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Sensitivity of the OMI ozone profile retrieval (OMO3PR) to a priori assumptions

T. Mielonen^{1,*}, J. F. de Haan¹, and J. P. Veefkind^{1,2}

¹Royal Netherlands Meteorological Institute (KNMI), De Bilt, The Netherlands

²Delft University of Technology, Delft, The Netherlands

* now at: Finnish Meteorological Institute, Kuopio, Finland

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Correspondence to: T. Mielonen (tero.mielonen@fmi.fi)

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We have assessed the sensitivity of the operational OMI ozone profile retrieval (OMO3PR) algorithm to a number of a priori assumptions. We studied the effect of stray light correction, surface albedo assumptions and a priori ozone profiles on the retrieved ozone profile. Then, we studied how to modify the algorithm to improve the retrieval of tropospheric ozone. We found that stray light corrections have a significant effect on the retrieved ozone profile but mainly at high altitudes. Surface albedo assumptions, on the other hand, have the largest impact at the lowest layers. Selection of an ozone profile climatology which is used as a priori information has small effects on the retrievals at all altitudes. However, the usage of climatological a priori covariance matrix has a significant effect. Based on these sensitivity tests, we made several modifications to the OMO3PR algorithm: the a priori ozone climatology was replaced with a new climatology (TpO3), the a priori covariance matrix was calculated from the climatological ozone variance values, and the surface albedo was assumed to be linearly dependent on wavelength in the UV2 channel. We found that the a priori covariance matrix basically defines the vertical distribution of degrees of freedom for a retrieval. Moreover, all the studied versions of the OMO3PR algorithm were equally effective in reducing uncertainty in the retrieved ozone profile. This implies that the posterior error values depend mostly on the assumed a priori errors. Our case study over Europe showed that the new version produced over 10 % smaller ozone abundances which reduced the systematic overestimation of ozone in the OMO3PR algorithm and improved correspondence with IASI retrievals.

1 Introduction

Atmospheric ozone is distributed both in the stratosphere and the troposphere. In the stratosphere, ozone acts as a shield that protects the surface from energetic ultraviolet radiation. Tropospheric ozone, on the other hand, is a greenhouse gas that warms

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spectrometer, which provides daily global coverage with high spatial and spectral resolution (Levelt et al., 2006a, b). It has been measuring since 2004.

A detailed description of the OMI ozone profile algorithm (OMO3PR) is given by Kroon et al. (2011). Briefly, the retrieval is based on the strong decrease in the ozone absorption cross section between wavelengths of 270 nm and 330 nm. The radiation at the longer wavelengths goes through the whole atmosphere while the shortest wavelengths are only affected by the highest layers of the atmosphere. Therefore, spectral information of UV radiation can provide information on the vertical distribution of ozone. The measurements are taken from the UV1 channel (270.0–308.5 nm) and the first part of the UV2 channel (311.5–330.0 nm). The retrieval algorithm uses optimal estimation (Rodgers, 2000; termed maximum a posteriori method in the book), where the difference between the measured and modeled sun-normalized radiance is minimized by adjusting the amount of ozone in 18 atmospheric layers. This method requires a priori information on ozone profiles and other parameters like the surface albedo in order to constrain the retrievals. The operational ozone profile retrieval uses the LLM ozone climatology (McPeters et al., 2007), which varies with month and latitude. The a priori ozone profiles are given constant relative variability of 20 % except for ozone hole conditions. Ozone hole conditions are assumed to occur between August and December at latitudes south of 50° S. There, the variability is 60 % for altitudes between 21 km and 50 km, and 30 % for the other altitudes. The vertical correlation length of ozone is an a priori constraint and it is set to 6 km. To ensure that the retrieved ozone volume mixing ratios are positive, the algorithm operates with logarithm of the volume mixing ratio for each layer.

Surface albedo is also fitted in the retrieval and the OMI surface albedo climatology (Kleipool et al., 2008) is used as an initial value for the surface underneath the atmosphere. The wavelength dependence of the albedo in both UV1 and UV2 channels is described with a second order polynomial. Surface albedo is fitted for all wavelengths (although the shortest ones do not “see” the surface) to partly account for the presence of aerosols and clouds which are not known or modeled in the retrieval.

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Stray light refers to light of other wavelengths that is scattered by the imperfect OMI optics onto the detector of a specific wavelength. This effect is more pronounced in the UV1 channel than in the UV2 channel because the detected radiances at the shorter wavelengths are smaller and, therefore, the measured signal is affected more by radiation from other wavelengths. The shortest wavelengths are reflected only from the highest altitude layers in the atmosphere, thus, stray light has the largest effect on the retrieval of ozone at these altitudes. Dobber et al. (2006) have provided a detailed description of stray light features in the OMI instrument. Regarding the ozone profile retrieval, correction for stray light is done in two steps. The first correction is done during the production of the L1B spectra (OML1BRUG; van der Oord et al., 2006). In this correction, specific wavelength ranges are used to define so-called source and target regions. For the source regions averaged signals are calculated using the information over the whole swath. These signals are multiplied by a polynomial that distributes the stray light over the target regions and then they are subtracted from all pixels in the corresponding target areas. The second stray light correction is done during the processing of the Level 2 ozone profile retrieval by fitting second order polynomials to both UV1 and UV2 channels separately.

