

RECENT DEVELOPMENTS TO THE RAL JOINT IASI+GOME-2 OZONE PROFILE RETRIEVALS USING TIR, UV AND VISIBLE SPECTRA

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ABSTRACT

We present results from recent developments of the RAL Ozone Profile optimal estimation retrieval scheme. The algorithm produces both a GOME-2 only and a joint IASI and GOME-2 profile product, both of which have sensitivity to tropospheric ozone. The joint product has been selected for the ESA Climate Change Initiative Ozone nadir prototype product, for which data will be disseminated to the climate modelling community. Time-series and highlights from several years of the single and joint MetOp-A GOME-2 and IASI retrievals are presented. We further present results of the introduction of measurements from the Chappuis ozone bands to add near-surface ozone information to the retrieval under certain atmospheric and surface conditions.

1. RAL UV OZONE PROFILE RETRIEVAL

The RAL Ozone Profile (RALOP) algorithm has a long and successful heritage, where sensitivity to tropospheric ozone was first demonstrated for the Global Ozone Monitoring Experiment (GOME) by [1]. The scheme has been subsequently developed, and has been applied to SCIAMACHY and GOME2 (on MetOp-A and B) measurements. As part of the ESA CCI project, RALOP was selected as the Ozone ECV (Essential Climate Variable) prototype algorithm for processing the entire GOME, SCIAMACHY and GOME-2 for Level 2 users.

RALOP is optimised to be sensitive to tropospheric ozone which requires high precision fitting in the Huggins bands. It is a sequential algorithm, where a direct fitting of the Hartley bands (270-306nm) is performed to establish a good stratospheric ozone profile, followed by a quick surface albedo fit at 335nm with the final stage being the Huggins bands fit (323-335nm). Information from the shorter wavelength and surface albedo fit are used as prior and input into the final step. The Huggins bands fit is a fit to the logarithm of the sun normalised radiance with a polynomial removed, which makes this part of the retrieval less sensitive to absolute radiometric calibration (which is potentially problematic for UV spectrometers of the GOME class), however due to the tight fitting

requirements for tropospheric ozone good wavelength registration of the measurement is very important. As such, both a wavelength registration and an off-line slit function retrieval are performed using the direct solar measurement. Indeed, accurate characterisation of the instrument response function was identified as a crucial requirement for reducing errors for tropospheric ozone retrieval in the GOME-2 Error Study performed at RAL [2]. A degradation correction is derived and applied to GOME-2 Band 1 measurements based on forward modelling from a climatological profile. Finally, the tight fitting precision in the Band 2 fit is achieved by fitting additional scaling factors for the leading principle components derived from a data subset of ozone profile retrieval residuals over 1 year. These patterns account for a range of instrumental artefacts and aspects of the atmosphere that are not sufficiently represented in the forward model. The absolute magnitude of these patterns is small and the pattern shapes are robust with time and space.

Fig. 1 shows monthly mean ozone sub-columns that demonstrate some characteristics of the RALOP sensitivity to tropospheric ozone for two months in 2008 (March and July). During Northern Hemisphere (NH) spring it is a challenge in the UV to detect tropospheric ozone at high latitudes because of the very high stratospheric ozone burden in addition to the relatively low tropopause to observe a relatively small ozone column below. The NH summer tropospheric ozone distribution is well characterised, with characteristically high ozone in the Mediterranean region – which is in good agreement with the spatial distribution and amount suggested by chemistry transport models (e.g. [3]).

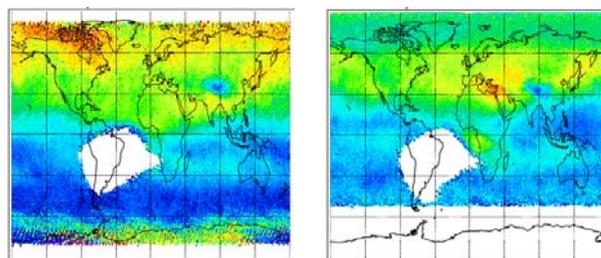


Figure 1 Monthly mean surface to 450hPa ozone (Dobson Units) for March (left) and July (right) in 2008 from RALOP

