Review of MTG UVS Mission Requirements

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1 INTRODUCTION

This report comprises a critical review of the specification for the MTG-UVS mission requirements' in relation to the objective of providing routine observations for operational air quality and atmospheric chemistry applications in the 2015 – 2025 era. The intention of this review commissioned by Eumetsat was to:

- Assess the extent to which currently-defined User Requirements are likely to be met through observations by UVS according to its current specifications
- Identify deficiencies or missing specifications
- Recommend possible improvements to the current specifications
- Recommend appropriate scientific studies to analyse in suitable depth the potential impact of the specifications on UVS products

The following set of nine specific issues has been addressed:

1. Value which could potentially be added by UVS to IRS for CO and CH₄.
2. Whether Chappuis bands could add worthwhile information on tropospheric O₃.
3. Whether spectral measurements in two polarisations could add worthwhile information on tropospheric O₃, and what additional instrument requirements would be needed for this.
4. Spectral resolution and spectral (over)sampling
5. Sensitivity to instrumental errors (nb radiometry, spectral stability & slit-function shape) and resulting requirements on accuracy/knowledge.
6. Variation with season of illuminated latitude range
7. Requirements for additional information to facilitate trace gas retrieval (nb aerosol, cloud, temperature, surface BRDF) and whether data auxiliary to MTG UVS and IRS will be required.
8. Initial assessment of potential for synergy with polar orbiting nadir-uv and/or limb-emission sounders to constrain the stratospheric and upper tropospheric distributions of O₃ and other targeted trace gases.
9. Ground pixel size as a function of latitude/longitude and corresponding variation in cloud(-free) occurrence.

The review has been conducted by Dr. B.J.Kerridge and Dr. R.Siddans of the Remote-Sensing Group in the Earth Observation and Atmospheric Science Division, in consultation with other members of the Group. It has focused mainly on O₃ profile retrieval, drawing primarily on experience from polar orbiting nadir-viewing uv spectrometers eg:

1. Development and large-scale application of GOME-1 processing scheme which delivers height-resolved O₃ spanning the troposphere as well as the stratosphere.
2. Practical demonstration of synergistic use of stratospheric O₃ L2 products from MIPAS to constrain tropospheric O₃ retrieval from GOME-1 and SCIAMACHY (Huggins bands)
3. Eumetsat GOME-2 Error Study, in which a number of instrumental and radiative transfer issues were addressed, with a view to assessing their impacts on error budgets of retrieved trace gases and recommending operational settings and actions to mitigate errors.
2 VALUE WHICH COULD POTENTIALLY BE ADDED BY UVS TO IRS FOR CO AND CH₄

RSG has recently co-ordinated the 2nd extension to the ESA study “Definition of Mission Objectives and Observational Requirements for an Atmospheric Chemistry Explorer Mission”. In this study, the potential of near-ir nadir sounding was quantitatively assessed through detailed simulations, with particular regard to the information which could be added to observations by IASI on MetOp. One of the key findings of this study was that, despite the fact that short-wave measurements tend to be more sensitive near the surface than mid-ir observations (which depend on temperature contrast), the relative strength of the 4.7 micron CO band compared to that 2.35 microns means that IASI can provide better retrievals even in the boundary layer (<2km) than the current concept for a grating instrument measuring the short-wave band. The resolution of IRS (0.6cm⁻¹) is sufficient for sounding CO with similar quality compared to that of the FTS simulated for the ESA study. It is therefore considered unlikely that the UVS measurements of CO will contribute significant information over that provided by IRS (though detailed retrieval simulations based on the specific instrument concepts would be required to confirm this).

The retrieval of CH₄ by an optimised nadir near-ir sounder was found to be rather promising, with precision on boundary layer mixing ratios being adequate to meet climate-related user requirements (~3%). However useful precision could only be achieved over high-reflectance land (albedo 0.3) or under sun-glint conditions. This achievable precision is comparable to that reported for IRS in [3].

The rationale for the stated user requirement to monitor CH₄ with better than daily temporal sampling is not clear: 12 hours is the most stringent temporal sampling requirements identified for CH₄ in the current ESA “CAPACITY” study to define requirements for operational chemistry monitoring. 6 hours is the resolution assumed in [3] at which useful signal to noise is achieved.

The initial assessment here is that measurements of CO at 2.3 microns would probably not add information to retrievals from IRS. There might be some benefit to CH₄ retrievals under specific (high-albedo) observing conditions but that it is not clear that such observations would meet a well-defined user requirement.
3 WHETHER CHAPPUIS BANDS COULD ADD WORTHWHILE INFORMATION ON TROPOSPHERIC O₃

Although studies have suggested that some information on tropospheric O₃ might be available from the Chappuis bands, this has never been demonstrated in practice to be useful compared to Hartley-Huggins observations by GOME, SCIAMACHY or other nadir spectrometers. Some simulations which demonstrate both the potential and the difficulty in practical exploitation are shown in Figure 3-2. Typical absorber optical depths are shown in Figure 3-1. Although, in the ideal case, precision in the lower troposphere could improve from ~40% to ~20% on including the range 460-540nm, extraction of this information depends on highly precise knowledge of all processes which impact the observed radiance on spectral scales broader than ~10nm, including:

- Radiometric calibration and stability. Neither GOME-1 nor SCIAMACHY have proved adequate in this specific respect.
- The surface albedo (which in practice has spectral structure as a function of surface type)
- Spectral structure in aerosol back-scatter

Note that a priori surface albedo precision of much better than 0.1% (at 10nm spectral scale) is required to recover similar information to the “No albedo fit” case shown in the figure. This implies an analogous requirement on radiometric calibration accuracy. (Note that absolute peak optical depth of the Chappuis feature at 600nm is ~0.05 implying radiometric accuracy requirements at the few % level even to begin to extract information, before information is added to the Hartley-Huggins signal.)

Other means exist to improve the information content in the troposphere including measurement of polarisation and combining the Harley-Huggins information with that from other sensors to better constrain the upper part of the profile (e.g. limb sounders, or IRS, making use of the differential sensitivity to the boundary layer of the uv / mid-ir nadir sounding techniques). We consider these approaches to be more likely to prove successful than attempting to exploit the Chappuis bands.

However, the Chappuis spectral range is contiguous with that which will be required to observe NO₂ and could be restricted to <540nm while retaining most of the information content, provided radiometric calibration is adequate. Spectral resolution requirements for the range should be modest. It would be desirable to more fully assess the radiometric requirements which would be adequate for useful Chappuis retrieval before finally concluding that extension of the spectral range is not justified.
Figure 3-1: Vertical optical depths for a typical mid-latitude atmospheric scenario.
Figure 3-2: Precision on ozone profile retrievals on a 6km vertical grid. Left hand panels show how estimated precision improves as more and more spectral coverage is included starting from 100% a priori error. In the standard case surface albedo represented by a piece-wise linear function on a 10nm grid is retrieved, with 100% a priori error. In the second case the albedo is assumed to be perfectly known. Only in the latter case does the Chappuis band significantly improve the estimated $O_3$ precision. Note that similar precision to the standard case is assumed even when an a priori of 0.1% is assumed for surface albedo. Signal to noise of the measurements is assumed to be as predicted by a GOME instrument model, for typical mid-latitude observing conditions and surface albedo 0.3. Averaging kernels for the “standard” case are shown on the right for the 240-340nm range (top) and 240-700nm range (bottom). From 4.
4 WHETHER SPECTRAL MEASUREMENTS IN TWO POLARISATIONS COULD ADD WORTHWHILE INFORMATION ON TROPOSPHERIC O₃, AND WHAT ADDITIONAL INSTRUMENT REQUIREMENTS WOULD BE NEEDED FOR THIS.

