48h forecast started on January 1, 2001 at 1200UTC. Units of mixing ratios are mg/kg. Distributions appear to be reasonable. Maxima of desert dust concentrations appear in proximity of the biggest sources and maxima of sea salt concentrations appear over Greenland and around the Aleutian Islands, due to storm activity. In general, however, the maxima of sea–salt concentration are correlated with areas of higher wind activity over the main oceanic regions.

3. Statistics for aerosol background fields derived using the Parrish and Derber method

The Parrish and Derber method (Parrish and Derber, 1992) is applied here to the aerosol forecasts described above to obtain a proxy for aerosol background statistics. The method consists in taking pairs of forecasts differences, usually 48h and 24h forecasts verifying at the same time, averaged over 6 months. This provides a total of 180 occurrences which is a reasonable sample size to build global statistics for a 3D variable at 60 vertical levels (a minimum of 60 samples would be required to build a full-rank covariance matrix at low wavenumbers). In general, it is better to have as large a sample as possible, hence the choice of 6 months to build the matrix. In this section, however, we show examples for January only. The month of July 2001 was also analysed in detail and results show small seasonal differences, but very similar patterns in the vertical and horizontal distribution of the errors. While one month is not enough for robust statistics, it can however reveal pathologies in the aerosol background statistics built from the forecast differences.

We note that the time lag of the forecast differences is not ideal since it is longer than the short–term forecasts used to provide the background fields of the analysis (typically 6 to 12 hours). Due to this discrepancy, the horizontal and vertical correlations of these longer–range forecast differences might be broader than those of the “true” background error. However, it is best to avoid use of 12-6h forecast differences because of the possibility of including the effects deriving from spin–up and diurnal cycle. The other known problem of the Parrish and Derber method is that the differences between the two forecasts are likely to be very small in data-sparse regions since there the analysis will not have “seen” enough observations to change the initial conditions ostensibly for the two forecasts. For this reason it is likely that this method underestimates the background variance in poorly observed regions. Moreover, if there are no observations related to the variable the background statistics are being build for, there is even a larger chance that the background errors would be underestimated. However, these shortcomings are well compensated by the possibility offered by the Parrish and Derber method of building large sample statistics by simply running short–range forecasts for several months. This is a powerful tool for a preliminary analysis of the background statistics and as a first step toward defining those statistics for “new” model variables.

For this study, the differences between the 48h and 24h forecasts valid at the same time were collected for the sum of the mixing ratios of all aerosol species. Mean, standard deviation and vertical and horizontal correlations

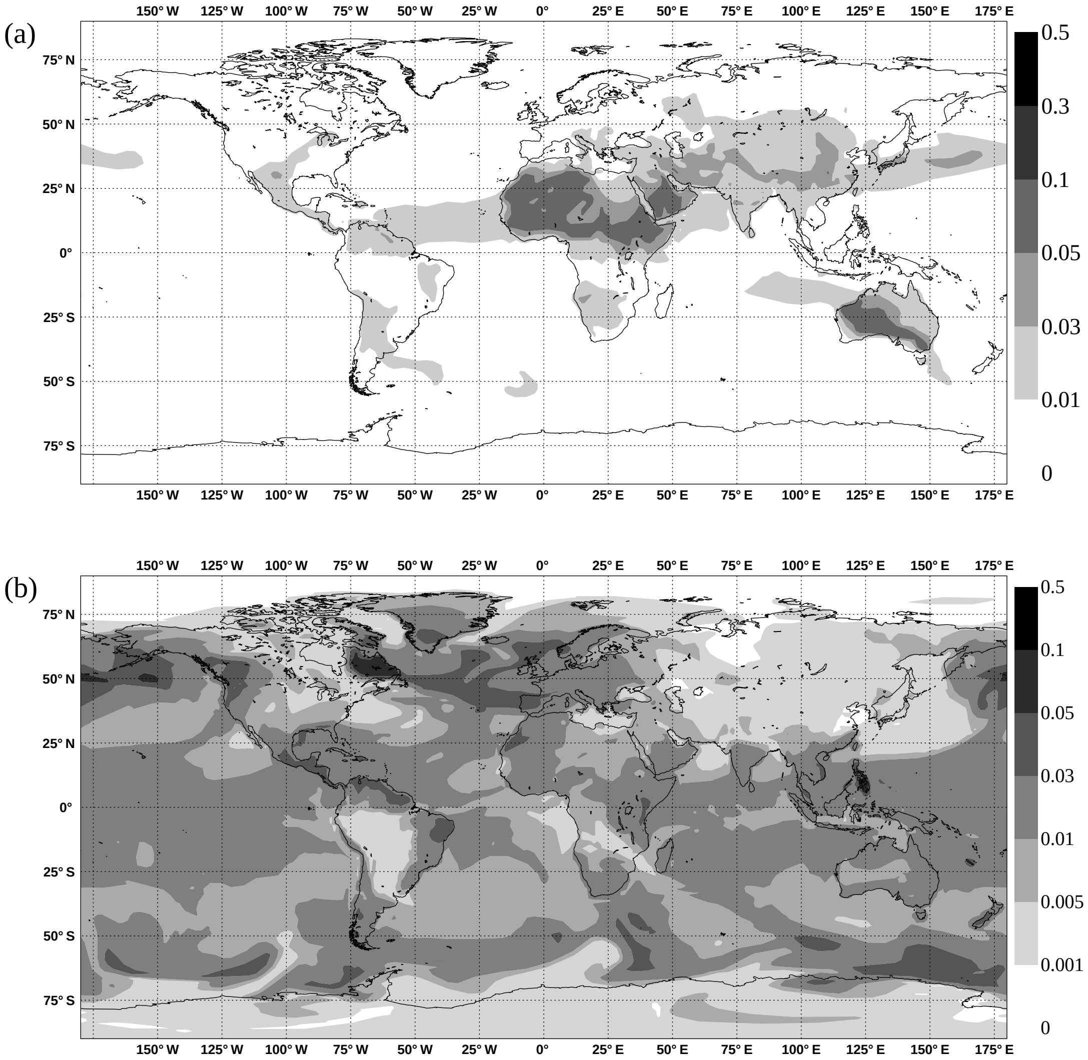

Figure 1: Horizontal distribution of aerosol mixing ratios in mg/kg at 1000 hPa. (a): 2-day forecast started on 01 January 2001 at 1200 UTC for desert dust; (b): 2-day forecast started on 01 January 2001 at 1200 UTC for sea salt.

were then calculated from this sample using standard definitions (Wilks, 1995). Note that due to the absence of aerosol removal processes and the relatively short time lag of the forecasts, the total average of the mean differences is not zero as one would expect from mass conservation consideration. However, this does not represent a problem since over the assimilation window of 12 hours it should not be expected that aerosol fields are balanced. The covariance was computed by subtracting the average over the sample size from the expected value of the forecast differences.