Table 2 summarizes the above mentioned information. It presents the content of the optimal estimation state vector used in the OMO3PR retrieval. The state vector contains the ozone profile with 18 layers and six values for surface albedo and for stray light parameters. If the cloud fraction is lower than 0.2, surface albedos are fitted. Otherwise, cloud albedo values are fitted. In the operational retrieval, the effect of NO₂, SO₂ and aerosols are not considered. In addition to the actual ozone product, the OMO3PR algorithm produces metrics, like posterior error and averaging kernel, that can be used to evaluate the retrieval.

3 Sensitivity of the OMO3PR algorithm to a priori assumptions

3.1 Stray light

To study the sensitivity of the retrieval to the stray light corrections we turned off the two corrections separately and at the same time and processed an orbit (18 October 2005, orbit 06704, 1496*30 pixels) with all the different versions of the algorithm. Then, we studied how the retrieved ozone profiles changed on average and in six different latitude bands. Figure 1 presents the difference between the operational and modified ozone profile retrievals for the whole orbit. The error bars in the plot represent the standard deviation of the difference for each layer. Figure 1a shows that turning off both stray light corrections introduced large and oscillating changes into the retrieved profiles. When compared with the operational retrieval, the changes are 10–20 % on average. Moreover, the number of reliable retrievals dropped dramatically, from 40 000 to about 13 000 in the studied orbit (06704). This confirms that stray light correction is essential for the convergence of the algorithm. When compared with the OMI-MLS comparison results presented by Kroon et al. (2011) in their Fig. 9, it seems that these oscillating changes would decrease the difference between OMI and MLS retrievals at some latitude bands while increase it at others. Even though the signs of the changes in the ozone amounts seem to reduce oscillation in the difference between the instruments at some latitude bands, the retrieval without stray light correction could change the results too much and turn underestimated retrievals into overestimated and vice versa.

Turning off the Level 1 (L1) stray light correction while doing the Level 2 (L2) correction caused only minor changes in the ozone profiles, as can be seen from Fig. 1c. As the plot shows, the systematic changes are small at higher altitudes and almost nonexistent in the troposphere. Moreover, the usage of the Level 2 stray light correction reduces variability at all altitudes as can be seen by comparing plot 1c with 1a and 1b. The large variations at the lowest altitudes are caused by cloud-free retrievals (cloud

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value at UV2 channel (Fig. 2b). The largest decrease in ozone levels was found close to the poles but near the equator the changes were small. At high latitudes the changes were in the range of 20 %. If a first order polynomial was used for the surface albedo at both channels, the amount of tropospheric ozone increased up to 10 % on average, as Fig. 2a shows.

We also studied how the posterior errors were affected when the albedo assumptions were modified. Figure 3 shows the averaged posterior errors (solid lines) and a priori errors (dashed lines) for the studied orbit (06704). The peaks in the a priori error profiles at 3 hPa are caused by the assumption of larger a priori errors for the ozone hole conditions. We found that all three albedo assumptions produced identical posterior errors for pressure levels smaller than 30 hPa. Between 100–30 hPa pressure levels the assumption of linear albedos for both UV bands produced the largest posterior errors while the usage of a second order polynomial at UV1 band and a constant value at UV2 band produced the smallest errors. For pressure levels over 100 hPa the situation is the opposite and the assumption of linear albedos produces the smallest errors and the constant albedo at the UV2 channel the largest. This means that the usage of a constant albedo at the UV2 band decreases the amount of ozone in the troposphere (Fig. 2) but it increases the posterior errors. The situation is the opposite when using linear albedos at both bands.

3.3 Ozone climatologies as a priori information

To constrain the retrievals, the OMO3PR algorithm uses climatological ozone profiles as a priori. In addition to the profiles themselves, a priori information on the variability of ozone at each layer is used. Recently, two new ozone climatologies became available: McPeters and Labow (2012) (henceforth ML), and Sofieva et al. (2014) (henceforth TpO3).

The ML climatology is formed by combining ozone soundings and MLS data. The climatology consists of monthly average ozone profiles and standard deviation for ten

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degree latitude zones with altitudes from 0 to 66 km. A more detailed description of the climatology is given by McPeters and Labouw (2012).

The TpO3 climatology is based on a combination of ozone soundings and SAGE II (McCormick et al., 1989) satellite data. Mean ozone profiles and standard deviations are given for ten degree latitude zones and for each month. The ozone mixing ratio profiles are presented on a 1 km vertical grid. In addition, the profiles are grouped for tropopause heights in 1 km intervals. This is an important addition because variation in the tropopause height is the main driver for variability in climatological ozone values in the upper troposphere and lower stratosphere (Sofieva et al., 2014). This variability increases the a priori errors in this altitude range. The tropopause heights have values between 6 and 17 km but the number and altitude of the tropopause heights varies for different latitude bands and months. In order to have constant dimensions for the a priori ozone look-up table in the OMO3PR algorithm, all latitude and month cases were assigned with 12 tropopause heights. Tropopause height was calculated in the retrieval algorithm using temperature profiles from ECMWF data following the guidelines given by Sofieva et al. (2014). If a calculated tropopause height was outside the range of the climatological tropopause heights, the nearest climatological value was assigned for it or an average of the two closest ones was used.