4.1 Background and qualitative assessment

The potential of adding q, the ratio of 1st and 2nd Stokes parameters (Q/I), to a measurement vector containing log(I/Iₒ), where Iₒ is the direct-sun irradiance, was assessed by SRON⁵. Although we do not agree with statements made in this paper in regard to: (a) how to formulate the O₃(z) retrieval problem to best extract information from spectrally-resolved backscattered solar UV measurements and (b) impact of spectroscopic uncertainties in ozone Huggins bands, we share the SRON view that addition of q to the measurement vector could, in principle, offer an incremental increase to tropospheric O₃ information and that, for design of MSG-UVS, this should be carefully evaluated.

Comments on the specific approach adopted by SRON are as follows:

1. The simulations undertaken by SRON do not exploit fine structure controlled by ozone in either the q spectrum or the reflectance (I/Iₒ) spectrum. Because it does not exploit differential structure, the SRON approach would, in practice, be more susceptible to broad-band errors in (a) the characterisation of instrument properties (ie radiometric and polarisation key data) and (b) in-flight calibration of q and reflectance spectra. The scheme developed by RAL has demonstrated that exploitation of the temperature-dependent Huggins bands dramatically improves tropospheric O₃ retrieval quality for GOME-1, and simulations confirm this will also be so GOME-2. We report below results of simulations which demonstrate that the same would be true for spectral measurements by MTG-UVS, irrespective of whether spectra in two orthogonal polarisations are used explicitly by the retrieval scheme or are combined to form a single spectrum of total intensity, I.

2. It was demonstrated in the GOME-2 Error Study for a conventional (reflectance only) O₃ profile retrieval that tropospheric data quality deteriorates quite rapidly for spectral resolution worse than 0.5nm. In simulations reported below, the impact of spectral resolution is assessed in simulations for measurements in dual (orthogonal) polarisations as well as for a conventional retrieval in which the two components are combined to form a single spectrum of total intensity, I. In both cases, the implicit assumption is that instrument polarisation has been corrected for perfectly.

3. Spectrally-resolved measurements of orthogonal polarisation to generate a single spectrum of I, in which the instrument’s polarisation response is corrected for, have been shown in the Eumetsat GOME-2 Error Study to be critical for achieving required accuracy in a conventional retrieval².  

4. The impact of aerosol on the polarisation signature of radiation emerging from the atmosphere has not been considered by SRON (or in simulations reported here), and nor has inhomogeneity in surface (polarised) reflectance within a ground pixel.

¹ GOME-2 has been under-specified in this regard, even though the spectral sampling/resolution of its PMDs are much better than GOME-1.
4.2 Retrieval simulations for single and dual polarisation spectral measurements

Vector radiative transfer calculations of sun-normalised radiances using a model developed by RAL from the RT3 model have been performed using a similar set-up in terms of instrument viewing geometry and geophysical scenarios to that employed in the Eumetsat GOME-2 Error Study. A number of instrument configurations have been examined by performing vector radiative transfer calculations at 0.2nm (band b1a/b) or 0.05nm (band 2b) resolution and convolving with an instrument spectral response function of FWHM equal to the specified resolution. Retrieval diagnostics have been calculated for synthetic spectral measurements of: (a) total intensity and (b) the combination of two orthogonal polarisations.

The nominal wavelength range used was 265-315nm in band 1a/b and 315-334.6nm in band 2b. In one simulation a large band 2b noise floor is applied, effectively removing the contribution from O3 differential spectral structure in band 2b (Huggins band), to attempt to replicate one of the configurations used by SRON (265 - 315 nm). In all cases, photon noise has been included, while additional noise contributions specific to GOME-2 have been neglected.

Figure 6-2 shows the full range of scattering angles, which drives the change in polarisation, over the full disc to be observed by MSG-UVS from geostationary orbit. At any given time there is little variation in scattering angle across the disc, except at the extreme edges. However, a complete range of scattering angles is experienced during the course of a day. The latitude and longitude of the minimum (and maximum) scattering angle, and hence polarisation, vary with both time of day and season. A diurnally and seasonally varying bias might therefore be expected if the instrument’s polarisation response is not accounted for accurately in the calibration of spectra. The view geometries used in the vector calculations are those applicable to the GOME-2 nadir view and (1920km) swath extremes, which span the range of scattering angles relevant to UVS as shown in Figure 6-2.

Figure 4-1 and Figure 4-2 compare Estimated Standard Deviations (ESDs) for different cases. The ESD at each retrieval level is defined as the square-root of the diagonal element of the error covariance matrix at that retrieval level, and is therefore a measure of precision on a single O3 profile retrieval. Columns from left to right correspond to across-track positions (viewing geometry indicated in each panel). Rows indicate either a specific noise floor level or the slit width which has been applied to band 2b. (The individual panels are included in section 11 as full page plots for extra clarity.)

Figure 4-1 shows the sensitivity to the band 2b noise floor at each spectral resolution, while Figure 4-2 show the sensitivity to spectral resolution for each band 2b noise floor.

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2 It should be noted, however, that O3 profile retrieval from backscattered uv measurements is an underconstrained inversion problem, and the off-diagonal elements in the error covariance matrix contain important information about the correlation of errors between different retrieval levels.
Figure 4-1 Comparison of ESDs for retrievals using dual polarisation measurements (tvec) or total intensity only (vector_i). Sensitivity due to band 2b noise floor (b2efl) varying from 0.0005 to 0.01 for stated spectral resolutions (nm) shown for three different viewing geometries.
Figure 4-2 Comparison of ESDs for retrievals using dual polarisation measurements (tvec) or total intensity only (vector_i). Sensitivity due to different spectral resolutions shown for stated band 2b noise floor (b2efl) for three different viewing geometries.
Dual polarisation measurements are seen to improve the ESD, although generally not significantly, (only up to 10%, depending on scattering angle). The largest impact is for scattering angles close to 90°, as expected theoretically.

The largest improvement in tropospheric ESD is obtained when the band 2b noise floor is reduced to below 0.001. Degrading spectral resolution beyond 0.48nm is seen to seriously degrade tropospheric information content.

The calculations presented here show markedly less impact from the explicit addition of polarisation information than those presented previously by SRON. This is due to important differences between the two sets of simulations. Most importantly, the SRON simulations neglect the large contribution to tropospheric information which is attainable from fitting the temperature dependent structure in the Huggins bands to high precision (<0.1% RMS). The RAL “baseline” simulations (total intensity modelled by scalar radiative transfer) do exploit the Huggins band structure extensively, and the incremental value of measuring spectra in dual polarisations and exploiting atmospheric polarisation information explicitly through a vector radiative transfer model is modest by comparison. SRON simulations were for nadir view exclusively, with a changing solar zenith angle, so variations in relative azimuth (and the associated impact on polarisation, U) were neglected. Differences between SRON and RAL formulations of the state vector and a priori constraint are also relevant.

Given the non-linear nature of O3 retrieval from reflectance spectra spanning Hartley and Huggins bands, and sensitivity to aerosol and surface reflectance and other geophysical and instrumental parameters, a necessary next step in the evaluation of dual polarisation measurements should involve iterative, non-linear retrievals in which auxiliary parameters were jointly retrieved and a thorough investigation of instrumental, geophysical and spectroscopic uncertainties and how they would propagate onto O3. A second, related issue to be assessed would be the impact of inhomogeneity within a ground pixel of (polarising) surface reflectance. In the simulations reported here, each ground pixel has been assumed to be spatially uniform in its surface (polarised) reflectance properties. We anticipate that a more sophisticated analysis would further reduce the increment in tropospheric information attainable from explicit use of dual polarisation measurements.

4.3 Requirement for dual polarisation measurements at high resolution for standard retrieval approach

Although the increment to tropospheric O3 information directly attainable from dual polarisation measurements would be modest, even if the Huggins band structure was fully-resolved in both polarisations, results from the Eumetsat GOME-2 Error Study have clearly demonstrated such measurements to be necessary in order to account accurately for polarisation in this wavelength range and apply a standard retrieval approach (with scalar radiative transfer model) which exploits the Huggins band structure to retrieve tropospheric O3.