To investigate the regional structure of the covariances, zonal averages were also computed for four areas: global, tropics (30S-30N), extra–tropics Southern Hemisphere (30S-90S) and extra–tropics Northern Hemisphere (30N-90N). Vertical correlations were computed on pressure levels to limit the computational cost, and are shown as functions of pressure. Horizontal correlations are shown at 1000 and 200 hPa.

a. Aerosol background standard deviation

Figure 2a shows the horizontal distribution of the forecast differences averaged over the month of January at 1000 hPa. The main patterns are connected to storm activity and transport as expected and show the largest values around the Equatorial belt, especially over Amazonia, Central Africa and Indonesia, and high latitudes over Greenland. It is also possible to notice areas of large differences over mountainous areas, partially connected to orographic uplift, but also a likely artefact of the interpolation to pressure levels. The corresponding standard deviation at 1000 hPa, shown in figure 2b, shows aerosol forecast uncertainty. The noticeable pattern is the low variance over the oceanic regions. This is connected to the fact that the forecast differences are small in these data–sparce areas, i.e. the wind fields from the initializing analyses for the 48h and 24h forecasts do not vary much, as well as the fact that the background aerosol load is small.

Figure 3 shows the profile of the integrated standard deviation for the four areas listed above. The globally integrated profile differs little from the tropical and northern-hemisphere integrated values, except at middle and lower levels where the NH values are larger, possibly due to higher storm activity in the winter hemisphere. The southern–hemisphere values are generally smaller at lower levels, but show little differences with the other profiles at middle and upper levels.

b. Aerosol background error correlations

The error correlations are an important aspect of the background covariance matrix: while the variance determines the relative weight that the background exerts, the correlations determine the way the information contained in the observation is spread spatially into analysis increments. For example, if the observations represent a vertically integrated quantity, the vertical structure of the increments depends entirely on the background error covariance matrix, since there is no constraint regarding that structure in the observation itself. Correlations also play an important role in spreading the information contained in one observation at a given location into analysis increments at a different location. If the horizontal correlations are too narrow, then the influence of the observation is limited to the nearby grid–points; conversely if the correlations are too broad, there is the risk of propagating the information too far from the point it was relevant for, hence introducing spurious analysis increments. In this section, the vertical and horizontal correlations for the background aerosol for the month of January 2001 are analysed to detect any obvious pathologies. To this end we show zonally averaged correlations and profiles of globally (and regionally) integrated vertical correlations at selected levels (1000, 500 and 200 hPa); also shown are maps of horizontal correlations at 1000hPa and 200hPa for 200 and 500-km radii. Zonal averages of vertical correlations are shown in figure 4: correlations at upper levels (200 hPa) show a rather homogeneous structure while at 500 and 1000 hPa, they appear more erratic, due to the influence of orography. In the Tropics, correlations at 1000 hPa show generally a broader structure in the ver-

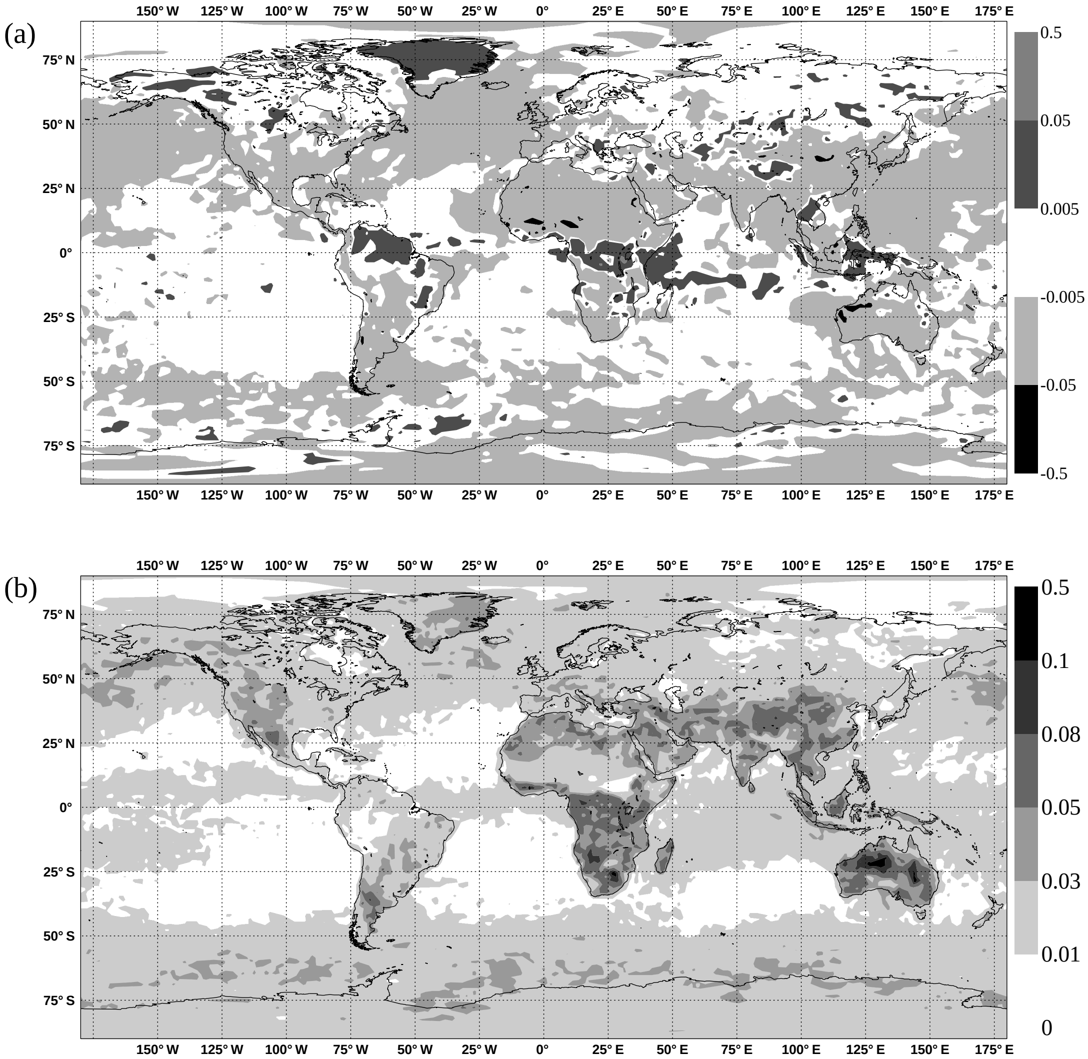

Figure 2: (a): Horizontal distribution of differences between 48 and 24h forecasts of aerosol mixing ratios at 1000 hPa; and (b) corresponding standard deviation in mg/kg for January 2001.

