



# GOME-2 Error Assessment Study

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## Phase V: Final Report Executive Summary

Version 1-1

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Date: April 2004



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## Executive Summary

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## Executive Summary

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## 1 Introduction to Phase V

In Phase I to Phase IV of the GOME-2 Error Assessment Study, a number of issues of potential importance to GOME-2 operational settings and error mitigation were investigated. The findings raised additional issues which required further work. The methodology and findings of Phase I to Phase IV were reported in main Final Report [Kerr&Al02]. This present Executive Summary outlines the findings from the work conducted under the Phase V study extension, which was added to the main study to consolidate the findings from Phase I to Phase IV. In the main part of Phase V (Task 2) five specific topics were addressed:

### 1. Type of Diffuser Plate

The potential improvement in trace gas column retrieval, when using a quasi-volume diffuser (QVD) in place of the originally proposed ground aluminium diffuser, was assessed.

### 2. Uncertainty in Characterisation of Diffuser BSDF

Information from the GOME-2 FM1, FM2 and FM3 calibration activities was used to quantify current uncertainties in characterisation of diffuser BSDF.

### 3. Residual Error from Polarisation Correction

The analysis performed in the main study was based on information from GOME-1 and GOME-2 (at component level). This was updated by using new information at instrument level from the GOME-2 calibration activities [TPD01, TPD03] and a polarisation study [Har&Al03].

### 4. Spatial Aliasing via Polarisation Monitoring Detectors

Spatial aliasing via the spectrometer (FPA detectors) had been analysed in the main study. In Phase V, spatial aliasing via the PMDs was analysed in an analogous way

### 5. Requirements for Characterisation of Slit Function Shape

The main study determined that slit function knowledge at sub detector pixel resolution was required to avoid serious errors in ozone profile retrieval. In Phase V, requirements were derived for laboratory measurements of the slit function shape.

As in the main study, most simulations in Phase V were performed for a set of realistic and representative geo-temporal scenarios (12 in total) which spanned a diverse range of observing conditions, including several surface albedos (typically 0.05 and 0.8), for view angles of nadir and the two (1920 km) swath extremes. The conclusions and recommendations from this study are therefore expected to be applicable to GOME-2 observing conditions generally (though not universally).

In all cases, the methodology was to:

- a. Generate spectral signatures for a particular error or uncertainty
- b. Propagate error signatures onto retrieved tracegas columns and O<sub>3</sub> profiles by *linear mapping*.

The significance of estimated errors was gauged by comparing these to the User Requirements, and to the Estimated Standard Deviations and Baseline Error Budgets, which had been compiled in the main study.

In support of these Task 2 activities, preparatory work to develop necessary software and datasets was conducted under Task 1.

In Task 3, recommendations were made in relation to operational settings and error mitigation, based on a review of the recommendations from the main study (Task I - IV) and the new results from Task 2 of Phase V.

Phase V of the study was conducted by a consortium comprising the following members:

<b>Serco Europe Ltd</b>	Prime Contractor; Study Administrator
<b>RAL</b>	Technical Coordinator; Ozone Profile Analysis; Methodology to Derive Slit-Function Measurement Requirements; Generation of Spectral Signatures of Diffuser BSDF Measurement Uncertainty
<b>IUP/IFE-UB</b>	Trace Gas Column Analysis; Analysis of Errors from different Diffuser Types
<b>SRON</b>	Generation of Residual Polarisation Error Signatures with/without Spatial Aliasing



## 2 Choice of type of diffuser plate

The diffuser type baselined for GOME-2 is made of ground aluminium. For GOME-1, this type of diffuser has been demonstrated to exhibit small-scale spectral structures which vary with sun-angle, and therefore season. The wavelength scales of these structures are comparable to those of trace gas absorption signatures, and their amplitudes are significant in relation to the fitting precision and the absorption amplitudes of trace gases other than ozone. Spectral correlation with trace gas absorption signatures has therefore been found to cause serious, seasonally dependent biases in trace gas columns retrieved from GOME-1<sup>1</sup>.

For the quartz quasi-volume diffuser (QVD), the amplitudes of these BSDF spectral structures have been measured to be four times smaller than the ground aluminium diffuser baselined for GOME-2. Errors on trace gas columns were estimated in Phase V of this study to be correspondingly lower for the QVD than the aluminium diffuser. These reductions were found to be worthwhile and important for O<sub>3</sub> (visible), NO<sub>2</sub>, BrO and H<sub>2</sub>CO.