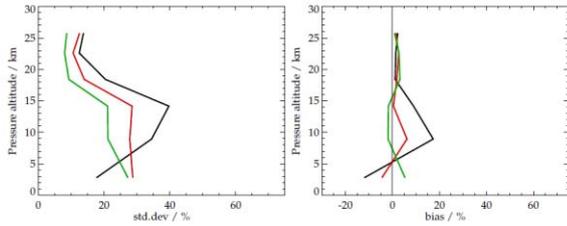


Figure 2. Standard deviation (left) and bias (right) for the RALOP scheme as compared to ozonesondes in 2007-2008. The prior agreement is indicated black, the red is the direct comparison between the retrieved profile and sondes, and the green line indicates the comparison with sondes with the GOME-2 averaging kernels applied. Collocation criteria are indicated in the text.

Fig. 2 indicates the quality of the ozone profiles retrieved by RALOP in a validation with ozonesondes. The data used have been cloud-cleared and the collocation criteria are 200km and 2 hours. The sondes convolved with the GOME-2 averaging kernels yield a bias of 6% in the lower troposphere and less in the sub-columns above. The standard deviation from sondes is also smallest for the convolved profiles and is an indication that the ozone variability is better captured by the retrieval than the prior in all but the lowest sub-column.

2. RAL JOINT IASI+GOME-2 PROFILE RETRIEVAL

RALOP produces ozone profiles from the infrared (IR) instrument IASI, in addition to UV instruments. The nature of the vertical information that can be obtained in the IR from IASI is different from in the UV, and may be considered to be complementary. cursory inspection of averaging kernels for each instrument shows the greater sensitivity for IASI over GOME-2 in the upper troposphere/lower stratosphere (UTLS) region in particular. The sensitivity of IASI to ozone lower in the troposphere can depend upon the thermal contrast in the field of view. By combining information from both instruments in a joint retrieval (the Huggins bands step of the conventional UV profile retrieval) this complementarity can be exploited.

Fig. 3 shows an example of how this complementary sensitivity can improve ozone retrieved in the UTLS region. Better separation of the tropospheric and stratospheric ozone is achieved in the NH region which is traditionally challenging for the UV instrument alone. Better representation of upper tropospheric ozone in the tropics is also evident. As with the IASI-only retrieval scheme, the joint scheme is more sensitive to the presence of cloud and certain surface types which can affect the retrieval quality, and making the scheme more

robust in these conditions will constitute further development of the scheme.

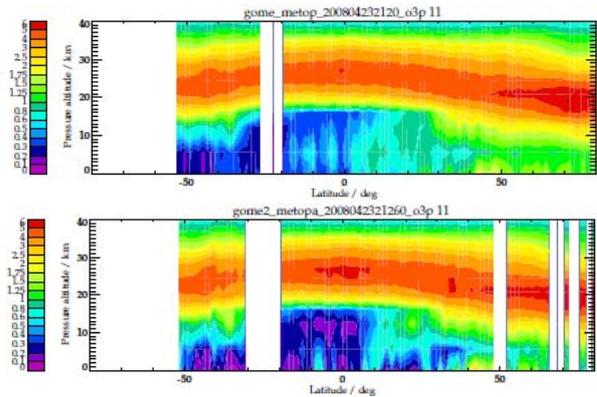


Figure 3. An orbit cross-section of ozone across the East Pacific and over Southeast Asia for GOME-2 only (top) and that retrieved jointly with GOME-2 and IASI (bottom) on 23rd April 2008. The improved separation in the UTLS in the NH is evident, and the lower ozone retrieved in the tropical upper troposphere for the joint scheme.

3. RETRIEVAL OF OZONE USING THE VISIBLE CHAPPAUIS BANDS

It has been identified that the Chappuis ozone bands (~440-750nm) represent a unique opportunity to obtain information about near-surface ozone concentration [4] that cannot be obtained by passive sensors in any other spectral region. The minimum reflectance is higher (specifically over land), and there is lower Rayleigh/aerosol scattering.