The recommendation from this review is therefore to retain the requirement for spectrally-resolved measurements in the Huggins bands at <0.5nm resolution in a polarisation orthogonal to the main spectrometer, to enable an accurate correction for polarisation. (The recommendation from this review does not therefore conflict with the current specification, even though the basis for this requirement is different.)
In the wavelength range <320nm, the spectral resolution required for measurements in the polarisation orthogonal to the main spectrometer is >0.5nm, because the polarisation signature in outgoing uv radiation is controlled by broad structure in the O3 Hartley band.
### 5 SPECTRAL RESOLUTION AND SPECTRAL (OVER)SAMPLING

At present the requirements on spectral resolution are as follows:

<table>
<thead>
<tr>
<th>UVS- Mission Bands</th>
<th>Central wavelength (nm)</th>
<th>Spectral Resolving Power at Central Wavelength</th>
<th>Resolution nm</th>
<th>Resolution cm⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>UVS-1A</td>
<td>292.5</td>
<td>731.25</td>
<td>0.4</td>
<td>47</td>
</tr>
<tr>
<td>UVS-1B</td>
<td>298.5</td>
<td>746.25</td>
<td>0.4</td>
<td>45</td>
</tr>
<tr>
<td>UVS-1C</td>
<td>306</td>
<td>765.0</td>
<td>0.4</td>
<td>43</td>
</tr>
<tr>
<td>UVS-2</td>
<td>319</td>
<td>797.5</td>
<td>0.4</td>
<td>39</td>
</tr>
<tr>
<td>UVS-3</td>
<td>330</td>
<td>825.0</td>
<td>0.4</td>
<td>37</td>
</tr>
<tr>
<td>UVS-4</td>
<td>347.5</td>
<td>868.75</td>
<td>0.4</td>
<td>33</td>
</tr>
<tr>
<td>UVS-5</td>
<td>440</td>
<td>1100.0</td>
<td>0.4</td>
<td>21</td>
</tr>
<tr>
<td>UVS-6A</td>
<td>755</td>
<td>151</td>
<td>5</td>
<td>87</td>
</tr>
<tr>
<td>UVS-6B</td>
<td>766</td>
<td>13000</td>
<td>0.059</td>
<td>1</td>
</tr>
<tr>
<td>UVS-6C</td>
<td>775</td>
<td>155</td>
<td>5</td>
<td>87</td>
</tr>
</tbody>
</table>

These requirements are considered separately for ozone profile, trace-gas column and O2-A band retrievals separately, below.
5.1 Ozone Profile Retrieval

Spectral resolution and impact of under-sampling errors were addressed in the GOME-2 Error Assessment study\(^7\). This study showed that 0.4nm resolution in the Huggins range was adequate (even optimal) for ozone profile retrieval. The impact of neglecting undersampling error does not change dramatically over the range of sampling ratios 4-8 (see Figure 5-1). The current requirement to oversample by a factor of 6 might therefore be relaxed to 4. Note that this error can (and is for GOME-1) be corrected by modelling the impact of undersampling using a high-resolution solar reference spectrum, so the 10-20% errors indicated in Figure 5-1 are considered an upper limit. Undesampling error is considered further in section 5.4.

On the basis of experience with GOME-1 ozone profile retrievals, it would be possible to relax resolution requirements to 1nm below in bands measuring below 306nm. Again an oversampling ratio of 6 does not seem necessary (baseline 4 would be adequate).

The omission of measurements between 265-290nm will have significant consequences for the quality of stratospheric ozone profile retrievals (see Figure 5-3). This deficiency might be partly recovered by using the IRS 9-10 micron band, but the resolution of IRS (0.5cm\(^{-1}\)) is not ideal for stratospheric retrieval and vertical resolution in poorer than obtainable from the Hartley band. On the other hand, the relative sensitivity of the mid-ir to altitudes above the lower troposphere might provide improved information on tropospheric ozone when combined with Huggins bands measurements (see Figure 5-2).

Further work to assess the combined of information content of the two sounders is recommended. This would lead to definitive requirements for spectral coverage of the Hartley band by UVS. At present however it does not seem that the omission of measurements below 290nm is critical given the emphasis of user requirements for geostationary ozone observations on the mid-lower stratosphere and below.

Figure 5-1: Estimated precision (ESD) on ozone profile retrieval and impact of undersampling errors from the GOME-2 error study. Panel labelled “MISREGISTRATION” shows the impact of neglecting undersampling error (which coupled to Doppler shift between back-scattered and solar reference spectra). In principle (an in practise to some extent) this error can be corrected using a high-resolution solar reference spectrum.
Figure 5-2: Estimated relative precision (1 corresponds to 100%) from test simulation of IRS 980-1070cm\(^{-1}\) band at 0.5cm\(^{-1}\) resolution (0.2K NEBT) and the combination of IRS with GOME-2 Huggins bands observations between 315 and 334nm. Standard mid-latitude profiles and GOME-2 observing conditions assumed.

Figure 5-3: % precision on height resolved O\(_3\) as spectral coverage is extended from long to short-wave. Mid-stratospheric precision improves from 30% to better than 10% on including the spectral range 290-250nm.
5.2 Trace-gas Column Retrieval

0.4 nm resolution was found to be adequate for the column retrieval of BrO, NO₂ (H₂CO was not assessed). It was noted that resolution for these species could be relaxed somewhat further if this was achieved by opening the slit (rather than defocussing), hence increasing the number of photons detected. NO₂ was shown to be most sensitive to degrading spectral resolution beyond 0.4nm (precision changed from 21 to 23% on defocussing from 0.5 to 0.8nm but this effect was more than compensated by increased light if the resolution was similarly degraded by opening the slit).

More information on the resolution trade-off for trace gases is contained in [8]. It is difficult to draw immediate conclusions from the plots in this report since signal to noise and the oversampling factor was kept fixed while spectral resolution was varied. (In the absence of fundamental change in information content with spectral resolution, this would result in a sqrt(resolution) improvement in precision towards finer spectral resolution.).

Figure 5-4 shows results from this study scaled by sqrt(resolution/nm) to provide results for which the total number of measured photons within a given band-pass is conserved. In the absence of strong a priori influence, this allows the fundamental information added by improving resolution, rather than simply by increasing the number of photons measured. In each case these simulations assume 100% a priori errors on the tropospheric amount. Where the estimation precision after the retrieval is dominated by the a priori, this scaling shows an apparent improvement in precisions as resolution is degraded which should be ignored for current purposes. Results indicate that only the species retrieved in the near-ir (H₂O & CO) are strongly sensitive to varying resolution over the simulated range. There is some indication that HCHO requires a resolution better than 2nm. The independence of the tropospheric ozone error on spectral resolution is presumably due to the inclusion of the Chappuis bands. As indicated in section 3 it will be extremely difficult to use the Chappuis bands in practise and so these simulations should not be used as a basis for relaxing the requirement on spectral resolution in the Huggins bands to sound tropospheric ozone.

The trade-off was also assessed in [9]. Plots from this report are shown in Figure 5-5, with lines indicating the expected dependence from the implied increasing total number of photons as resolution and sampling is improved while signal to noise (on each channel) is conserved. For NO₂ at signal to noise 1000 there is a clear benefit of improving resolution to 100cm⁻¹ (approximately 1.6nm at 400nm), since curves are steeper than the sqrt(resolution) case. An optimum spectral resolution is difficult to identify for the other species.

