How important is to use diagnosed background error covariances for the atmospheric ozone analysis?

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1 Introduction

The background error covariance matrix is a key component of any assimilation system. It accounts for the variance and for the correlations and these two contributions can be assessed and estimated separately. The background error variance has to be compared to the observation error variance in order to evaluate their relative weight in the analysis produced by the assimilation process. The background error correlations carry to the neighbouring gridpoints the information brought in by the obervations at their locations. They also transfer the information to other variables not directly measured, if these are physically related to the measured ones.

The assessment of background (and analysis) error is an interesting feature of ensemble data assimilation systems. This flow-dependent information can be exploited in a cycle assimilation system to improve the estimate of the background error covariance matrix. Lorenc (2003) and Buehner (2005) illustrated how an ensemble-estimate background error covariance matrix can be used in a variational assimilation system. Rather than using the ensemble directly to construct an estimate of the covariance matrix, it may be used indirectly to calibrate specific parameters of a covariance model (Fisher, 2003; Belo Pereira and Berre, 2006).

The use of ensembles in combination with a variational assimilation scheme is relatively unexplored in atmospheric chemistry data assimilation. The main purpose of this study is to investigate the potential of an ensemble of atmospheric ozone analyses to provide useful flow-dependent estimates of the background error variance and correlations, in a four-dimensional variational assimilation suite. Therefore, we propose to assess the analyses sensitivity to the choice of fixed or estimated variance and correlations. Our results are based on stratospheric and upper tropospheric ozone analyses realized during a five months period from January to May 2008.

2 The assimilation system

Valentina is a modular variational data assimilation suite developed at CERFACS. In this study, it is coupled to the Météo-France Mocage Chemistry Transport Model (CTM). Mocage is used as the forecast model that produces the atmospheric ozone concentrations. It is combined with ozone profile measurements from the Microwave Limb Sounder (MLS) instrument, using a four-dimensional variational assimilation scheme.

2.1 Atmospheric ozone forecast

The CTM Mocage covers the planetary boundary layer, the free troposphere and the stratosphere. It provides a number of optional configurations with varying domain geometries and resolutions, as well as chemical and physical parameterisation packages. In this study, we worked with a 2° by 2° global version of Mocage, with 60 vertical levels (from the surface up to 0.1 hPa). The meteorological forcing fields are provided by the operational European Centre for Medium Range Weather Forecasts (ECMWF) numerical weather prediction model. To compute the ozone fields, we adopted the linear ozone parameterisation developed by Cariolle and Teyssèdre (2007) in its latest version. This parameterisation is based on the linearisation of ozone production/destruction rates using an altitude/latitude chemical model.

2.2 Observations

The MLS instrument has been flying onboard the Aura satellite in a sun-synchronous polar orbit since August 2004. Vertical profiles of several atmospheric parameters are retrieved from the millimeter and sub-millimeter thermal emission measured at the atmospheric limb (Waters et al., 2006). Measurements are performed between 82° S and 82° N. This gives about 2000 profile measurements per day.

For our study we have used the latest version (v2.2) of the screened MLS ozone product. We restricted the data selection to the pressure range from 215 hPa to 0.5 hPa, which represents measurements at 16 pressure levels per profile. Four of these pressure levels are located in the Upper Troposphere-Lower Stratosphere (UTLS). The error at these levels has values from 5% to 100% below 100 hPa, from 2% to 30% at 100 hPa. Below, the MLS ozone data have small biases, with a random error of the order of 5% (Froidevaux et al., 2008; Livesey et al., 2008).

2.3 Data assimilation method

In this study, we produced atmospheric ozone analyses with the Valentina assimilation system coupled with Mocage. The version in use is similar to the one used in our previous studies (Massart et al., 2007, 2009). It is based on the Mocage-Palm system developed jointly by CERFACS and Météo-France in the framework of the FP5 European project ASSET (Lahoz et al., 2007). It was then extended with the support of the Ether centre for atmospheric chemistry products and services. As a difference from previous studies based on Valentina, we use here a four dimensional variational method (4D-VAR) instead of its FGAT (first guess at appropriate time) variant. The size of the 4D-VAR assimilation windows was set at 12 hours.