In contrast to the Huggins bands, which have relatively high differential spectral structure, the Chappuis bands are very broad with limited differential structure. There are many other atmospheric constituents which have broadly varying spectral structure in this region which can interfere with an attempt to accurately fit ozone here. Furthermore, the principle challenge of accurate spectral fitting for ozone in the Chappuis bands is the highly variable spectral shape of the surface itself, which can also change with time. [5] sought to fit ozone with the Chappuis bands but found the errors that arose due to surface characterisation and influence from other absorbers made the quality of ozone retrieved too large to make the ozone product useful.

Here we present an alternative approach and indicate the way in which the Chappuis ozone column can be used to improve upon the UV (and potentially UV+IR) profile product. The first part of this work is a study to identify the conditions in which one could expect to

obtain increased information about near surface ozone from the Chappuis bands in addition to that provided in the UV. The second part of the work is to show that the total column ozone retrieved from the Chappuis bands only can be fit to the precision defined in the prior study that is required to be able to add information to the UV-retrieved ozone profile, and suggests a method of implementation. The method is presented in detail in [6].

Joint retrieval using simulated measurements in the UV and visible part of the spectrum for a range of signal to noise (snr) ratios and surface types predict the averaging kernels under these ranges of conditions. Samples of these averaging kernels are shown in Fig. 4 for a European climatological ozone profile over a “grass-like” surface. These simulations for a fitting window of 450-550nm demonstrated that a snr of greater than 300 is required for the averaging kernels representing the 0-2km and 0-6km sub-columns to become significantly large. Although this threshold snr is smaller for a wider spectral fitting, a fit with real measurements is likely to become more difficult above 550nm where it would additionally have to incorporate GOME-2 Band 4.

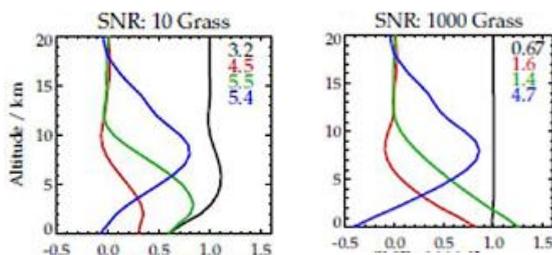


Figure 4. Simulated averaging kernels for a joint retrieval of ozone for sub-columns 0-2km in red, 0-6km in green, 6-12km in blue and total column in black. The inset numbers in corresponding colours indicate the estimated error on the sub-columns.

Since it is unlikely that it would be either practicable or possible to apply the retrieval approached simulated here to all 4 GOME-2 channels simultaneously (principally due to instrumental issues), it would be more sensible to use an approach that would separate the fitting of both parts of the spectrum, particularly as the Chappuis bands can only provide one piece of information about ozone. The simulations of averaging kernels are repeated for a Chappuis-only retrieval. It can be shown that in this case the break-through snr value corresponds to a column fitting precision of between 2 and 4 DU (depending upon surface type). After this is established, it then becomes necessary to demonstrate that this can be achieved with real measurements.

The approach presented here involves a DOAS methodology where many spectral patterns are required

to be fit which represent atmospheric constituents and surface characteristics that occur in this spectral region. Patterns for O_3 , O_4 , NO_2 are used. Since the water vapour spectrum in the Chappuis bands can exhibit strong line absorption that has temperature and pressure related characteristics, a mean cross-section is derived and fit from simulations from a training set of atmospheric profiles, in addition to two leading eigenvectors that can represent the main variability characteristics. A similar approach is used for the Ring spectrum. A set of 0-3rd order polynomials are fit, the shape of which are able to represent the spectral behaviour of Rayleigh scattering, aerosol and cloud. Finally, a set of patterns are fit that represent surface spectral behaviour within a scene. They are the leading patterns derived from a set of surface and mineral spectral databases (ASTER and USGS references to go here). These patterns are fully described in [6].