It should be noted that all these trade-off assessments are based on the assumption that measurement errors are spectrally uncorrelated. In practise it can be expected that better spectral resolution will bring benefits in the presence of spectrally correlated errors (systematic or otherwise) which are not quantified in these simulations. Care should therefore be taken before concluding e.g. that a resolution of 5nm is adequate for NO₂ retrievals. At present however, it is not clear that a resolution finer that 1nm is required except for ozone profile retrieval, where the requirement is 0.4nm.
Figure 5-4: Trade-off between spectral resolution and precision on tropospheric retrieval of each trace gas. Dashed lines show data scanned from the plots of [8]. Solid lines are the same data, scaled by \( \sqrt{\text{resolution/nm}} \). Where the 100% a priori error is not significant, the solid lines show the trade-off for fixed total number of photons entering the instrument. (Curves are identical at 1nm, by definition).

Figure 5-5: Figures 9-12 from [9]: “Standard deviation \( \sigma_p \) of the posterior distribution for the H2CO tropospheric column density, expressed as a fraction of the prior tropospheric column density \( u_o \). The horizontal blue line indicates the prior standard deviation, while the red line indicates the required accuracy threshold”. Grey lines are added to each panel showing \( \sqrt{\text{resolution}} \) curves.
5.3 Oxygen A-band

At present 1cm\(^{-1}\) resolution is required in the \(O_2\) A-band. The reviewers recognise that such high resolution (if coupled to high signal to noise and very stringent radiometric accuracy requirements) could, in principle, provide useful information on aerosol and thereby improve tropospheric trace gas retrievals. Height-resolved aerosol retrieval was also assessed in the ESA study [2]. In that study, more information was found to be present in the stronger \(H_2O\) absorption bands at longer-wavelengths in the near-ir, however the \(O_2\) A-band could still provide useful information. A general finding of the ESA study was that aerosol retrieval from optically thick near-ir bands is very sensitive to radiometric and spectral calibration errors, since the technique relies on the absolute sun-normalised radiance being well calibrated (not only differential structure). In general, the quality of the absolute radiometric calibration must be comparable to the required signal to noise, before significant errors are introduced.

On the basis of experience with aerosol retrieval from GOME A-band observations, it is certainly the case that the A-band observations would need to have finer spectral resolution than GOME to offer better information on aerosol than is likely to be available from the FDHSI imager.

The reviewers are not currently in a position to comment more quantitatively on the spectral and radiometric requirements necessary for high-resolution measurements of the A-band to improve trace-gas retrievals by better constraining aerosol retrieval. Evaluating the A-band retrieval capability was identified as a topic for further work from the Eumetsat GOME-2 error study and we suggest again that further studies in this area would be useful before strictly defining an instrument concept.

If the A-band observations are primarily to provide information on cloud, it is questioned whether the channel provides additional information compared to FDHSI or the combination FDHSI+IRS (which would also provide sub-ground-pixel information for UVS).
5.4 Further Consideration Of Undersampling Error

Some further calculations have been performed to assess the requirement for spectral oversampling. The need to oversample is driven by Fraunhofer structure in the solar irradiance spectrum coupled to the need to interpolate measured radiances. Interpolation of measured radiances is required for two reasons:

(a) to form sun-normalised radiance accounting for any shift in the wavelength calibration of the instrument or Doppler shift of one or other spectrum (in the GOME polar orbiting case, the solar spectrum was always shifted by ~0.007nm due to Doppler shift).

(b) to model rotational Raman scattering given that radiation scattered into the Raman lines is offset by up to ~2nm.

Interpolation errors have been estimated here by appropriately convolving and sampling the solar reference spectrum of [10] which has a resolution of 0.01nm. A range of spectral resolutions (0.25, 0.5, 1.0, 2.5 and 5.0nm) and oversampling factors (1, 2, 4, 6, 8, 10) are simulated.

Interpolation errors are determined as follows:

- A nominal spectrum is obtained by convolving and sampling the solar spectrum according to a given resolution and oversampling factor.
- A shifted spectrum is obtained by offsetting the spectral sampling.
- The shifted spectrum is simulated by interpolating the nominal spectrum.
- The interpolation error is given by the relative difference between the “true” shifted spectrum and that simulated by interpolating from the nominal spectrum.
- The rms of the interpolation error over integer 10nm wavelength intervals from 240-790nm is determined and plotted.

Interpolation errors are strongly dependent on the assumed slit-function shape as well as width. 3 cases have been simulated: “Box-car” (in fact a trapezium with 0.01nm edge taper), triangular and gaussian (+/- 2 FWHM are considered).

Two cases of spectral offset are considered:

(a) an offset of 0.01nm (comparable to the GOME Doppler shift). This is considered a reasonable upper limit for a tolerable variation in the wavelength calibration of the instrument. This error should be smaller than that implied by the signal to noise requirement for a given species in the appropriate spectral range.

(b) all offsets in 0.01nm steps up to the resolution of instrument are considered and the maximum rms variation in each 10nm interval, considering each of these offsets, is reported. This should be considered as an absolute upper limit on the error which might feed into the modelling of Ring effect. These errors can be at least an order of magnitude larger than implied by signal to noise requirements before they impact

---

3 Note this spectrum is contaminated by atmospheric O₂ absorption in the A-band and results in this region should therefore not be considered realistic.
constituent retrieval, since the amplitude of Ring effect is at least an order of magnitude smaller than the sun-normalised radiance for all resolutions considered here.

Results are plotted twice for each offset, to clearly illustrate the dependence on over-sampling for fixed resolution and vice-versa. See Figure 5-6-Figure 5-9.

For box-car slit functions, interpolation errors are appreciable for all oversampling ratios at resolutions <5nm. As might be expected, errors are much smaller for triangular slit functions and smaller still for a Gaussian slit. This illustrates the desirability of defocussing to some degree the slit-image onto the detector arrays (a clear conclusion from [7]). An oversampling of 6 is sufficient to ensure errors for the 0.01nm offset are smaller than 0.1% at 0.5nm resolution across the whole spectral range. Errors generally become smaller with increase wavelength.

It is emphasised that implied errors are upper limits on the real impact on retrievals, since a high-resolution solar reference spectrum can be used to model (and substantially mitigate) the interpolation error, and this is done in practise for GOME-1. Nevertheless it would be desirable to be able to neglect undersampling error entirely in MSG-UVS data analysis, provided this was straightforward to implement by instrument design and was not achieved by sacrificing the spectral resolution which is actually required e.g. to retrieve tropospheric O_3.
Figure 5-6: Interpolation errors for 0.01nm wavelength shift; each panel corresponds to a specific spectral resolution and slit function shape.
Figure 5-7: Interpolation errors for 0.01nm wavelength shift; each panel corresponds to a specific oversampling ratio and slit function shape.
Figure 5-8: Maximum interpolation errors for wavelength shifts of magnitude up to the spectral resolution; each panel corresponds to a specific spectral resolution and slit function shape.
Figure 5-9: Maximum interpolation errors for wavelength shifts of magnitude up to the spectral resolution; each panel corresponds to a specific spectral resolution and slit function shape.
6 SENSITIVITY TO INSTRUMENTAL ERRORS

These issues are addressed following the structure of [1]:

6.1.2.1 Spectral requirements

6.1.2.1.1 Spectral bands, resolving power
Discussed under section 5, above.

6.1.2.1.2 Spectral calibration
MRD_UVS.30
The wavelength of each spectral channel shall be known better than 0.002 nm for wavelengths below 400 nm and 0.004 nm at longer wavelengths.

For channels other than 6B, these requirements are probably adequate and necessary for the knowledge of the difference between the centroid of neighbouring pixels\(^4\). However, a less stringent requirement could be imposed on the absolute (mean) spectral calibration of entire band (baseline ~ spectral resolution/2).

For channel 6B we would assume at least an order of magnitude more stringent requirement given the high spectral resolution.

6.1.2.1.3 Spectral stability and uniformity
MRD_UVS.60
The ISRF centroid of each spectral channel shall not vary by more than 1/20 of a spectral sample.

The origin of this requirement is not clear. It is probable that the knowledge requirement above is adequate.