**Recommendation V1** The quasi volume diffuser should be used for GOME-2

	DIFFrms / DODrms*100 [%]	
	GOME-1	QVD
O <sub>3</sub> UV	0.5	0.1
O <sub>3</sub> VIS	15	4
NO <sub>2</sub>	82	22
BrO	255	67
H <sub>2</sub> CO	82	22
DIFFrms	1.64e-4	0.43e-4

**Table 1:** Estimated percent error on trace gas columns from the RMS ratio of diffuser over differential optical depth (DOD) and RMS of differential spectral structures for different diffuser types

With the new diffuser mounted, seasonally-dependent biases in minor trace gases should be reduced by a factor of ~ 4. However, these biases will still not be negligible, and so will need to be carefully quantified. It is assumed that a dedicated validation campaign will be conducted for each GOME-2 flight model in the period soon after launch, and that this will reveal any biases in columns of the minor absorbers NO<sub>2</sub>, BrO, OClO, H<sub>2</sub>CO, and SO<sub>2</sub> arising from this and other error sources. To characterise the *seasonal-dependence* of errors arising from diffuser spectral structures, ground-based measurements of these minor absorbers will need to be made regularly for each flight model at a range of latitudes for several years<sup>2</sup>.

**Recommendation V2:** Measurements of NO<sub>2</sub>, BrO, OClO, H<sub>2</sub>CO and SO<sub>2</sub> columns should be made regularly for several years by ground-based instruments to characterise the *seasonal-dependence* of errors arising from diffuser spectral structures for each FM in flight.

<sup>1</sup> Structures of this magnitude may also cause a seasonally-dependent tropospheric ozone bias in profile retrieval, as indicated in this study by simulations of BSDF error (see Sect 3).

<sup>2</sup> Extending the existing NDSC network to make regular column measurements of these minor absorbers in the free troposphere and stratosphere would enable the quality of GOME-2 trace gas column data to be maintained over the entire MetOp-1,-2 & -3 mission duration. When tropospheric concentrations of HCHO, SO<sub>2</sub> and NO<sub>2</sub> are elevated by pollution, their tropospheric columns can be derived from GOME-2. Extending the existing ground-based network to include (DOAS) measurements of these trace gases would therefore enable tropospheric columns derived from GOME-2 to be validated



### 3 Uncertainty in characterisation of diffuser BSDF

The bi-directional spectral distribution function (BSDF) of the GOME-2 QVD has been measured with two different optical stimuli during calibration activities for FM1, FM2 and FM3: (i) the FEL lamp, and (ii) the sun-simulator (SS)<sup>3</sup>. In the ideal case, these two measurements would be identical, but in practice they are not.

The deviation of the FEL:SS ratio from 1 was taken as a measure of the current uncertainty in BSDF. The magnitude and wavelength dependence of this deviation was different for FM1, FM2 and FM3, although in all three cases its magnitude was ~ few %. From the Baseline Error Budgets for retrieved products derived in the main study, it could be anticipated that broad-scale BSDF errors of this magnitude in Band 1 would cause significant errors in stratospheric O<sub>3</sub> profile retrieval, and this was confirmed to be the case in Phase V.

In addition, fine-scale spectral structure in the FEL:SS deviation in other bands was also discovered to cause errors in retrieved products, depending on the degree of spectral correlation with trace gas absorption signatures. In the Huggins bands, the spectral signature of FEL:SS deviation was found to give rise to large errors in tropospheric O<sub>3</sub> profile retrieval. Deviations in Bands 2 and 3 were found to also give rise to errors in columns of BrO and NO<sub>2</sub>, respectively, which were significant in relation to their baseline error budgets.

The above approach has identified the potential importance of erroneous fine-scale spectral structure in GOME-2 BSDF characterisation<sup>4</sup>. However, propagated errors on O<sub>3</sub> profile and trace gas column retrievals should be considered as indicative, at best.

It is important that measurements by the FEL and the sun-simulator (and also NASA integration sphere) are mutually consistent within their respective error bars, and also that the sun-angle dependence of the diffuser BSDF is accurately characterised on fine spectral scales. Pre-flight measurements on ground of zenith-sky and direct-sun spectra should permit diffuser BSDF and the Level-1 radiometric calibration algorithm to be verified to a useful level.