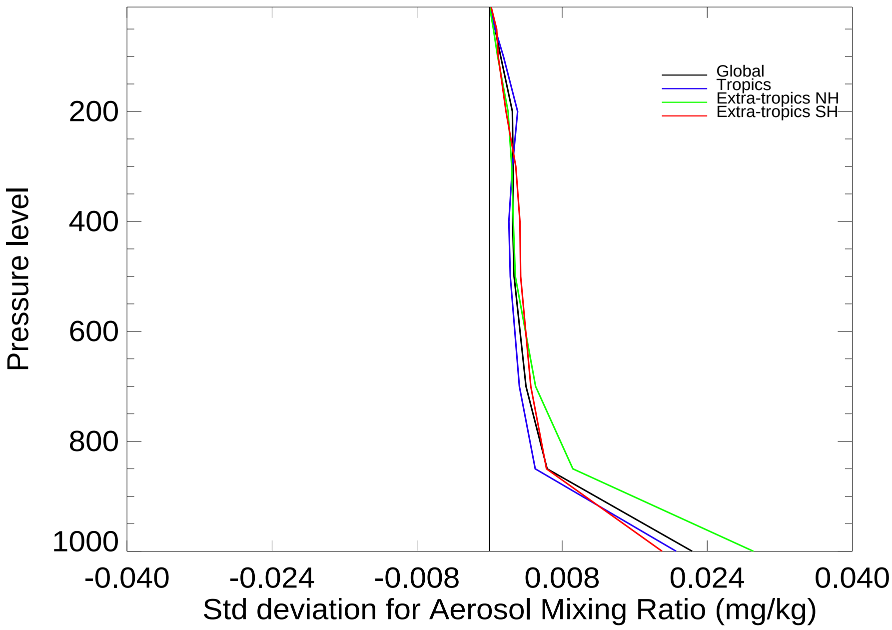

Figure 3: Profiles of integrated aerosol mixing ratio standard deviations for different regions as functions of pressure level for January 2001. The green line is the extra–tropical northern–hemispheric region; the red line represents the extra–tropical southern–hemispheric region; the blue line represents the Tropics and the black line is the integral over the whole globe.

tical than correlations at midlatitudes, likely due to the influence of convection. Error correlations are mostly positive everywhere with exceptions of correlations between 500 hPa and 1000 hPa. This can also be seen in figure 5 which shows the vertical profiles of zonally integrated correlations for four regions (Tropics, Southern/Northern Hemisphere Extra–Tropics, Global). These profiles reflect the fact that correlations are more homogenous at 200 hPa, whereas they present more variability at 1000 hPa, especially in the middle troposphere. In particular, the northern–hemispherically integrated correlations differ from the tropically integrated correlations: the former tend to decrease to zero quite rapidly above the boundary layer whereas in the Tropics, the vertical correlations decrease less rapidly, indicating the influence of convection in maintaining a coupling between surface and middle troposphere (see panel (a) of figure 5). This higher variability is due to the more intense storm activity in the winter hemisphere. However, when a larger sample of statistics is consider some of this regional variability is smoothed out.

Maps of horizontal correlations are shown in figure 6 at 1000 hPa and in figure 7 at 200 hPa for a distance of 200 and 500 km, respectively. The computation of these horizontal correlations is performed under the assumption of isotropy, i.e. for each point within a given radius, the covariance between that point and all others inside the domain is calculated without considering the variations along a given direction. This is an assumption that might be unrealistic under certain atmospheric conditions (e.g. in the proximity of a front). However, it provides an idea of the global patterns of horizontal correlations and also offer a way to find out pathological behaviours, for example, non–zero correlations between points which are spatially far–removed. In general, it is expected that horizontal correlations asymptote to zero for distances much larger than the typical horizontal correlation length scale of the variable in question. For aerosols, Collins et al. (2001) quote a value of 200 km as a characteristic length scale for optical depth, supporting their estimate with a reference to observations from the Lidar In–Space Technology Experiment (LITE) (Winker et al., 1996). In their model for the aerosol optical depth background matrix, they assume an exponential decay of the off–diagonal elements, using 100 km as a typical length scale. This value ensures that the background errors decorrelate rapidly with separation on the model grid, which they run with 100 km grid spacing. In our study, we observe that the horizontal correlations for aerosol mixing ratio do indeed decrease with increasing horizontal separation; however, over areas of large aerosol load, for example over the Sahara, there are non–zero correlations even at 500 km, as shown in figure 6b. The other aspect to note is that horizontal correlations decrease more slowly at 200 hPa, but are more homogeneous, than at 1000 hPa (note the predominance of lighter greys in figures 7a/b with respect to figures 6a/b). For example, over Central Europe the error correlations at 1000 hPa vary between 0.1 and 0.5, whereas for the same are the error correlations at 200 hPa are between 0.7 and 0.9. Given these results, it would be incorrect to assign a pre-determined correlation length which is constant for every point in the domain. The same conclusion could be applied to the vertical correlation length scale.