MRD_UVS.70
For each of the UVS-mission bands, the integral of the absolute value of the difference of the UVS system PSF relative to the same pixel and two different channels (j and k) shall be less than 0.03.

The origin of this requirement is not clear.

6.1.2.2 Geometric requirements
It is assumed these are entirely driven by and consistent with user requirements and we do not comment.

6.1.2.3 Temporal requirements
It is assumed these are entirely driven by and consistent with user requirements and we do not comment.

\(^4\) The centre wavelength of a pixel being defined as the centre of gravity based on the first moment of the slit function.
6.1.2.4 Radiometric requirements

6.1.2.4.1 Reference scene radiances

The dark scene radiances in channels 1A-1C in table 3 of [1] are anomalously low and we do not understand their origin (4 orders of magnitude below the corresponding bright scene radiances through the short-wave radiance should be independent of surface albedo). The following tables are based on average radiances over the relevant spectral ranges from the scenarios used in the GOME-2 study. Although these relate to nadir-polar-orbiter viewing geometry, the radiances should be comparable to geostationary radiances for similar solar zenith. Values are in W/cm²/nm/sr.

6.1.2.4.1.1 Surface albedo : 0.05

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6.1.2.4.1.2 Surface albedo : 0.8

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6.1.2.4.1.3 Minimum, maximum and average radiances

The following tables show minimum and maximum scene radiance over all scenarios, but still separated into the two surface albedo cases.
6.1.2.4.1.4 Surface albedo : 0.05

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6.1.2.4.1.5 Surface albedo : 0.8

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</tbody>
</table>

6.1.2.4.2 Radiometric resolution

It is recommended that the average radiance value at 0.05 albedo quoted above be used as the basis for signal to noise requirements, since tropospheric retrievals depend on cloud-free conditions.

The maximum radiance at albedo 0.8 should be used to define the observable dynamic range.

The stated signal to noise values in [1] seem reasonable for channels 1-5. The reviewers cannot comment on the A-band requirement without further understanding the driving user requirement.

6.1.2.4.3 Polarisation

See section 4

6.1.2.4.4 Radiometric accuracy

MRD_UVS.220

The absolute calibration accuracy shall allow the determination of unpolarised irradiance within a spectral channel, to better than 3%, over the full dynamical range using the solar irradiance as a reference.

This requirement is adequate for DOAS retrievals from channels 2-5. 1% should be the requirement for channel 1. For channel 6B it is expected that a much better accuracy would be required for unbiased aerosol or pressure retrievals to be possible. Accuracy comparable to the signal:noise requirement is probably necessary for this class of observation.

MRD_UVS.230

The relative calibration between spectral channels of a band shall allow the determination of unpolarised radiance to better than 0.02% [TBR 1].

This is reasonable for bands 2-6. It could be relaxed to 1% in channel1.
MRD_UVS.240
For any wavelength and the maximum flux above, the contribution to straylight from all sources (spatial, spectral, outside FOV) shall not exceed 1% of the signal at the wavelength in question after characterisation and adequate straylight correction.
This is reasonable for channels 1-5, but should be more stringent in channel 6B.

MRD_UVS.260
Calibration differences between different samples of the same channel and at different scan angles shall be less than 0.02% [TBR 2].
Presumably calibration differences of a larger magnitude can be tolerated so long as they are characterised on ground and invariant in flight.

MRD_UVS.270
The relative radiometric accuracy of the same channel between two calibration cycles shall be better than 0.2 % [TBR 3].
This requirement is probably also not stringent enough for channel 6B.

6.1.2.4.5 Radiometric stability
MRD_UVS.280.updated
The long term stability of the channels over the complete lifetime of the instrument shall be better than 5% in the UVS-1 (A, B, C), UVS-2, UVS-3, UVS-4 and UVS-5 band and 1% in the UV6 (A, B, C) bands.
“Long term” should be defined. If it relates to the life-time of the instrument then this is adequate for bands 1-5.

6.1.2.5 Performance characterisation data
MRD_UVS.290.updated
The channels shall be characterised prior to launch to allow for an in flight calibration accuracy of 1.5%.
Should be 1% in channel 1 and probably much better in channel 6B

MRD_UVS.300
The spectral instrument response functions of all channels for each detector shall be characterised over the complete band path to better than 2%.

MRD_UVS.310
The half width full maximum positions of the spectral instrument response functions of all channels of each detector shall be characterised to better than 1%.
Requirements on slit-function knowledge are critical but these requirements are not specific enough. The requirements for slit function characterisation for GOME-2 were derived in [11], but are not straightforward to express in generic terms. Further attention is required to define requirements on knowledge of slit-function shape. Spectral correlation of errors must be specified together with uncertainties at a resolution higher than detector pixel FWHM.
6.1.2.6 Solar mode

MRD_UVS.xx

The UVS instrument shall measure the extraterrestrial full disk solar irradiance in the same bands defined in MRD_UVS.10 and spectral resolution defined in MRD_UVS.20 and spectral oversampling defined in MRD_UVS.50.update.

MRD_UVS.xx

The solar irradiance shall be measured once per day. It shall be possible to increase the frequency of the solar irradiance measurements during special campaigns.

The user requirement for more frequent observations than daily is not obvious.

MRD_UVS.xxx_new

When in Solar mode, the dynamic range of each of the UVS-Mission bands shall be optimised to measure the spectral solar irradiance as specified in Table 5.

We do not understand the origin of the dark (and hence reference) scene radiance values in table 5. The bright scene values seem to correspond to observing the sun via a perfect Lambertian diffuser.

The daily solar reference spectrum must be measured with at least a factor 2 better signal to noise than the back-scattered spectra. The stated signal to noise of 100 is certainly not adequate.

The frequency at which the solar spectrum is measured should by at least weekly to oversample variability associated with the 27 day solar rotation. The requirement to sample more frequently will be determined by instrument stability (especially under thermal variations) and so should be implied by the requirement that the error on sun-normalised radiance due to interpolating solar observations to the time and wavelength of any earth-radiance measurement shall be less than that implied by the signal to noise of the earth measurement. This in turn is related to whether oversampling is sufficient to account for any known change in wavelength calibration or whether a adequate high-resolution reference spectrum is available to adequately correct for undersampling.
6 VARIATION WITH SEASON OF ILLUMINATED LATITUDE RANGE

Figure 6-1 and Figure 6-2 illustrate the variation of solar zenith angle and scattering angle as sampled by UVS. The following points are noted:

- The whole observed latitude range is illuminated (SZA > 90) at mid-day throughout the year.
- The scattering angle varies only slightly (20 degrees) across the disk at a given time of day. In particular, the 90 degree scattering angle at which most information from polarisation measurements might be expected occurs only near dawn/dusk (where the signal is low and air-mass factors large). I.e. the benefit of measuring polarisation for ozone and aerosol retrieval should be assessed specifically for the geostationary view geometry, it is difficult to translate results for polar platforms to the geostationary case.
Figure 6-1: Variation of solar zenith angle during the day at equinox and solstice
Figure 6-2: Variation of scattering angle during the day at equinox and solstice.
7 REQUIREMENTS FOR ADDITIONAL INFORMATION TO FACILITATE TRACE GAS RETRIEVAL (NB AEROSOL, CLOUD, TEMPERATURE, SURFACE BRDF) AND WHETHER DATA AUXILIARY TO MTG UVS AND IRS WILL BE REQUIRED.

Required auxiliary data are identified and discussed below.

7.1 Aerosol
The impact of aerosol on ozone on trace gas retrievals was assessed in [7] and [8].

![Figure 7-1: Errors from aerosol based on assuming various MODTRAN scenarios in simulated measurements while the retrieval assumes the background case to apply.](image)

It is assumed that the imager on MTG would provide adequate information, although measurements in dual polarisation, as for POLDER, may improve aerosol optical thickness over land. A quantitative assessment would be needed to establish whether this would be needed in support of MTG-UVS trace gas retrievals.