The forecast error covariance matrix of Valentina is split into a correlation matrix and a diagonal matrix filled with the forecast error variance (square of the forecast error standard deviation). The correlation matrix is divided into a horizontal and a vertical operators, both modelled using a diffusion equation (Weaver and Courtier, 2001). These two operators require the specification of the length-scales to compute the forecast error correlation matrix.

The observation error variances are computed using the square of the the given standard deviations of the MLS observation errors. The random observation error of one measurement is assumed to be independent of the random observation error of other measurements along both the same profile and other profiles. This means that the off-diagonal terms of the observation error covariance matrix are equal to zero. Moreover, Froidevaux et al. (2008) showed that the averaging kernels' peaks are close to unity for the selected assimilated levels. This implies that we can use the MLS data without specifying the averaging kernels.

3 Diagnosed background error covariances

Over the five months studied period, we carried five assimilation experiments with different assimilated data sets. The five data sets were built by adding to the retrieved measures, a random centred Gaussian noise with a standard deviation equal to the standard deviation of the observation error. From this ensemble of assimilation runs, we computed an ensemble of forecast errors from which we calculated the variance and the length-scales associated to the correlations. With two forecasts per day and five runs, we had an ensemble of ten elements per day. We chose to extract monthly statistics, resulting in about 300 elements over the whole period. This choice was driven by the fact that we needed a number of elements large enough to produce significant statistics. But we did not want to loose the flow-depend aspect by computing the statistics over the whole five months period.

3.1 Diagnosed background error standard deviation

All the monthly diagnosed background error standard deviations present a similar shape (Fig. 1). The standard deviation is higher (in percentage of the field) in the UTLS region, especially over the equatorial region. This means that the confidence on the model forecast is lower in these regions. The differences from one month to another are localized in the Polar regions. There, higher values of the standard deviation spans a larger vertical range during the Polar night.

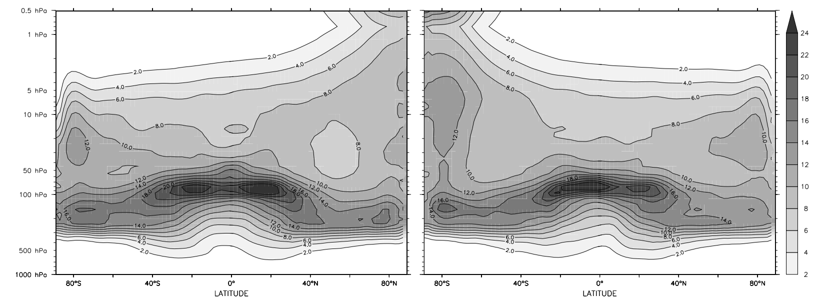

Fig 1. Zonal mean of the diagnosed ozone variance in % for January (left panel) and May (right panel) 2008.

3.2 Diagnosed background error horizontal correlations

To save computational time, we currently compute the horizontal correlations for each pressure level from the same two-dimensional latitude-longitude length-scale field. As the assimilated observations are mainly stratospheric, we averaged over the stratospheric levels the horizontal correlations of the diagnosed background error. We found that the monthly diagnosed length-scales associated to the horizontal correlations are strongly inhomogeneous in time and space (Figs. 2 and 3). In the zonal direction, the length-scales vary from 50 km to 600 km, with smooth variations with the latitude. In the meridional direction, they vary from 150 km to 350 km, with important spatial variations and from one month to others.