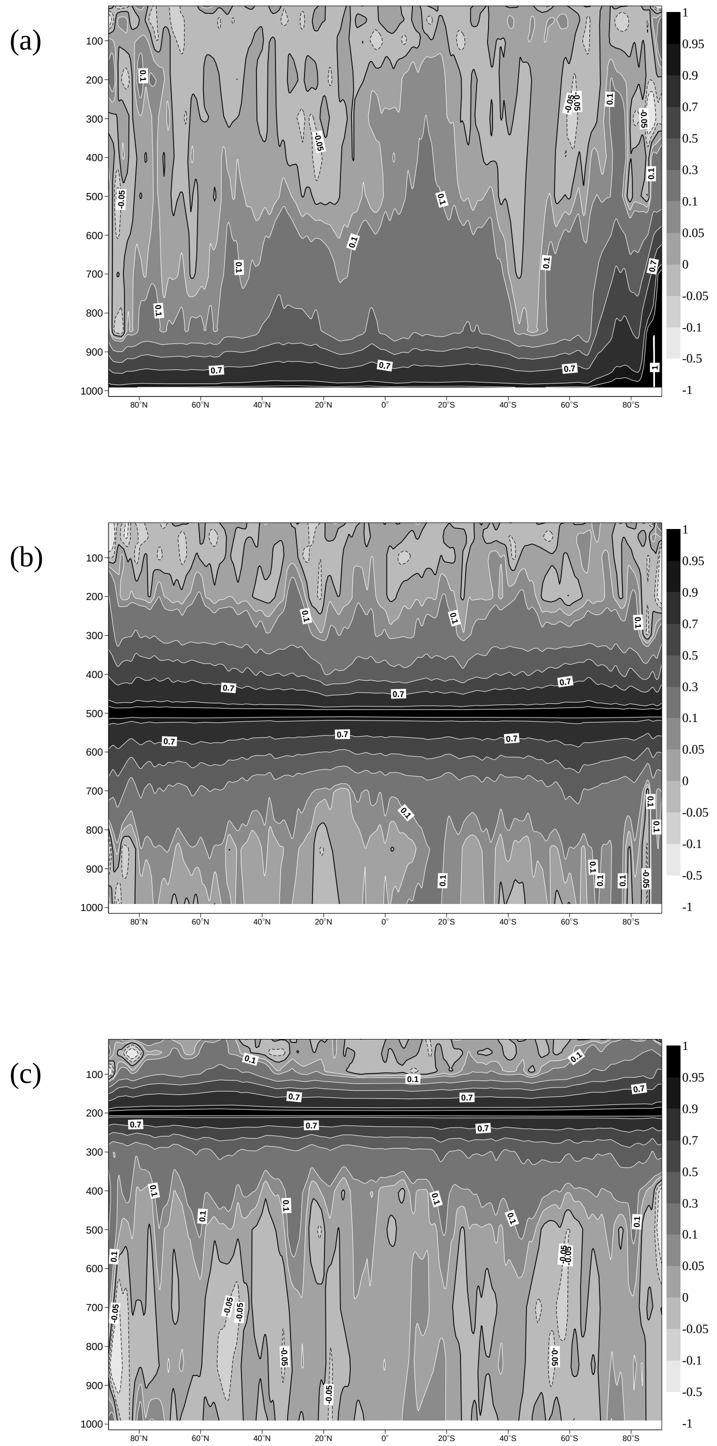

Figure 4: Zonal averages of aerosol vertical correlations for January 2001 at (a) 1000 hPa, (b) 500 hPa, and (c) 200 hPa. The white solid contour lines denote isolines of positive correlations and the black dashed lines denote isolines of negative correlations. The zero contour line is marked by the black solid line.

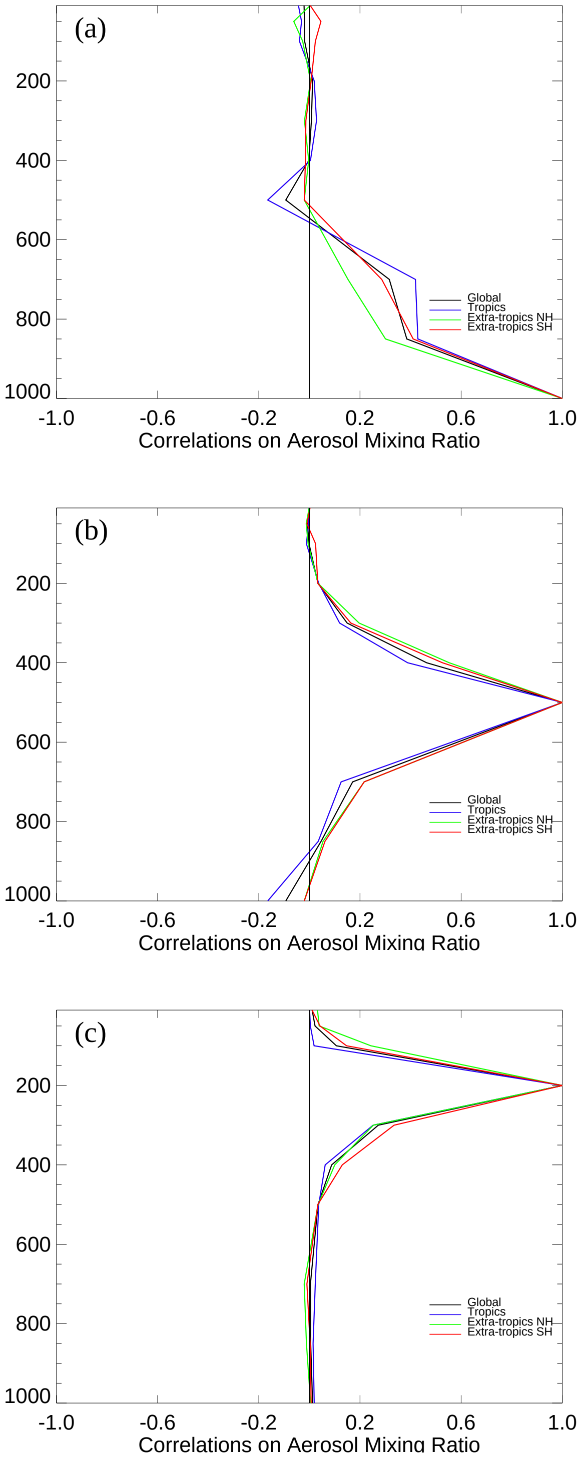

Figure 5: Profiles of integrated vertical correlations for January 2001 for (a) 1000 hPa, (b) 500 hPa, and (c) 200 hPa. Colour–coding as in figure 3.