7.2 Cloud
The issue of sub-pixel inhomogeneities in cloud and surface properties and their impact on measurements and retrievals from uv-vis spectrometers in polar orbit has been considered quite extensively in a number of studies. Characterisation of spectrometer ground-pixels by co-located measurements at much higher spatial resolution is essential. Such information is currently used (e.g. ATSR-2 for ERS-2 GOME-1, AATSR for Envisat SCIA) to identify and flag sub-pixel cloud so that this auxiliary information is available to users of trace gas data products from the spectrometer. In advanced data inversion or assimilation schemes to be applied to MTG-UVS, surface and cloud properties represented at sub-pixel resolution would be incorporated explicitly into the forward model.
A more subtle requirement for sub-pixel information has been identified and quantified in the Eumetsat GOME-2 Error Study through an assessment of spatial aliasing. It was found that, even if the integration and read-out of all detector pixels is perfectly synchronised (so there is no spatial aliasing), there can still be a significant error in O3 profile retrieval in scenes in which surface (cloud) reflectance inhomogeneity is large. This is due to non-linearity in radiative transfer which means, for example, that the spectrum for two adjacent sub-pixels with high and low surface (cloud) reflectance cannot be represented by a single calculation using their averaged surface (cloud) reflectance.

It is envisaged that the MTG vis/ir imager to fly alongside UVS would be adequate to characterise cloud and surface properties.

7.3 Temperature

The impact of temperature errors was assessed in [7]. Results for a typical atmospheric scenario are shown in Figure 7-2. The following cases were simulated:
- TEMP-10KM: Errors of 1K magnitude with 10KM correlation length.
- TEMP-2KM: Errors of 1K magnitude with 2KM correlation length.
- TEMP-FCBKG: Temperature errors according to an ECMWF forecast model background covariance (provided by A.Collard, pri. comm.).
- TEMP-IASI: Errors if information from IASI is added to the same forecast background.
- Errors from a 1% error in surface pressure were also simulated and shown to be negligible.

Note that the particular ozone profile scheme simulated in this study extracts information from the temperature dependence of the Huggins bands. Other schemes, particularly for other trace gases, are likely to be less sensitive to temperature errors.

It can be concluded that temperature information from an NWP forecast is required for tropospheric O3 retrieval. Even so, errors of less than or equal to 10% can be expected which could be mitigated further if operational sounder data or and NWP analysis could be used.
7.4 BRDF

In general, trace-gas retrievals from backscattered uv/vis measurements assume the surface to be Lambertian and retrieve an effective surface albedo independently. There is no requirement for prior knowledge of the surface albedo itself, assuming the surface to be Lambertian.

For GOME ozone profile and trace-gas column retrievals, the impact of assuming a Lambertian BRDF was assessed in [7] by simulating measurements with representative BRDFs for a number of surface types. The only case in which large errors were found (10s% for tropospheric O₃) was ocean under sun-glint conditions. Since sun-glint will occur for a significant fraction of geostationary observations within the tropics, it will be important to account properly for the ocean BRDF in sun-glint geometry. It is expected that the standard Cox and Monk model will be adequate. This model is dependent on wind-speed. It is probable that the UVS measurements themselves could be used to adequately fit wind-speed over ocean and an effective Lambertian albedo over land. If this is the case, auxiliary information on wind-speed and further information on BRDF would not be required for “traditional” O₃ profile or DOAS retrievals. This assumption should be confirmed by further study.

To extract information from polarisation measurements, it will be necessary to model the polarising effect of the surface. Further work would be required to assess whether auxiliary information is required to do so adequately.
To make use of the Chappuis bands signature to improve precision on tropospheric ozone, it will be necessary to model the wavelength dependence of the surface reflectance from 450 to 560nm with an accuracy varying from 0.1\% at spectral scales \~10nm to 1\% over that entire spectral range. It is not clear that this will be possible from any available auxiliary data-set.
8 INITIAL ASSESSMENT OF POTENTIAL FOR SYNERGY WITH POLAR ORBITING NADIR- AND/OR LIMB-EMISSION SOUNDERS TO CONSTRAIN THE STRATOSPHERIC AND UPPER TROPOSPHERIC DISTRIBUTIONS OF O3 AND OTHER TARGETED TRACE GASES.

8.1 Polar orbiting nadir-sounders

The polar orbiting operational missions EPS MetOp and NPOESS are planned to deliver data over the coming two decades. These include nadir-viewing spectrometers operating in the uv/vis (GOME-2, OMPS) and mid-ir (IASI, CrIS) to supply data on atmospheric composition globally. A continued need by the met services for global observations from advanced polar orbiting satellites can be anticipated for the post-EPS era. It is therefore worthwhile to consider User Requirements and design of MTG-UVS to address these in the context of observations likely to be made concurrently from polar orbit. The baseline assumption is that observations comparable in type to those of MetOp would be available in the MTG-UVS period.

8.1.2 UV/VIS

Assuming ground pixel sizes to be similar, and ignoring other factors which might differ between polar and geostationary orbit, the added value of MTG-UVS observations to those of a GOME-2 class polar orbiter would specifically be in terms of temporal coverage over the geographical region which is observable. The US NPOESS system will comprise three satellites whose equator crossing times are such as to observe at three very different local times of day (and for IR sensors, also three local times of night). Assuming this also to be the case for a post-EPS system, the added value of MTG-UVS therefore come from either:

1. Accumulating a larger number of (cloud-free) observations over the whole region viewed within a given time period, e.g. the assimilation time window used for NWP
2. Sampling a given location more frequently and/or for a longer duration than from polar orbit (~4hourly intervals)

The value added by MTG-UVS for Air Quality applications could depend on either of these criteria, since the manner in which satellite observations could benefit such applications has still to be determined. The coupled issues of ground pixel size and path length through the troposphere, which jointly determine the probability of cloud-free observations, are critical to the assessment (see Section 9), and hence to the definition of MTG-UVS design.

One particular issue which merits attention is the shortwave extent of Hartley band measurements needed by MTG-UVS if this band is covered by a nadir-uv spectrometer in polar orbit.

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5 At the peak of the Hartley band (~254nm) detected radiation is scattered from mesospheric altitudes. At progressively longer wavelengths in the Hartley band, detected radiation is scattered from decreasing altitudes in the stratosphere. The temporal scales of O3 variability at these altitudes is typically longer than in the lower stratosphere and troposphere.
8.1.3 IR

In addition to the temporal sampling dimension mentioned above, the distinctly different and complementary properties of radiative transfer in the IR and UV/VIS wavelength regions are worthy of serious study, having only been touched on briefly in Section 2 of the current report. For O<sub>3</sub>, a particular issue is, again, whether the Hartley band measurement by MTG-UVS could be dispensed with if equivalent information was forthcoming from a nadir-ir spectrometer in polar orbit, or indeed from MTG-IRS.

8.2 Polar orbiting limb-sounders

Limb-emission and nadir-uv techniques have highly complementary attributes for sounding the troposphere & lower stratosphere. The limb-emission technique has good vertical resolution and high sensitivity in the stratosphere, which extend downwards into the upper troposphere. However, the lower troposphere cannot be seen, due to obscuration by clouds and/or water vapour. In mid-IR windows, penetration of limb observations into the troposphere is controlled by clouds, although this is not the case at mm wavelengths<sup>6</sup>.

Nadir techniques, on the other hand, have comparatively good horizontal resolution and sampling, are less frequently affected by upper troposphere cirrus and have sensitivity to some trace gases and aerosol in the lower troposphere.