A DOAS retrieval of the Chappuis slant column is performed using a standard least-squares fit. The ozone slant column can be directly compared to the O3M-SAF operational slant column product. Initial comparisons were favourable, but the mean residuals of the fit indicated that there were unknown instrumental or atmospheric terms that were not being sufficiently fit. A month of these mean residuals were then used to introduce a further pattern into the DOAS fit. Only mean residuals from scenes of high tropical cloud were used to construct this pattern - from a retrieval where the ozone was constrained to the SAF L2 slant columns amount and the surface patterns were not fit - since the light path is relatively simple and unlikely to be very different between the visible and UV (where the L2 product is derived). Retrievals including this pattern, and a similar pattern over cloud-free ocean improved the agreement with the L2 product, an example is shown in Fig. 5.

The results in Fig. 5 indicate that the level of agreement in many scenes is within the limit specified previously in terms of the required precision to make the slant column estimate add information to the UV product. Some account must be taken of the differences in air mass factors (AMFs) in the spectral regions, which will limit the agreement between the slant columns derived in the UV and the visible. AMFs can be calculated using a radiative transfer model, both for clear-sky profiles and with a simulated cloud, should cloud information be available.

These AMFs have been calculated using ozone profiles retrieved by RALOP and can be shown to explain much of the remaining differences between the SAF L2 and Chappuis slant columns.

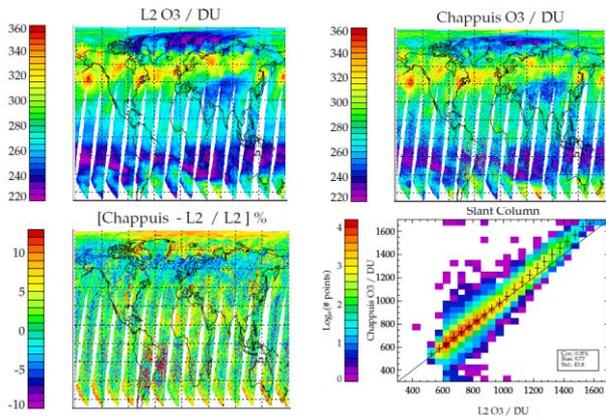


Figure 5. The top left and right panels show the SAF L2 and RAL Chappuis total column derived from the retrieved slant column using the geometric air mass factor. The bottom left panel shows the percentage difference, and the bottom right the correlation.

It is envisaged that the final step required to combine the information is to use the difference between the Chappuis slant column and the slant column predicted using the AMFs from the UV profile, in a linear retrieval step using the derivative of the light path in height in the Chappuis bands as a forward model. This step will form the basis of future work.

4. REFERENCES

1. Munro, R, R. Siddans, W.J. Reburn, B.J. Kerridge (1998). Direct measurement of tropospheric ozone distributions from space. *Nature*, **392**, No.6672, 168-171
2. Kerridge, B.J. R. Siddans, B. Latter, I. Aben, C. Tanzi, W. Hartmann, J. P. Burrows, M. Weber, R. de Beek, V. Rozanov, A. Richter (2004). GOME-2 Error Assessment Study, Phase V: Final Report, EUMETSAT Contract EUM/CO/01/901/DK
3. Richards, N., Arnold, S., Chipperfield, M., Rap, A., Monks, S., Hollaway, M., Miles, G., Siddans, R., (2013). The Mediterranean summertime ozone maximum: Global emission sensitivities and radiative impacts, *Atmospheric Chemistry and Physics*, 13, 2331-2345. doi: 10.5194/acp-13-2331-2013
4. Chance, K., Burrows, J et al., (1997). Satellite measurements of atmospheric ozone profiles, including tropospheric ozone, from ultraviolet/visible measurements in the nadir geometry: a potential method to retrieve tropospheric ozone, *J. Quant. Spectrosc. Radiat. Transfer* **51**(4), 461476
5. Richter, A., F. Wittrock, M. Weber, and J. P. Burrows (2012). Evaluating the potential of GOME-2 ozone column retrievals in the Chappuis bands, EGU2012-1747 AS3.0 XY71, EGU Conference 2012.
6. Miles, G., Siddans, R., Tuinder, O. (2013). Analysis of GOME-2 level-1b data quality and degradation effects on operational ozone profile retrievals. SAF Visiting Scientist Final Report (Available at <http://o3msaf.fmi.fi/VSreports.html>)