In order to see how the usage of these climatologies affect the ozone retrievals, we processed two orbits (18 October 2005, orbits 06702 and 06704) using all three climatologies. For the evaluation, every 10th measurement and 10 pixels for each measurement from the middle of the swath were taken into account. In the comparisons we used the new climatologies with the operational a priori covariance matrix and with error covariance matrices calculated from the variance values given in the climatologies. A correlation length of 6 km was used to calculate the non-diagonal elements of the a priori covariance matrix.

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3.3.1 ML climatology

In the first comparison, we only changed the average ozone profiles and used the operational a priori covariance matrix. This combination produced the largest differences at the highest altitudes when compared with the operational retrieval (Fig. 4a). This was expected because the largest changes to the climatology when compared with the LLM climatology are at the top of the profiles. In addition, the amount of ozone increases around 200 hPa.

In the second comparison, we replaced the operational a priori covariance matrix with a climatological one that was calculated from the variance values given in the climatology. For this case, as Fig. 4c shows, the highest altitudes do not change much. At altitudes below 10 hPa the difference with the operational retrieval shows an oscillating behavior that increases towards lower altitudes. This is caused by the larger a priori variance of ozone in the troposphere as can be seen from Fig. 5, which presents the a priori and posterior errors for the retrievals with different ozone climatologies. In the stratosphere the ML a priori errors (Fig. 5, green dashed line) are much smaller than the operational values but for pressure levels over 50 hPa the situation is the opposite. For the posterior errors (solid green line) the situation is similar. This can also be seen from Table 3 which presents the mean a priori and posterior errors for the different retrieval versions. The unweighted mean errors are calculated for the whole profile and for the lower part of the atmosphere in order to highlight the change at the lowest altitudes. Regarding the values for the whole profile, the ML errors are close to the operational ones, however, at the lowest altitudes ML values are significantly larger (a priori ~ 60 % larger, posterior ~ 35 % larger).

3.3.2 TpO3 climatology

For the first comparison, we used operational a priori covariance matrix with the TpO3 climatology. As Fig. 4b shows, the largest differences are seen around 200 hPa, TropO3 giving smaller ozone values than the operational retrieval.

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the stratosphere. As a whole, Fig. 7 shows that the distribution of degrees of freedom for a retrieval depend mainly on the selection of the variance values used in the a priori covariance matrix.

In addition to degrees of freedom, it is important to consider how these different a priori assumptions affect the a priori and posterior errors. Figure 8 presents the errors for the discussed versions of the retrieval (dashed lines for a priori and solid lines for posterior). Figure 8a shows the errors for the operational retrieval and for two versions with TpO3 climatology. The first version (TpO3) has the same albedo assumptions as the operational while for the second one (TpO3_alb) a linear albedo is assumed in the UV2 channel. As the dashed lines show, all the retrievals have the same a priori errors. The usage of the TpO3 climatology produces slightly smaller posterior errors than the operational version at some altitudes and the modified albedo only has a minor effect at the lowest altitude. Figure 8b shows the errors for the retrieval versions with the TpO3 climatology, modified albedo and climatological a priori covariance matrix. For the first version (TpO3_alb_covar), the a priori errors are taken directly from the climatological variance values, thus the a priori errors in the stratosphere are small. For the two other versions, minimum a priori errors were assumed to be either 10% (TpO3_alb_covar_10) or 20% (TpO3_alb_covar_20). As the plot shows, posterior errors are significantly different for these versions. In the troposphere, the posterior errors are larger than for the retrievals with the operational a priori errors. In the stratosphere, smaller a priori errors produce smaller posterior errors which is to be expected. Although the errors look significantly different for the retrievals with operational and climatological a priori error covariance matrices, the relative change between the a priori and posterior errors stay in the same range for all the versions, especially in the troposphere. In the stratosphere, the operational a priori covariance matrix produces slightly larger reduction in the uncertainty. Based on these results it seems that all the retrieval versions are as effective in reducing the uncertainty and that the posterior error values depend mostly on the assumed a priori errors.

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Based on the sensitivity tests discussed in this section and our aim to improve the accuracy of the OMO3PR retrievals in the troposphere, we decided to make the following modifications to the algorithm: (1) we replaced the LLM ozone climatology with the TpO3 climatology, (2) we replaced the operational a priori covariance matrix with a climatological version that is based on the variance from the TpO3 climatology (with min. 10 % standard deviation, separated tropo- and stratosphere), and (3) we replaced the second order polynomial for the albedo in the UV2 channel with a first order polynomial. The tropo- and stratosphere were separated in the climatological error covariance matrix, although, our sensitivity studies (not shown) did not show visible effects in ozone abundances caused by this modification. In addition, we updated the retrieval's vertical pressure grid to $P_i = 2^{-i \cdot 1.37/2} \times 1000$ for $i = 0.18$ which follows the principles presented by Liu et al. (2010) without changing the number of layers. We also tested how sensitive the retrieval is to the selection of the correlation length. The operational retrieval uses correlation length of 6 km, thus, we tested how the retrieved ozone abundances change if correlation lengths of 1 km, 3 km or 12 km are used instead. Our comparisons showed that only the selection of 1 km as correlation length had a significant effect on the retrieved ozone profiles. This selection increased oscillations in the profiles. Based on these results we decided to use the operational correlation length.