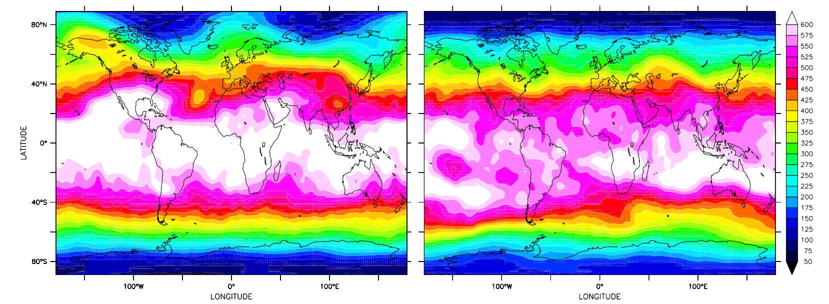

Fig 2. Stratospheric zonal length-scale (in km) diagnosed for January (left panel) and for May (right panel) 2008.

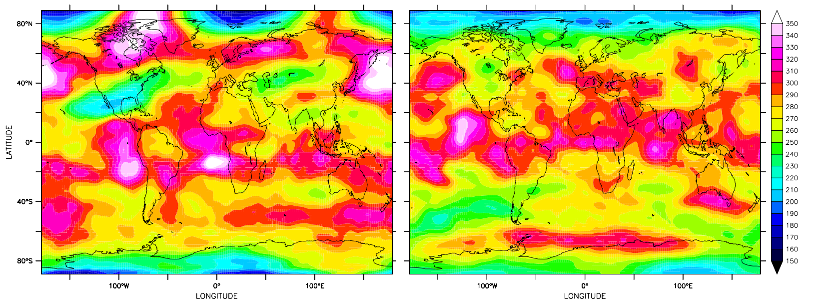

Fig 3. Stratospheric meridional length-scale (in km) diagnosed for January (left panel) and for May (right panel) 2008.

3.3 Diagnosed background error vertical correlations

The vertical length-scale represents the vertical correlation of the background error. In the stratosphere, it varies smoothly from 0.15 to 0.3 (in units of the logarithm of pressure) with the altitude. But it increases in the UTLS region. Its behaviour is similar for all the studied months (Fig. 4).

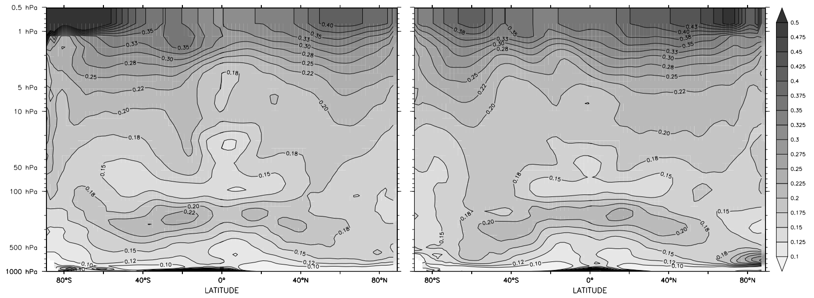

Fig 4. Zonal average of the vertical length-scale (in units of the natural logarithm of pressure) diagnosed for January (left panel) and May (right panel) 2008.

4 Background error covariances effects on the analysis

Our methodology consists in comparing three assimilation experiments, which differ only by the modelling of the background error covariance matrix. Experiments details are reported in Tab. 1. The criterion used to assess the improvements on the ozone analysis determined by

	length-scale			
Name	horizontal	vertical	variance	legend
reference	450 km	0.3	15%	- - - - -
partial	diagnosed	diagnosed	15%	-·-·-·-·-
full	diagnosed	diagnosed	diagnosed	———

Tab 1. Characteristics of the assimilation experiments.

the use of diagnosed length-scales and standard deviations is based on the evaluation of the bias and the standard deviation with respect to assimilated or independent data. A comparison with a direct simulation without any assimilation is also performed. The results of the direct simulation are represented as the grey shaded area.