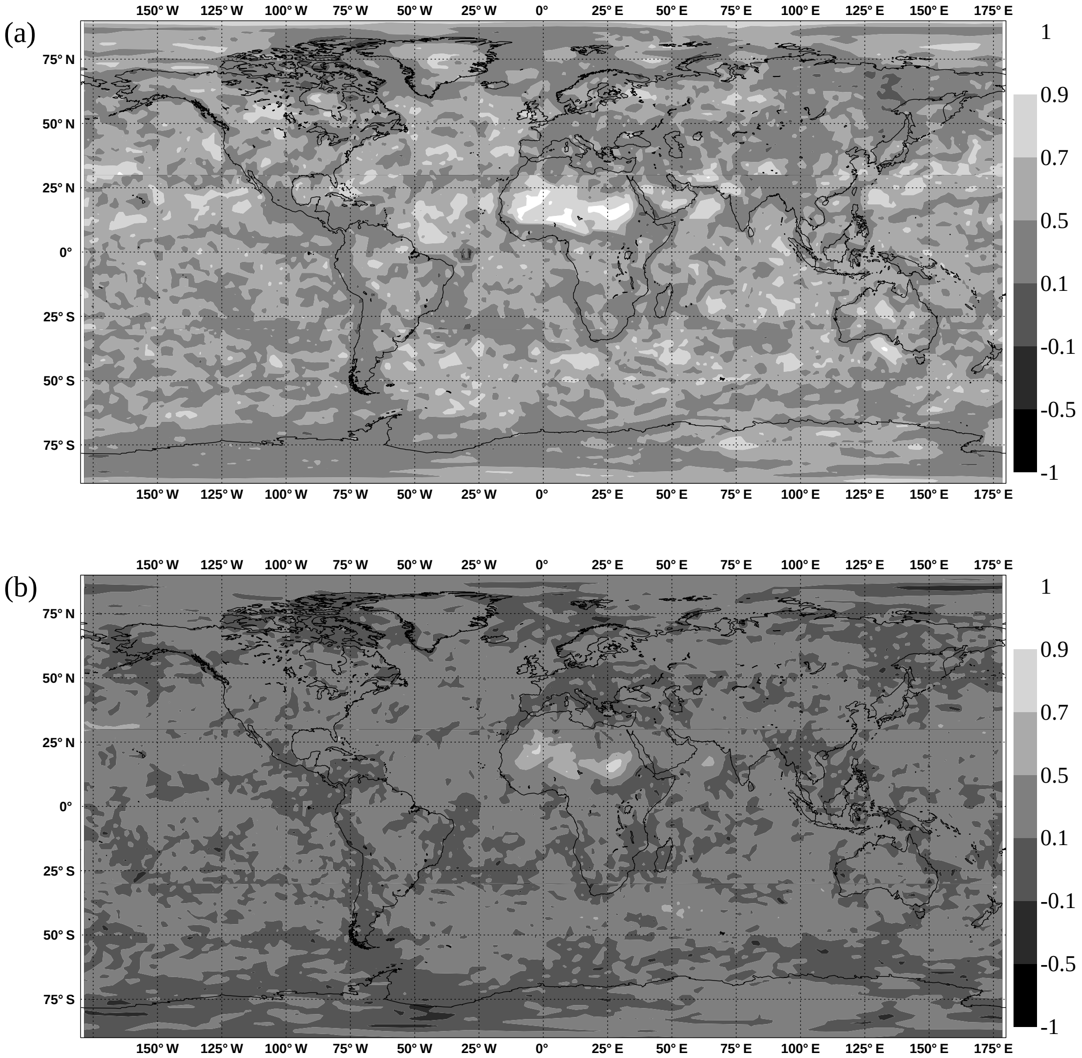

Figure 6: Maps of horizontal correlations of total aerosol mixing ratio at 1000 hPa for (a) 200, and (b) 500 km.

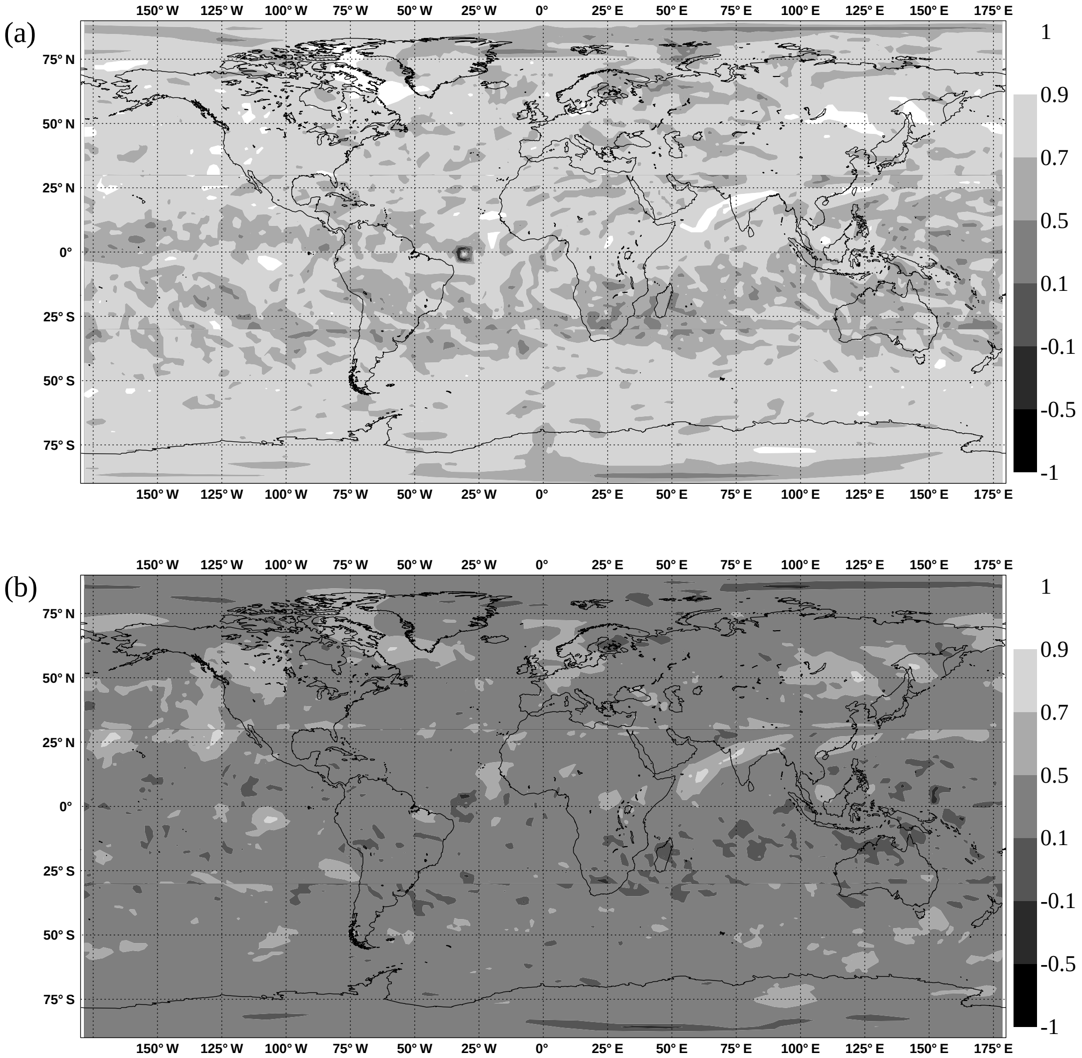

Figure 7: Maps of horizontal correlations of total aerosol mixing ratio at 200 hPa for (a) 200, and (b) 500 km.