4 Evaluation of the modified algorithm

In order to see if the modifications to the algorithm improved the correspondence of the tropospheric ozone profile retrievals with other methods, we compared our results with the results published by Eremenko et al. (2008). The modified version of the algorithm uses a different pressure grid than the operational one, thus we had to interpolate the profiles in order to compare values for the exactly same altitude range. This was done by calculating a cumulative ozone profile in Dobson units from the top of the atmosphere down to the bottom of each layer and interpolating it to keep the total ozone amount in the column constant. Then, the tropospheric ozone abundance was taken

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parametrization also has a significant effect on the retrieved ozone profile but mainly in the layers close to the surface. The selection of the a priori ozone profile climatology had a relatively small effect on the retrieved ozone profiles while the usage of climatological variance values in the a priori covariance matrix increased the differences significantly. Based on these sensitivity studies we modified the OMO3PR algorithm to improve the accuracy of tropospheric ozone retrievals. This was done by replacing the operational ozone climatology (LLM) with TpO3 climatology, by using climatological variance values in the a priori covariance matrix and by changing the wavelength dependency of surface albedo in the UV2 channel from a second order polynomial to linear. Our studies showed:

1. a priori covariance matrix basically defines the vertical distribution of degrees of freedom for a retrieval.
2. We were able to increase degrees of freedom significantly in the troposphere by increasing a priori errors in the troposphere and lower stratosphere, and by decreasing them at higher altitudes.
3. All the studied versions of the OMO3PR algorithm were equally effective in reducing uncertainty in the retrieved ozone profiles. This implies that the posterior error values depend mostly on the chosen a priori errors.
4. When compared with the IASI measurements presented by Eremenko et al. (2008) the new version produced over 10 % smaller ozone abundances in the troposphere over Europe which reduces the systematic overestimation of the OMO3PR algorithm.

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Table 1. The agreement between OMO3PR and other ozone profile observations in percents. Summarized from Kroon et al. (2011). The instruments used in the study are the Microwave Limb Sounder (MLS), the Tropospheric Emission Spectrometer (TES), the Stratospheric Aerosol and Gas Experiment (SAGE II; McCormick et al., 1989), the Halogen Occultation Experiment (HALOE; Russell et al., 1993), the Optical Spectrograph and Infrared Imager System (OSIRIS; Llewellyn et al., 2004), the Global Ozone Monitoring by the Occultation of Stars (GOMOS; Bertaux et al., 2010) and balloon-borne ozonesondes (ECC).

	Tropical	Mid-latitude	Polar
OMI – MLS [%]	±10	±10	±30
OMI – TES [%]	±20	±30	±60
OMI – SAGE II [%]	10–60	20–40	
OMI – HALOE [%]	> 30	> 30	
OMI – OSIRIS/GOMOS [%]		±10	–15–20
OMI – ECC [%]	5–80	5–60	10–20

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Table 2. Content of the Optimal estimation state vector and the related a priori information used in the OMO3PR retrieval.

Optimal estimation state vector Species	Number of elements	a priori information	a priori error
O ₃ profile	18	LLM climatology (McPeters et al., 2007)	20 % (For ozonehole conditions 60 % (21–50 km) and 30 % for other altitudes.)
Surface albedo (surface or cloud)	6	OMI surface albedo climatology (Kleipool et al., 2008)	100 %
Stray light	6	0	100 %

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Table 3. Mean a priori and posterior errors in percents for three retrievals: operational, with ML ozone climatology and with TpO3 climatology. Mean unweighted errors are presented for the whole profile and for lower atmosphere (> 100 hPa). The values are calculated from the data presented in Fig. 5.

a priori	Operational	ML	TpO3
Whole column	19.8 %	20.6 %	16.6 %
Lower atmosphere (> 100 hPa)	19.5 %	30.7 %	28.8 %
posterior			
Whole column	10.5 %	12.0 %	10.0 %
Lower atmosphere (> 100 hPa)	15.5 %	21.0 %	19.2 %

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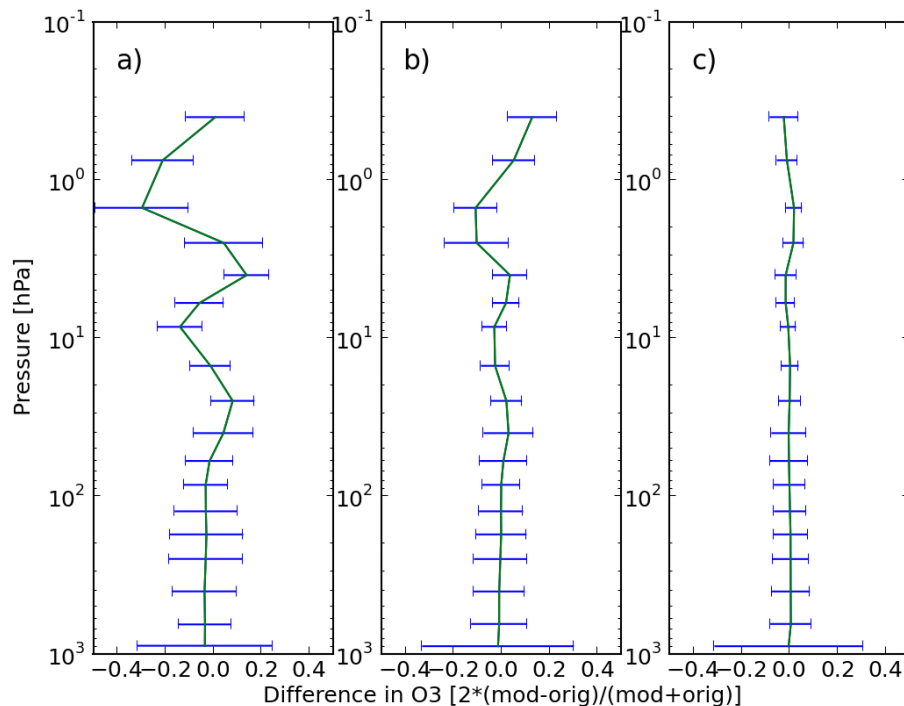