4.1 Effect on the analysed ozone profiles

In most of pressure levels where MLS data are assimilated, the ozone analysis is equal in average to the measurement (Fig. 5). Above 5 hPa, the data error increases. The analysis is then less constrained by the data. As a consequence, it is closer to the background. In the *full* experiment, the background error variance is lower than for the two other experiments at these pressure levels. This experiment gives thus more confidence to the background state. This explains why above 5 hPa the analysis bias and the standard deviation with MLS is higher for the *full* experiment compared to the two others (Figs. 5 and 6). This occurs for all latitudes.

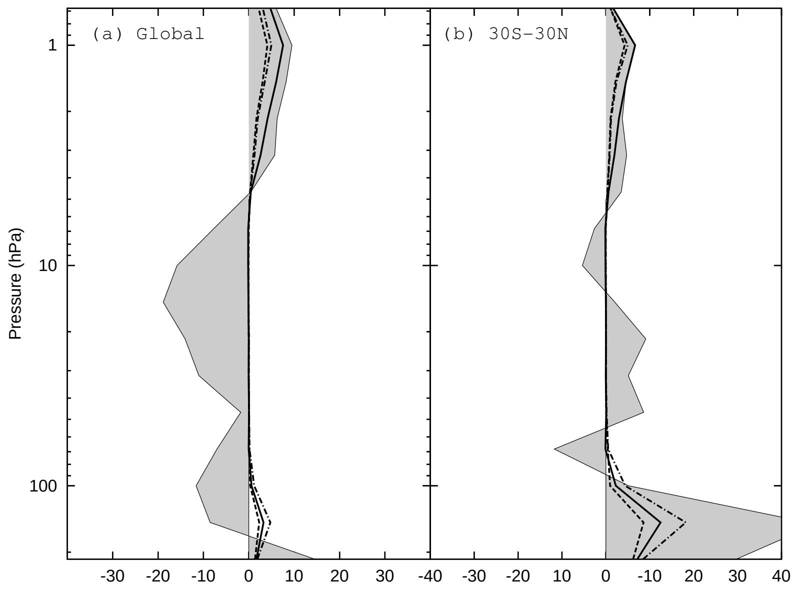

Fig 5. Average of MLS measurements minus ozone analyses normalized by the climatology (in %) as a function of pressure: (a) global domain and (b) 30°S-30°N latitude band. The number of used measurements is about 300 000 for (a) and 80 000 for (b).

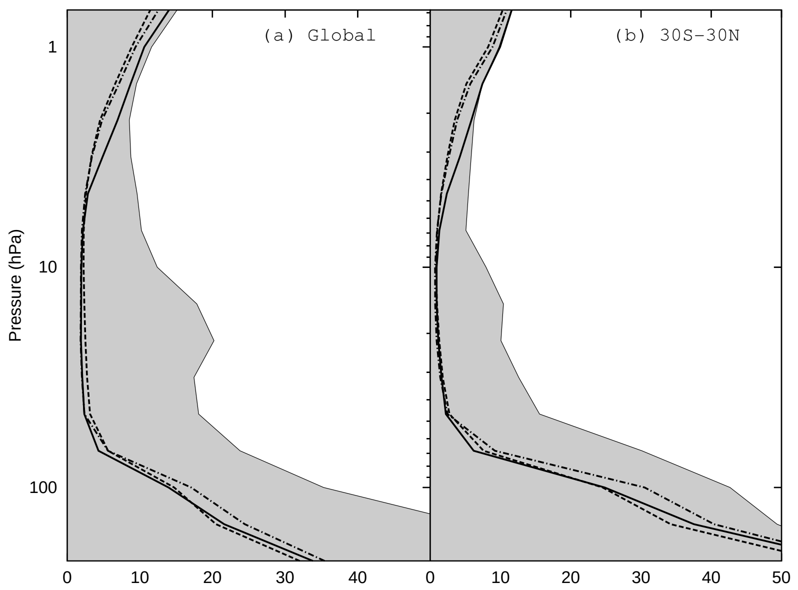

Fig 6. Same as Fig. 5 but for standard deviation.