4. A statistical model for the aerosol background error covariance matrix

In constructing a background error covariance matrix (**B**–matrix, hereafter), there are many constraints that one needs to keep in mind. In principle, this matrix should represent the error correlations between all pairs of model points; considering that the state vector of a typical analysis system has dimensions of 10^6, and that the corresponding **B**–matrix would have 10^{12} elements, it is clearly necessary to reduce the size of the problem to manageable proportions by constructing the **B**–matrix from a set of sparse matrices. In mathematical terms, one seeks to determine **L** such as

$$\mathsf{x} = \mathsf{x}_b + \mathbf{L}\chi \qquad (1)$$

$$\mathbf{B} = \mathbf{L}\mathbf{L}^T \qquad (2)$$

where x is the model state vector, x_b is the background state and **B** is the background error covariance matrix. In virtue of equations (1)-(2), the traditional cost function equation

$$J(\mathsf{x}) = (\mathsf{x}-\mathsf{x}_b)^T\mathbf{B}^{-1}(\mathsf{x}-\mathsf{x}_b) + (\mathsf{y}-H(\mathsf{x}))^T\mathbf{R}^{-1}(\mathsf{y}-H(\mathsf{x})) \qquad (3)$$

becomes

$$J(\chi) = \chi^T\chi + (\mathsf{y}-H(\mathsf{x}_\mathsf{b}+\mathbf{L}\chi))^T\mathbf{R}^{-1}(\mathsf{y}-H(\mathsf{x}_\mathsf{b}+\mathbf{L}\chi)). \qquad (4)$$

H represents the operator that transforms from model space to observation space; and **R** is the observation error covariance matrix which also accounts for errors introduced by H. The background error covariance matrix does not appear explicitly in equation (4) and is defined by the choice of the matrix **L**. There are no specific requirement on the matrix **L** but the purpose is to keep or model through **L** the main properties of the background errors. Correlations between model variables are taken into account through this process, so that the control variables can be assumed independent. The other important properties that need to be included in a statistical description of the **B**–matrix are non–separability, e.g. the tendency for broad horizontal error structures to be deep and for narrow horizontal structures to be shallow, and spatial variability, i.e. background error correlations have different spatial structures according to geographical location.

Due to the strict operational requirements at NWP centres, a large effort is devoted to the definition of the matrix **B** (or equivalently **L**). At ECMWF, the error covariance matrix model described in Derber and Bouttier (1999) was used until recently. A new formulation due to Fisher (2003, 2004), currently operational, allows a better representation of the spatial variability of horizontal correlations with respect to the more rigid Derber and Bouttier (1999) formulation, thanks to the introduction of the "wavelet" J_b. In this approach, the properties of the **B**–matrix are modelled by using the mathematical framework of wavelet–like non–orthogonal base functions with the property of having simultaneous localisation both in space and wavenumber. For a rigorous mathematical description of the "wavelet" J_b formulation, the reader is referred to Fisher (2003, 2004), while for a less mathematical general introduction the reader is referred to Fisher (2006).

In the following section we show results from the "wavelet"–J_b method applied to the error statistics described in section **3.**. Since a direct comparison with earlier results is not possible due to the fact that the **B**–matrix is computed on model levels rather than pressure levels, our goal is to use the results from the 4D–Var single observation experiment to show that some characteristics displayed by the aerosol background errors in the off–line analysis are captured by the "wavelet"–J_b formulation in the 4D–Var context and that the resulting **B**–matrix for aerosol mixing ratio can be used with confidence in the new aerosol analysis system. The following sections describe briefly the changes made to the ECMWF 4D–Var to accomodate the new control variables and show results from the single observation experiment.

5. The aerosol analysis system

The ECMWF 4D–Var system has been recently modified in order to include aerosol–related observations in the analysis. A more detailed description of these modifications will be presented in a separate article and is beyond the scope of this paper. For a theoretical description of the ECMWF 4D–Var the reader is referred to (Courtier et al., 1994). Of interest here is the notion that the ECWMF 4D–Var now includes total aerosol mixing ratio as a control variable in research mode. The introduction of this control variable has entailed modifications to several components of the IFS. First of all aerosols had to be included in the model as prognostic variables: this development was described in section **2.**.

A new pathway for aerosol–related observations had to be created, including observation operator model and its tangent linear and adjoint. As first step, it was decided to model aerosol optical depth. An *ad hoc* observation operator transforms the mixing ratio profiles into extinction and hence integrated vertically to obtain optical depth via use of pre–tabulated optical coefficients specific to the various aerosol species included in the forecasts. The optical coefficients depend on spectral wavelength and size bin, as well as relative humidity for hygroscopic species (i.e. sea salt). This operator is flexible and can be applied to total optical depth retrieved from various sensors at different wavelengths. For now, the chosen wavelengths are those of the MODIS instrument on board the Aqua and Terra satellites (0.47, 0.55, 0.66, 0.87, 1.24, 1.63, 2.13 microns). The tangent linear and adjoint models for aerosol optical depth were tested off-line to ensure that the stringent adjoint test (i.e. the equality of norms computed with the tangent linear and with the adjoint operators) was satisfied. The dependency of aerosol optical depth on relative humidity is only considered in the nonlinear model, but is neglected in the adjoint computation. Likewise, aerosol-specific physical processes, such as sedimentation, and wet/dry deposition, are only included in the nonlinear run.

The chosen control variable for the aerosol analysis is total aerosol mixing ratio defined as the sum of mixing ratios for all species and bins. The optimisation in terms of this variable is done by assuming that the relative contribution of the mass in a given bin and for a given species to the total aerosol mass does not change over the assimilation window (6 hours). This is a strong assumption in the sense that the increments in total mixing ratio will mainly come from "heavier" aerosols whose contribution to the total mass is dominant. However, it is a necessary assumption given the fact that not all aerosol species and bins can be included in the control vector to keep the cost of the minimisation at a reasonable level, also in view of a possible operational application.