Fig. 1. Effect of stray light corrections. Change in the ozone profiles when the retrieval has no stray light correction (a), only L1 correction (b), and only L2 correction (c). Error bars show the standard deviation of the difference.

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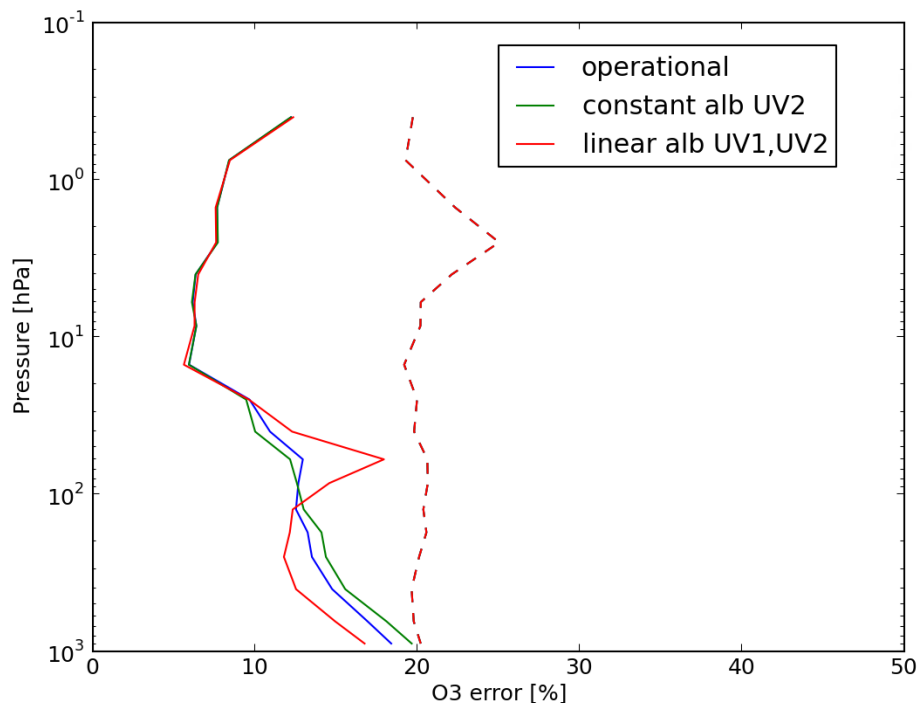


Fig. 3. Effect of albedo assumptions on posterior errors (solid lines). Operational retrieval is shown in blue, linear albedos at both UV1 and UV2 channels instead of second order polynomials shown in red, and constant albedo at UV2 channel instead of second order polynomial is shown in green. Dashed lines show the a priori errors.

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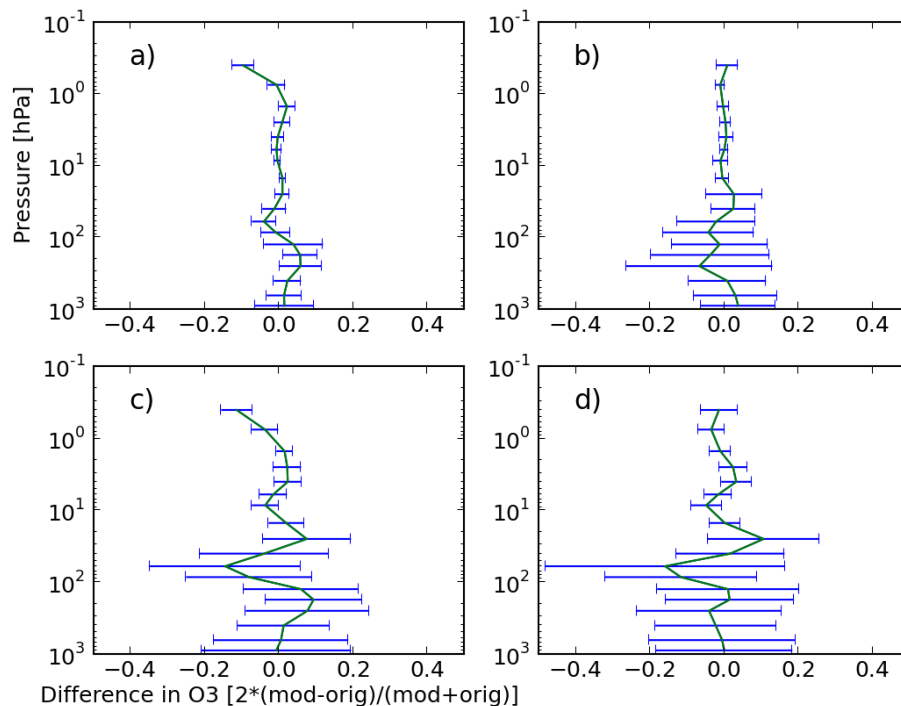