Bellow 70 hPa, the data error also increases. As the background error variance also increases in the *full* experiment, one can expect to obtain analysed ozone concentrations closer to the assimilated observations than for the two others experiments. But this is not the case. In fact, the comparison between the *reference* and the *partial* experiments shows that the use of the diagnosed length-scales increases the bias (only in the equatorial region) and the standard deviation (at all latitude bands) of the analysis with the MLS data in the UTLS.

The effect of the use of diagnosed length-scales on the UTLS region is confirmed when the ozone analysis is compared to independent measurements from ozonesondes. The analysis bias compared to ozonesondes is globally the same for the three experiments, with differences mainly localized in the UTLS of the equatorial region (Fig. 7). The bias is there lower for the *partial* experiment and increases when using the diagnosed standard deviation (*full* experiment). But it remains lower than the bias of the *reference* experiment. Concerning the standard deviation of the difference between the ozonesonde measurements and the analysis, the *partial* and the *full* experiments show similar values, systematically lower or equal than the values from the *reference* experiment (Fig. 8). This improvement is general, allover the globe.

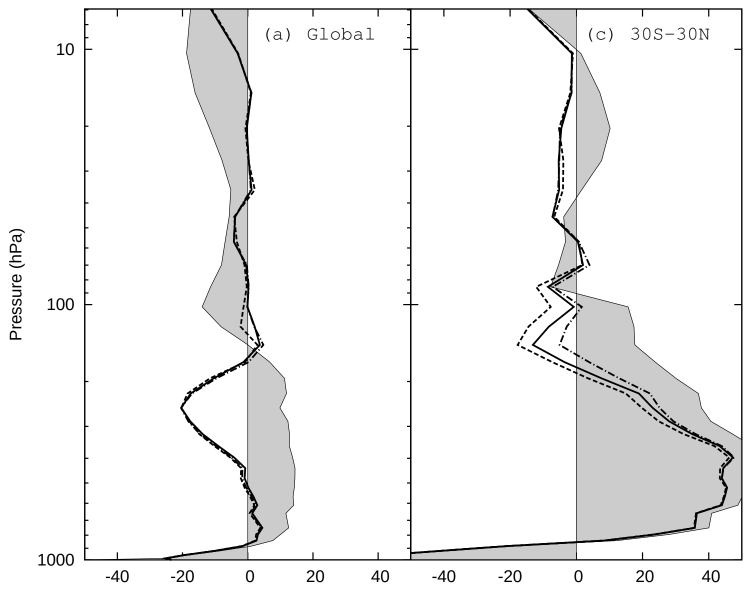

Fig 7. Average of ozonesondes measurements minus ozone analyses normalized by the climatology (in %) as a function of pressure: (a) global domain and (b) 30°S-30°N latitude band. The number of used measurements is about 360 for (a) and 47 for (b).

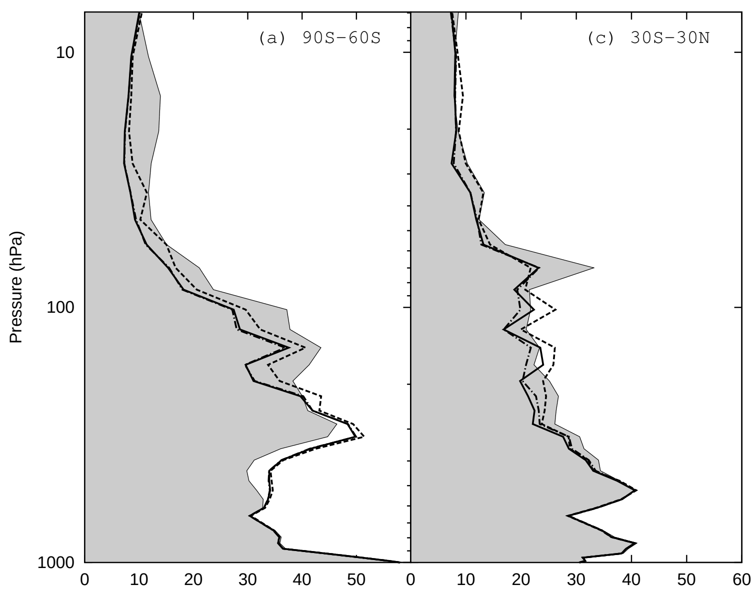

Fig 8. Same as Fig. 7 but for standard deviation.