Finally, background error correlations for total aerosol mixing ratio had to be prescribed for the definition and minimisation of the cost function of equation (**4.**): to this end the background error statistics from the Parrish and Derber method were used to define the wavelet–based aerosol **B**–matrix.

a. Single observation experiment

The functional test for the new aerosol **B**–matrix is its application in a 4D–Var experiment using the ECMWF 4D–Var. The experiment set–up consists of a single observation of aerosol optical depth at 0.55 microns. In this scenario, all increments in control variables other than aerosol mixing ratio are zero, since no contribution to, i.e., temperature or moisture increments comes from the aerosol optical depth.

Although not strictly necessary for this idealized test, we chose a value of aerosol optical depth which was actually observed on August 1, 2003 at the observing facility of Lampedusa, Italy (35.5N–12.6E). The model configuration for this single observation experiment consisted in two aerosol species (seal-salt and desert dust), each described by three size bins (with limits 0.03, 0.5, 5 and 20 microns for sea-salt and 0.03, 0.55, 0.9 and 20 microns for desert dust) initialised from a previous aerosol forecast.

The increments in total mixing ratio are shown in figure 8. Panel (a) shows the horizontal distribution of the increments at the surface while panel (b) shows a zonal cross section at 35.5N. As a general feature, it is possible to see that the spatially–varying horizontal correlations, implicit in the background error covariance matrix "wavelet" formulation do spread the information from a single–point observation to neighbouring points, thus enhancing the information that can be extracted from a given observation. The size of the increments decreases with distance following the decrease in horizontal correlations.

We also looked at the vertical distribution of the total aerosol mixing ratio increments over Lampedusa, and compared their structure with the standard deviation implied by the aerosol background error covariance matrix interpolated at the specific location. Figures 9 and 10 show profiles of standard deviation and increments, respectively. The vertical distribution of increments follows closely the standard deviation, showing the instrumental role of the background error covariance matrix in distributing increments from a vertically integrated observation. It can also be noted that the standard deviation implied by the wavelet formulation of the background error covariance matrix is similar in shape to that derived from the off–line calculation and based on the same Parrish and Derber method statistics (see fig. 3). Although a direct comparison is not possible due to the different vertical coordinates (model versus pressure levels), and to the globally–integrated versus specific–point values, it is possible to see the similarities of the profiles. In general, this single observation experiment shows that the aerosol **B**–matrix can produce meaningful analyses.

These results underline the importance of a correct definition of the background error correlations: if correlations are artificially included in the background matrix via an arbitrary correlation, which does not match the correlation length inherent to the model processes, then the information contained in the observations is not transferred consistently between levels and grid points, and the vertical and horizontal structure of the analysed fields will be not be realistic. If some vertical information is present in the observations, i.e. the observation comes from a sounder, radiosonde or radar, then the vertical structure of the increments will be a compromise between the background and the observations, according to the sensitivity of observational operator to the model variables, as implied by the Jacobian matrix; however, if no profiling information is contained in the observations, as it is the case for vertically–integrated quantities (for example, aerosol optical depth), then the vertical structure of the increments rely solely on the structure specified in the background matrix. If this structure is unrealistic or not consistent with the model, the structure of the increments will also be unrealistic.

6. Summary and future perspectives

This paper described the steps taken to define a background error covariance matrix for total aerosol mixing ratio, a variable recently introduced in the ECMWF IFS with the goal of constructing an aerosol analysis system. These steps included building aerosol error statistics from forecast differences following the Parrish and Derber method, i.e. using differences between the 48h and 24h forecasts valid at the same time. The forecasts included prognostic aerosols species, i.e. sea salt, desert dust and continental particulate, and were run for six months. The statistics were analyzed in depth for the month of January 2001 to understand the spatial characteristics of the aerosol background error correlations. It was shown that horizontal correlations have high spatial variability. In particular, error correlations at the surface are broader over areas of large aerosol load, close to sources, for example over desert areas. In general, however, horizontal correlations are "longer" at upper levels (i.e. 200 hPa) rather than at the surface. It was also shown that vertical error correlations show more variability in the lower troposphere and tend to be less variable in the upper troposphere.

The statistics from the forecast differences were used to define a total aerosol background error covariance matrix based on the "wavelet" J_b approach. This matrix was then applied in a single observation experiment to obtain aerosol mixing ratio analysis increments. The horizontal structure of the increments showed how information from a single point observation could be spread to neighboring points thanks to the **B**–matrix. The