Fig. 4. Effect of a priori ozone climatologies. Change in ozone profiles when ML (a) and TropO3 (b) are used with the operational error covariance matrices. Change in ozone profiles when ML (c) and TropO3 (d) are used with climatological covariance matrices. Error bars show the standard deviation of the difference.

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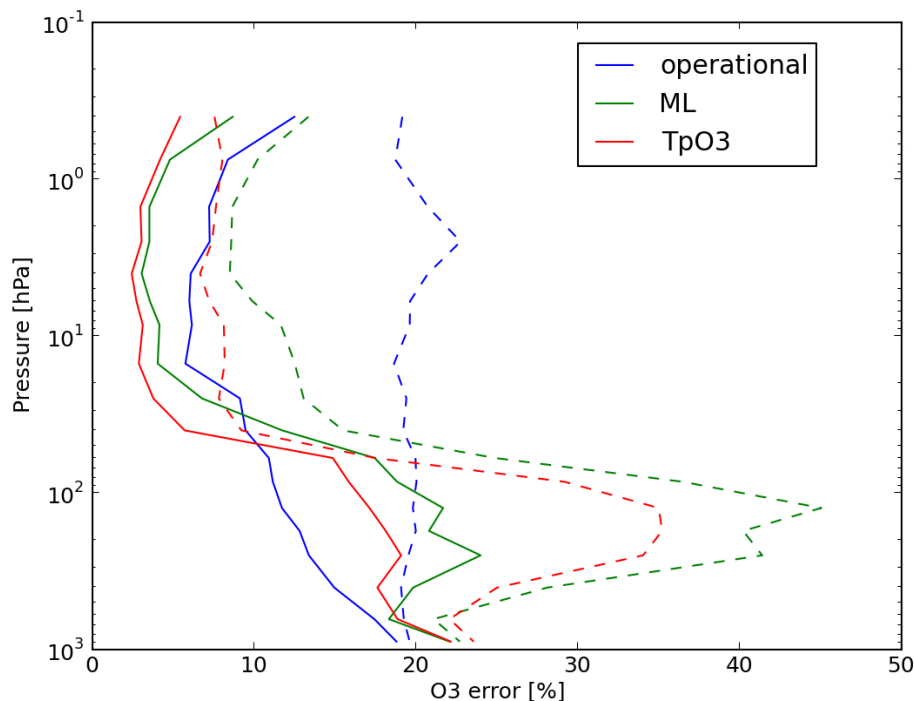


Fig. 5. Effect of ozone climatologies on a priori (dashed lines) and posterior errors (solid lines). Operational retrieval is shown in blue, ML climatology in green and TpO3 climatology in red. The a priori errors for ML and TpO3 climatologies are based on the ozone variability reported in the respective climatologies.

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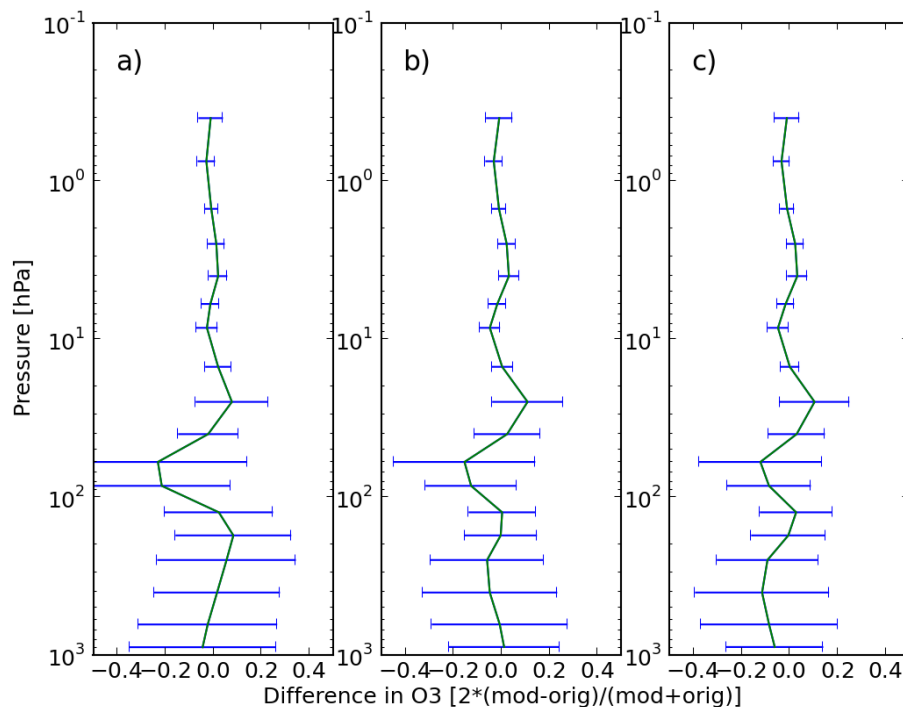


Fig. 6. Effect of albedo assumptions with the TropO3 climatology. **(a)** assuming linear albedos at both UV1 and UV2 channels instead of second order polynomials. **(b)** assuming constant albedo at UV2 channel. **(c)** assuming linear albedo at UV2 channel. Error bars show the standard deviation of the difference.