4.2 Effect on the analysed total column ozone

To further evaluate the effects of the diagnosed parameters of the model for the background error covariances, we also compared the different analyses from the different experiments to the data from the Ozone Monitoring Instrument (OMI). OMI is a nadir viewing imaging spectrograph that measures the solar radiation backscattered by the Earth's atmosphere and surface (Levelt et al., 2008). In this study, we used the OMI total ozone columns (data available from `http://www.temis.nl`) produced with the KNMI DOAS method (Veefkind et al., 2006). The OMI-DOAS total ozone columns showed a globally averaged agreement better than 2% with the ground-based observations (Balis et al., 2007). The data show no significant dependence on latitude except for the high latitudes of the Southern Hemisphere (SH) where there is a systematic overestimation of the total ozone value by 3% to 5% . Due to the high resolution of the OMI data, we averaged each OMI measurement scene (60 ground pixels) on a 4° by 4° horizontal grid. This means that we used about 100 measurements at the equator and about 300 measurements over the polar regions for each cell of the 2° by 2° horizontal grid, for the five months comparison period.

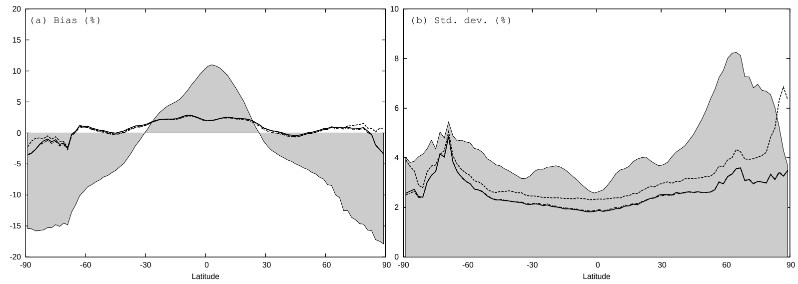

Fig 9. Comparison with OMI total ozone column data. Bias (left panel) and standard deviation (right panel) in % of OMI data.

In terms of total ozone columns, all the assimilation experiments reduce the bias with the OMI data compared to the direct simulation (Fig. 9). The biases of the three experiments are quite similar with values under 4%. They differ over the Polar region where the bias of the *reference* experiment is lower. Nevertheless, this experiment has a higher standard deviation than the two others in this region. Over the North polar region, the standard deviation is even higher than the one from the direct simulation. The use of diagnosed length-scales (*partial* and *full* experiments) sensibly improves the standard deviation of the difference with OMI. The difference is then near 3% with high values under 5% near the edge of the South polar vortex.

5 Conclusions

We carried on three assimilation experiments over a five months period during which we analysed atmospheric ozone concentrations using the MLS data. The aim of these experiments was to realize a sensitivity study of the scores of our model to the background error covariances. We found that the use a constant horizontal length-scale for modelling the background error correlations, reduces the analysis error (in terms of standard deviation) with independent data compared to the direct simulation (without any assimilation) except over the polar regions. In these regions, the diagnosed horizontal length-scales have very low values compared to the constant one. The use of these diagnosed length-scales seriously reduces the error in the polar regions and allover the globe. Their effect is mainly localized above 5 hPa and below 70 hPa. Below 70 hPa, they also affect the ozone average but only over the equatorial region. The further use of the diagnosed ozone standard deviation does not sensibly modify the analysed ozone fields. It little increases the equatorial UTLS bias compared to ozonesondes. But it slightly decreases the standard deviation compared to the OMI total columns. The specification of appropriate length-scales to model the background error correlations seems thus to be the most important contribution to improve the quality of our atmospheric ozone analysis.

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