In principle, the optimal approach for sounding tropospheric trace gases such as O<sub>3</sub> is therefore to combine information from limb-emission sounding (eg MIPAS) and nadir-sounding (e.g. GOME / SCIAMACHY). To demonstrate this concept, the standard RAL two-step scheme to retrieve O<sub>3</sub> profiles spanning troposphere and stratosphere from GOME has been adapted. The standard scheme, as applied in simulations reported elsewhere in this review, is as follows:

1. O<sub>3</sub> Hartley band 240-300nm:
   - A traditional “buv” approach is applied first to retrieve an O<sub>3</sub> profile from the Hartley band
   - O<sub>3</sub> weighting-function (and averaging kernel) peaks span the stratosphere, so profile information is of good quality in the stratosphere.

2. O<sub>3</sub> Huggins bands 325-335nm:
   - The profile and error covariance matrix from the Hartley band step are used as <em>a priori</em> for the Huggins band step.
   - Valuable information in the troposphere and lower stratosphere is added, provided that a fitting precision of <0.1% RMS is achievable (cf ~1% in Hartley band)

MIPAS retrievals can replace the Hartley-band step, offering a stratospheric profile of higher vertical resolution and accuracy. This synergistic approach goes beyond simplistic

<sup>6</sup> Investigation in a recent study for ESA through limb radiative transfer calculations based on temperature, humidity and cloud fields from ECMWF analyses spanning one year has recently demonstrated that cirrus has a relatively small effect on limb emission sounding of the upper troposphere at mm-wavelengths by comparison to IR wavelengths.
differencing of a (limb-derived) stratospheric column from a (nadir-derived) total-column. The vertical profile shape, surface albedo & aerosol are properly accounted for in radiative transfer during the iterative retrieval. This eliminates air-mass factor errors in the total column (vital for extracting the small tropospheric signal). The Huggins bands T-dependence is found to add two pieces of independent information in the troposphere/lower stratosphere.

For the Huggins band step in the synergistic scheme, the O$_3$ *a priori* profile is as for the standard GOME scheme at 0, 6, 12 km and the MIPAS L2 product (on MIPAS levels) at 16 km & above. The *a priori* error covariance matrix is as defined by the MIPAS retrieval errors at 16 km and above and 100% below 16 km. In all other respects the Huggins band step is identical to the standard two-step GOME scheme.

RAL’s synergistic scheme has been applied to both MIPAS + GOME and MIPAS + SCIAMACHY. Since only two full orbits of adequately calibrated SCIA data were available at time of this analysis, only a limited demonstration of the technique has been possible so far.

![Figure 8-1](image_url)

**Figure 8-1** Comparison of O$_3$ retrieval from the synergistic MIPAS/SCIA scheme to the standard GOME retrieval for the corresponding ERS-2 orbit. The top-left panel shows the *a priori* for the standard two-step GOME retrieval, which is based on a monthly climatology for 10° latitude bins. The bottom-left panel shows the O$_3$ cross-section retrieved from the standard two-step scheme applied to GOME. The top-right panel shows the MIPAS L2 O$_3$ product with GOME *a priori* substituted <16 km, as used as a priori to the SCIA Huggins bands retrieval. The bottom-right panel shows the O$_3$ cross-section retrieved from SCIA measurements in the Huggins bands.
Figure 8-2 $O_3$ at the surface\(^7\) retrieval level for three partial orbits of ERS-2 and the corresponding orbits of Envisat. The left-hand panel shows the GOME-only retrieval and the right-hand panel shows the MIPAS+SCIA(Huggins bands) retrieval.

The GOME-only, MIPAS+GOME (not shown) and MIPAS+SCIA exhibit rather similar features in troposphere. Since the GOME-only scheme has been extensively validated, this is considered to offer a satisfactory initial demonstration of limb-nadir synergy. The advantages are: to combine the attributes of MIPAS in the stratosphere with those of nadir-uv in the lower troposphere; to by-pass the sensitivity of MIPAS to cirrus in the UT; to by-pass the ongoing radiometric calibration issues of SCIA <310nm; to permit retrievals in the South Atlantic Anomaly region (important for tropospheric $O_3$), where dark-current noise in band 1 is too high for use of GOME-1 measurements. SCIA offers higher across-track sampling than GOME, although frequent gaps in its along-track sampling have to be accepted, which are caused by alternation between nadir-mode and limb-mode.

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\(^7\) The retrieval at surface level represents a vertical average over the lower half of the troposphere, due to the intrinsic width of the averaging kernel.
9 GROUND PIXEL SIZE AND CLOUD-FREE PIXEL OCCURRENCE. AS A FUNCTION OF LATITUDE/LONGITUDE

Aspects of the UVS viewing geometry are illustrated in Figure 9-2. The following quantities are shown:
- Pixel size on ground: Assuming FOV are equiangular from the satellite, this shows the pixel size on the ground (in the radial direction) when the size at nadir is 6km (as required). i.e. distance $d_1$ in Figure 9-1.
- Horizontal LOS distance 0-10km: The distance travelled along the line-of-sight between 0 and 10km (i.e. notionally within the troposphere); distance $d_2$ in Figure 9-1.
- The ground pixel area assuming a pixel dimension in the radial direction is $d_1 + d_2$.
- The line-of-sight zenith angle at the ground; $\Theta$ in Figure 9-1.
- The fraction of pixels which can be expected to be cloud-free. This is an approximate estimate of the cloud-free sampling frequency derived as follows: The probability of a scene of given area being completely cloud free was determined from ATSR-2 data on 14 December 2004 in 3 latitude bands, 20°S-20N, 20-40° North & South, 40-60° North and South. (Both northern and southern latitude are included to approximate an annual mean from the 1 day of data, assuming there is no hemispheric asymmetry in cloud sampling). Each 1km pixel in the ATSR-2 data is classified as cloudy or cloud-free using ratios of the 3 ATSR-2 visible channels at 5.5, 6.7 and 8.7 microns.

Ideally a much larger data-set would be used to generate seasonal and better resolved latitudinal dependencies however this was not feasible within the time-scale of this project. Nevertheless the results give an indication that while the tropics and Southern Europe will be sampled quite well by the UVS instrument, sampling north of the Mediterranean will be strongly limited by cloud.

An assessment of the temporal correlation of cloud occurrence should be carried out to establish (a) with what frequency (and under which observing conditions) the geostationary platform can provide at least one measurement per day of a given location on the ground (since temporal and spatial correlations are high it is not obvious that the frequency will be much larger than the instantaneous probability of a cloud free scene as shown). (b) How often more than one sample of the diurnal cycle is obtained at a given location (sampling the diurnal cycle is the major justification of geostationary measurements and this benefit should be properly quantified, accounting for cloud).

![Figure 9-1: Definition of some parameters in Figure 9-2](image-url)
Figure 9-2: UVS viewing geometry: Left: Radial dimension of pixel at earth surface for fixed spacing in off-nadir angle, assuming 6km dimension at nadir. Centre: Distance along the LOS between altitudes 0 and 10km, projected onto the Earth surface. Right: Estimated percentage of cloud free scenes based on (a) the total of the two radial dimensions being used to represent the horizontal dimension of the pixel (b) a statistical relationship between % cloud free scenes and ground-pixel size derived from ATSR-2 data (see text for details)
10 RECOMMENDATIONS FOR FURTHER SCIENTIFIC STUDY

To follow-up on this initial review of MTG-UVS requirements, it is recommended to Eumetsat that consideration be given to investigating the following topics in greater depth, in parallel with pre-Phase A system studies for MTG.

1. More extensive simulations modelling polarised radiative transfer e.g. to assess impact of aerosol and surface inhomogeneities on:
   a. Polarisation correction <350nm
   b. Added value to tropospheric O₃ of spectral measurements in two polarisations
   c. Added value for retrieval of aerosol

   The vector radiative transfer calculations performed in this initial study were for a very limited set of viewing geometries and geophysical scenarios and they accounted only for polarisation due to Rayleigh scattering and a surface assumed to be homogeneous across the ground pixel. This is also the case for the previous analysis performed by SRON. However, spectra of polarised outgoing uv radiation will also be affected significantly and in a non-linear way by aerosol and by inhomogeneities in (polarised) surface reflectance. It would also be desirable to perform calculations for a representative range of viewing geometries (azimuth & zenith angles), solar zenith angles and geophysical scenarios.