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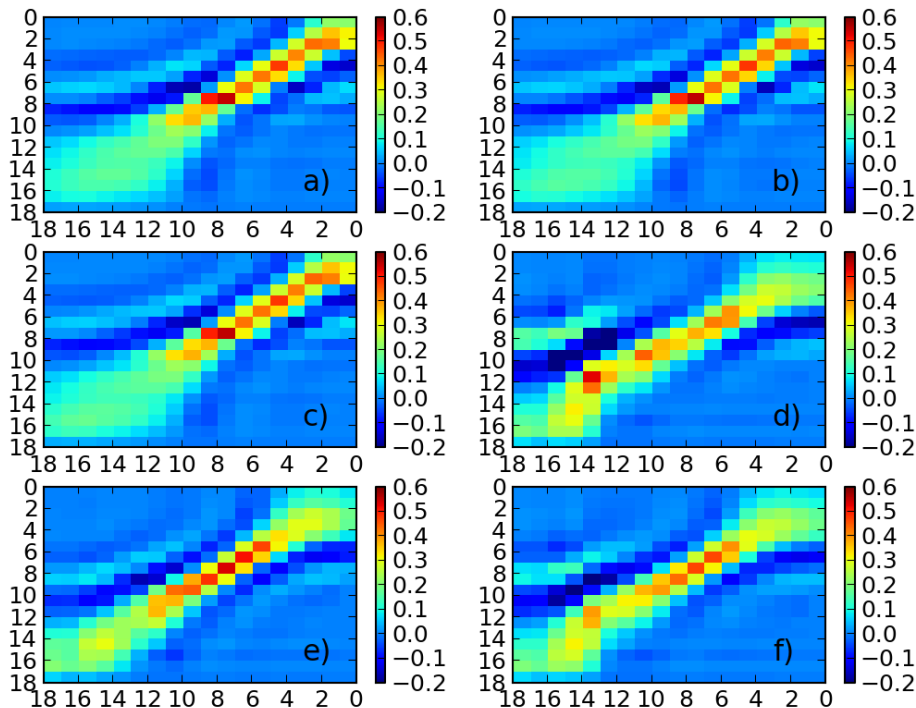


Fig. 7. Mean averaging kernels from 34 pixels on the 17 July 2007 (45–55° N, 20–30° E) for the operational retrieval **(a)**, with the TpO3 climatology **(b)**, with TpO3 and linear albedo in UV2 channel **(c)**, with TpO3, linear albedo in the UV2 channel and a climatological error covariance matrix **(d)**, with a climatological error covariance matrix and minimum of 20 % variance **(e)** and with a climatological error covariance matrix and minimum of 10 % variance (TpO3_alb_covar_10), **(f)**. Axis are the layer indexes, 18 being the layer closest to the surface.

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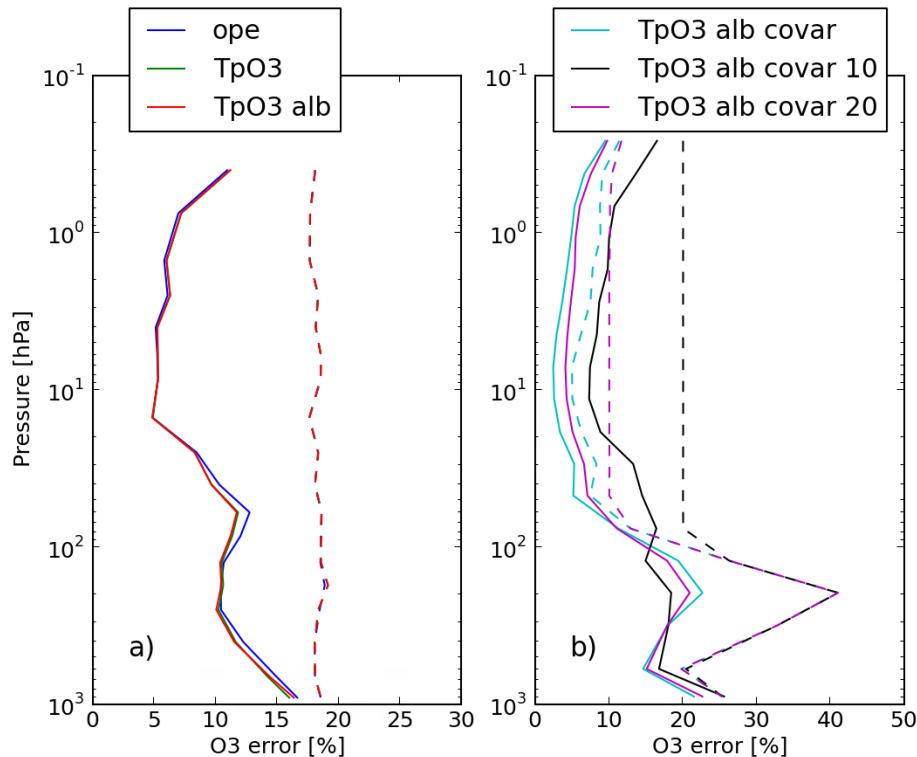