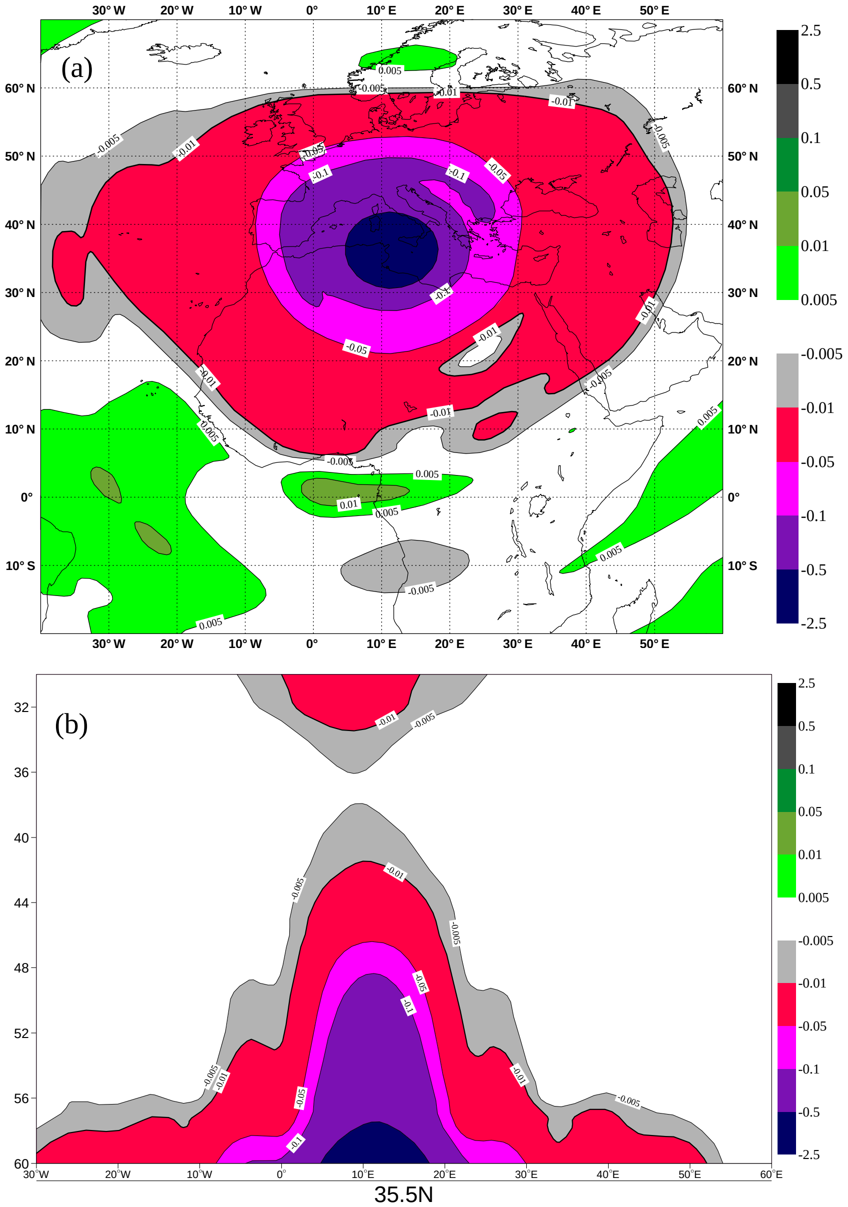

Figure 8: Increments in total aerosol mixing ratio (mg/kg) for a single observation experiment on August 1, 2003 at 1200UTC. The observation is located over the island of Lampedusa (Italy, 35.5N-12.6E). (a) Horizontal structure of increments at the surface; and (b) zonal cross section.

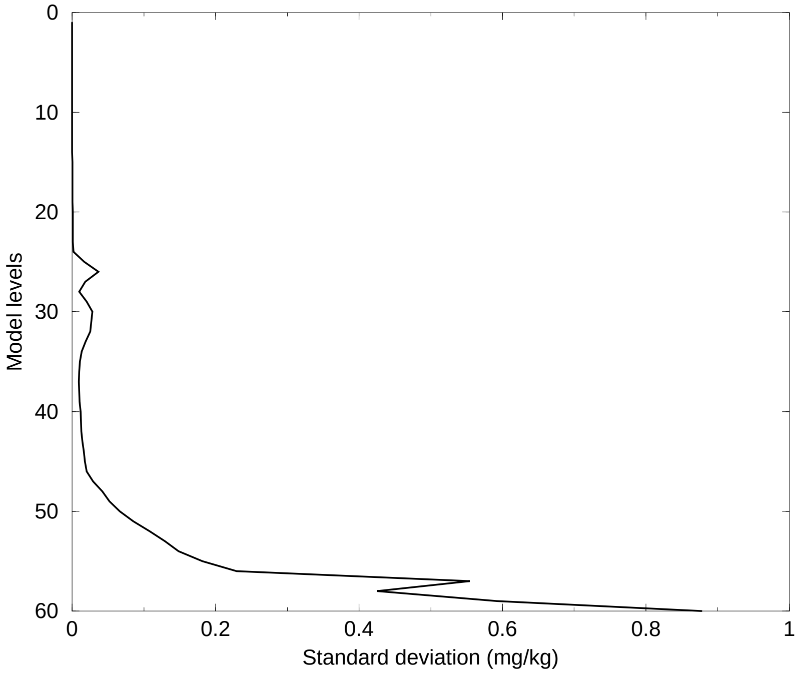

Figure 9: Background standard deviation of aerosol mixing ratio (mg/kg) at Lampedusa (Italy, 35.5N-12.6E).

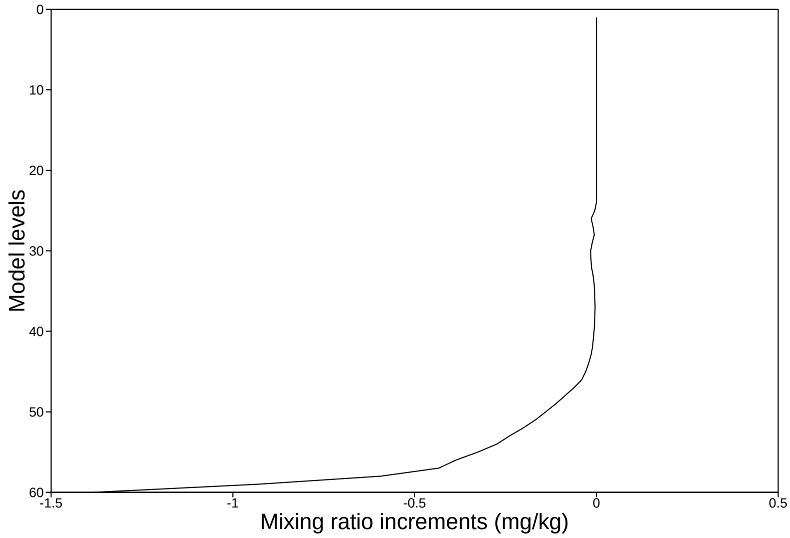

Figure 10: Profile of increments in total aerosol mixing ratio (mg/kg) as functions of model levels for Lampedusa (Italy, 35.5N-12.6E).

vertical profiles of the increments were consistent with the profiles of aerosol mixing ratio variance observed in the off–line computations. Overall, the results proved that the aerosol **B**–matrix based on the NMC error statistics could be used with confidence to obtain preliminary aerosol analyses.

In view of the requirements for two years of aerosol reanalyses as part of GEMS, the aerosol **B**–matrix will require several refinements, which will also depend on the improvements and changes in the aerosol model. It is likely that there will be the need to define error statistics for new aerosol control variables other than the total aerosol mixing ratio, for example the fine and coarse mode aerosol mixing ratios which allow to discriminate between aerosols of maximum size larger than 1 micron and larger aerosol. In this case, the Parrish and Derber method might be used again to re–create the error statistics. Some tuning of the aerosol background error covariance matrix might be required to ensure the necessary spatial variation of the error correlations.

Possible improvements notwithstanding, this first attempt at generating error statistics and an error covariance matrix for aerosol mixing ratios described in this paper represents an advancement toward the assimilation of "non–conventional" observations of atmospheric constituents, such as aerosol, into a NWP global model.

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