2. Analysis using MSG-SEVIRI data of the frequency and duration of cloud-free ground-pixels as a function of: geographical location (lat,long), time of year, time of day and ground-pixel size.

   For air quality applications, a dedicated study is needed to quantify statistics of observation to ground-level (i.e. into the boundary-layer) from geostationary orbit, since the temporal and spatial sampling requirements for these applications differ from those for NWP applications. These statistics would determine the ground pixel size and observing strategy which would be needed to meet User Requirements on trace gases and aerosol for air quality applications. Analysis using MSG-SEVIRI data would be directly relevant to MTG in terms of its observational geometry and could address most of the required dimensions, which has not been possible in the initial study performed here using a small sub-set of ATSR-2 data.

3. Potential for retrieval of trace gas information in the troposphere by combining information from:
   a. UVS & IRS
   b. MTG & post-EPS polar orbiter

   a) In this study, a very preliminary assessment has been made through retrieval simulations of the potential value to tropospheric O₃ of combining UVS with IRS observations. The principle being that O₃ weighting functions for the two sensors have vertical profiles which differ in one crucial respect. In the IR, sensitivity to trace gas absorption is negligible at ground-level where temperature contrast with the surface is very low, whereas, in the uv, multiple-scattering by molecules and aerosol increases sensitivity to trace gas absorption near ground level. It would be

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8 The analysis could be performed for synthesised, larger ground-pixels by combining individual SEVIRI pixels.
desirable to undertake a more extensive set of simulations to: (1) establish for a representative set of geophysical scenarios the potential advantage of combining observations from these two sensors through considering joint retrievals; (2) perform a realistic error analysis (ie including errors other than noise) and (3) optimise certain instrument specifications, taking into account of complementary information available from the two sensors. Synergy between GOME-2 and IASI on MetOp. Results from synergistic use of real flight data from the instruments GOME-2 and IASI on MetOp will become available in due course (~2006/7) for verification of simulations for O₃ which combine UVS with IRS.

b) In this review, results and conclusions have been cited from ongoing studies at RAL to use flight data from the polar orbiting instruments ERS-2 GOME, Envisat MIPAS and SCIAMACHY to demonstrate synergistic use of IR limb-emission (MIPAS) and uv nadir-backscatter (GOME / SCIA) observations to retrieve O₃ vertical profiles which span the troposphere and stratosphere. The principle being that:

- Retrieval of O₃ in the middle & lower troposphere is critically dependent on how accurately O₃ is represented in the upper troposphere and stratosphere.
- O₃ in the stratosphere and UT can be retrieved most accurately from limb-emission measurements

For O₃ profiling, it has been demonstrated from MIPAS and GOME, and also from MIPAS and SCIA, that the advantages of limb-emission and nadir-backscatter techniques can be combined and some of their disadvantages overcome through synergistic use of their data. However, there are several further dimensions which it would be worthwhile to explore further at an early stage in preparation for design of MTG for operation in the post-EPS era:

Limb-mm – nadir synergy for O₃

- In the recent ESA UTLS study¹², it was shown that the comparatively low sensitivity to cirrus of mm-wave measurements offered a significant advantage for limb-sounding O₃ (also H₂O and CO) in the UT. These and other attributes were found to complement those of IR limb-sounding, so it is envisaged that a mm-wave limb-sounder might be one component of a polar orbiting mission in the era post-EPS. It would therefore be desirable to look at potential for limb-nadir synergy between UVS (and IRS) and mm-wave as well as IR limb-sounders in polar orbit.

Limb-nadir synergy for uv/vis target trace gases other than O₃

- From absorption in a uv/vis spectrum observed in nadir, the line-of-sight column amount can be derived directly and a vertical column amount can then be derived, subject to assumptions about the vertical profiles of atmospheric absorbers and scatterers. However, for weak absorbers (i.e. all uv/vis detectable trace gases except O₃) the spectra themselves contain no height-resolved information.
- Several weakly-absorbing trace gases (e.g. NO₂, SO₂, HCHO) targeted by MTG-UVS have distributions in the stratosphere and upper troposphere which can be retrieved from polar orbiting limb-emission sounders, making them additional candidates for limb-nadir synergy. In particular, NO₂ and SO₂ (following
volcanic eruptions) have stratospheric concentrations which exceed those in the lower troposphere.

- Combining limb-emission information with nadir uv/vis information would enable concentrations in the lower troposphere to be attributed.

- In the absence of co-located limb observations, vertical profiles of these trace gases in the stratosphere and upper troposphere could be constrained only by (assimilation) models. Chemistry of the upper troposphere and lower stratosphere is very complex, however, and it seems rather unlikely that the evolution of chemistry schemes within (assimilation) models will be sufficient for them to replace co-located limb observations, if the latter are available.

Value added by MTG to polar orbiters and vice versa

- The value which could potentially be added by geostationary observations to those from polar orbit has yet to be quantified. This could be done through simulations in which the 3-D tropospheric and stratospheric distributions of trace gases are modelled as a function of local time of day for a representative set of days throughout the year. Existing analyses of temperature, wind, humidity, cloud and ozone (e.g. ECMWF) together with trace gases from a regional air quality forecast model could be used to generate radiances and retrieval simulations undertaken for a set of realistic case studies. The simulations could be done for limb- and nadir-sounding polar orbiting instruments and for MTG instruments, separately and in combination.

4. Refine requirements for correlative aerosol and cloud information

   At present quite stringent requirements are placed on the spectral resolution in the O$_2$ A-band to provide information on cloud and aerosol for the constituent retrieval. The extent to which the current spectral resolution is required is not very clear, and it is likely that to make use of such information the requirements on absolute spectro-radiometric accuracy will be very strict. On the other hand additional information on cloud and aerosol could come from other sensors on board MTG (e.g. imagers and IRS). A retrieval simulation study should follow the assessment of cloud statistics (point 2 above) to
   a. quantify constituent errors in partially cloudy scenes
   b. quantify extent to which errors mitigated by sub-pixel cloud information being used in retrieval
   c. define requirements for O$_2$ A-band measurements for UVS constituent retrieval in the light of available information from other sensors. If other sensors are required then co-registration requirements would be defined.

5. Refine Geometrical / sampling requirements

   The basis for current geometrical / sampling requirements is not clear at present. Work should be carried out to refine these including
   - shape of point spread function
   - pointing knowledge
   - co-registration between channels & other MTG instruments - c.f. sub-pixel scene homogeneity
   - strategy for image acquisition (c.f. 3s sample time for all channels)
6. **Perform full error assessment study**

The current MTG-UVS instrument requirements are defined in a quite general manner in an attempt to allow industrial studies a free hand in arriving at the most suitable instrument concept to meet user requirements. Once the design becomes more clearly defined it is expected that areas for trade-off will emerge (e.g. between spectral resolution, coverage & oversampling) which are constrained by the specific instrument concept. Retrieval simulations studies to assess these trade-offs in terms of retrieval errors vs user requirements (like those performed for GOME-2) will be required to refine the instrument design and operation.
11 APPENDIX 1: POLARISATION ERRORS

ESDs: slit=0.239 nm

Figure 11-1 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-2 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-3 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-4 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-5 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-6 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-7 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-8 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-9 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-10 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-11 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-12 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-13 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-14 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-15 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-16: Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-17 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-18 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-19 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-20 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-21 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-22 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-23 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11.24 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-25 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-26 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-27 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-28 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-29 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
Figure 11-30 Retrieval ESD for indicated slit-width, noise floor and viewing geometry.
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