Fig. 8. Effect of a priori covariance matrix assumptions on a priori (dashed lines) and posterior errors (solid lines). Operational retrieval is shown in blue, TpO3 climatology in green, TpO3 with linear UV2 albedo in red (a), TpO3 with climatological a priori errors in cyan, TpO3 with climatological a priori errors with minimum of 20 % in black and TpO3 with climatological a priori errors with minimum of 10 % in magenta (b).

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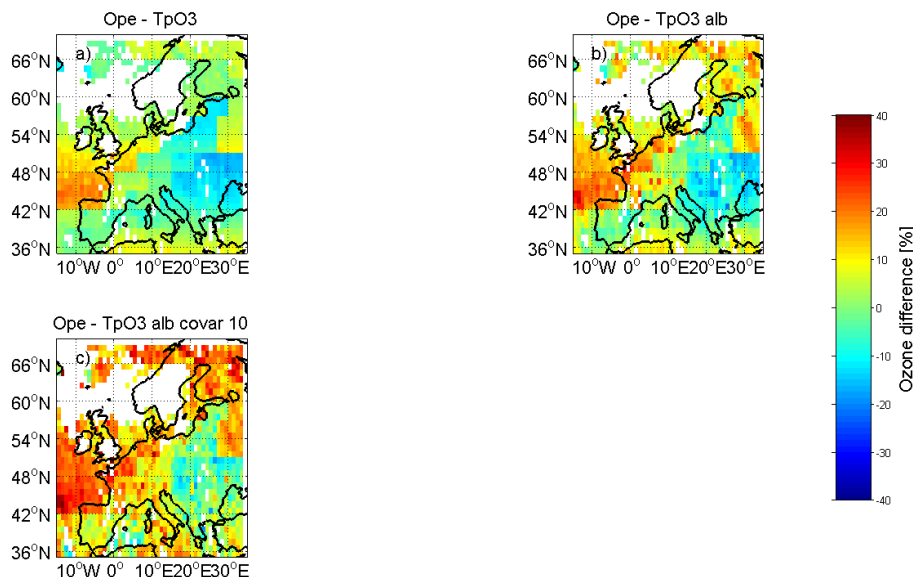


Fig. 9. Difference in tropospheric ozone abundances (up to 400 hPa) between operational (ope) and modified OMO3PR retrievals on 17 July 2007. Modified versions of the OMI retrieval algorithm are: TropO3 climatology and operational albedo (a), TropO3 climatology and linear albedo in UV2 (b), and TropO3 climatology, linear albedo in UV2 and climatological error covariance matrix (c). Daily data averaged on 1×1 grid. Averaged differences are given in Table 4.

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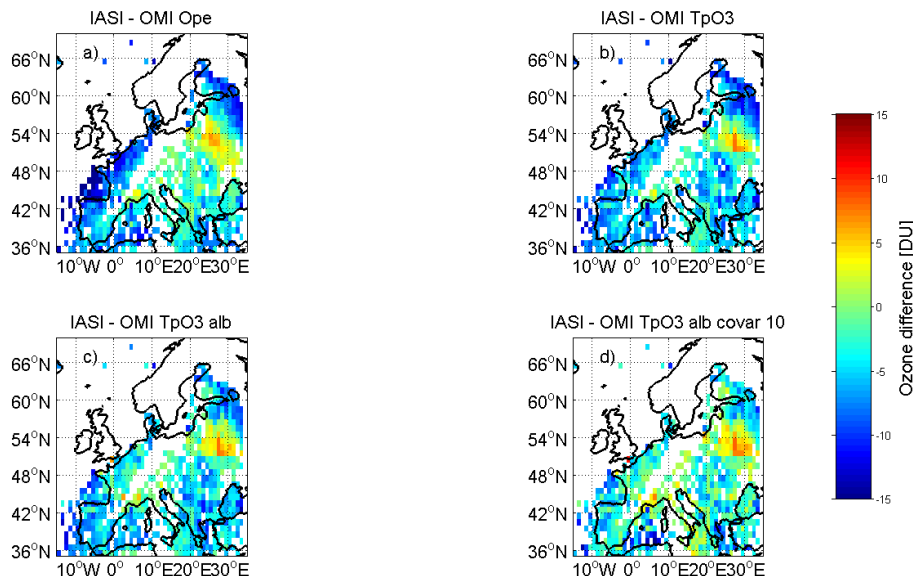


Fig. 10. Difference in tropospheric ozone abundances (up to 400 hPa) between IASI and OMI on 17 July 2007. Four different versions of the OMI retrieval algorithm are used: operational **(a)**, TropO3 climatology and operational albedo **(b)**, TropO3 climatology and linear albedo in UV2 **(c)**, and TropO3 climatology, linear albedo in UV2 and climatological error covariance matrix **(d)**. Daily data averaged on 1×1 grid. Statistics of the differences are given in Table 4.