**Recommendation V3:** *Realistic error budgets should be defined for FM1, FM2 and FM3 diffuser BSDF, paying particular attention to fine-spectral scales.*

**Recommendation V4:** *Zenith-sky and direct-sun measurements should be made with flight models on ground to verify BSDF calibration and to test the Level-1 algorithm<sup>5</sup>.*

### 4 Residual error from Polarisation Correction

Residual error signatures, in sun-normalised radiance spectra arising from the polarisation correction, depend upon the polarisation responses of the FPAs and PMDs, and errors in their pre-flight measurement (i.e. errors in polarisation Key Data). An important aspect of Phase V was to use the polarisation responses, which had been measured at *instrument level*<sup>6</sup> for FM2, in place of information on individual *optical components*, which had been combined together in a theoretical way for use in the main study.

The location of the lowest wavelength PMD near 311 nm (c.f. ~ 350 nm for GOME-1) means that wavelength interpolation yields smaller polarisation errors for GOME-2 in Band 1. In the main-study, errors simulated for GOME-2 were almost always better than for GOME-1 and always less than 20% (in almost all cases < 10%).

The unpolarised radiation from the sun becomes polarised when scattered/reflected. The type and degree of polarisation depends on the nature of the scattering/reflecting medium and therefore on height. *The polarisation signatures in monochromatic spectra of backscattered solar radiation are therefore controlled by the absorption of ozone and other trace gases.* To the extent that the GOME-2 PMDs under-resolve and under-sample these atmospheric absorption signatures (e.g. ozone in the Huggins bands), smooth wavelength interpolation of the derived polarisation correction will be in error. Residual errors from application of the current

<sup>3</sup> A third stimulus, NASA's integrating sphere, has also been used but results were not available in time for Phase V.

<sup>4</sup> This is consistent with the previous finding in regard to diffuser type.

<sup>5</sup> Measurements need to be made and analysed early enough for a feasible response to be possible, if necessary (e.g. repeat measurement).

<sup>6</sup> This also included the measured U sensitivity, which was not accounted for in the main part of the study.



polarisation correction algorithm (PCA) were synthesised using calculations on a sufficiently fine spectral grid by a polarisation-dependent radiative transfer model.

Because residual errors are spectrally correlated with the O<sub>3</sub> Huggins bands, the tropospheric part of the O<sub>3</sub> profile retrieval and the O<sub>3</sub> total column retrieval, which both make use of differential structures in the Huggins bands, were both found to be very sensitive to propagation of residual polarisation errors.

The possibility was assessed to reduce these errors by reading out every PMD detector, instead of the currently-selected sub-set. However, this was found to give very little improvement, because of the more fundamental problem of limited spectral resolution, ~ 4 nm in the Huggins bands, which is not sufficient.

The main findings from Phase V can be summarised as follows:

1. The new, more reliable, simulations for GOME-2 indicate that mapping errors can be much larger than simulated in the main study, particularly for eastward pixels. In some cases, errors are unacceptably high in the troposphere.
2. It was originally expected that residual errors from the polarisation correction would be most serious in the Band 1 region, due to the interpolation from the theoretical point to the lowest wavelength PMD ~ 311 nm. However, the mapped errors showed that, for GOME-2 FM2, the largest contributions are actually from Band 2. This is driven by the large amplitude in some cases (notably extreme east pixels) of fine-structure in the error signatures which is correlated with the Huggins bands.
3. Although GOME-2 improves on GOME-1 in capturing polarisation on broad spectral scales, it does not improve on GOME-1 in capturing the fine-scale polarisation signature caused by atmospheric absorption in the Huggins bands, because the spectral resolution of the PMDs is not sufficient.
4. Errors in polarisation Key Data were not addressed explicitly in Phase V. However, the residual errors depend also on the Q/I ratio<sup>7</sup>, and noise in the measured polarisation responses “blows up” when Q/I tends to zero<sup>8</sup>.
5. GOME-2 views much closer to 90° scattering angle towards the eastern edge of the 1920 km swath and earlier local time of observation than does GOME-1 in its 960 km swath.
6. Errors due to low Q:I ratio are generally large, but not as significant as those driven by large amplitude Huggins structure.

It is recommended that further work be carried out with respect to residual errors in sun-normalised radiance arising from polarisation because, although these are generally quite small (< 1%), in a number of cases they cause errors in O<sub>3</sub> total columns and profiles which exceed User Requirements. At present, for example, errors of 10's% are found in tropospheric ozone retrieved from the extreme east view. These large errors are caused by Huggins structure in the residual polarisation error which cannot be corrected with the current scheme, even if all PMD pixels were to be made available and used in the correction. This is a consequence of the low spectral resolution (~ 4 nm) of the PMDs in the Huggins range.

Possible approaches to mitigate these errors would be:

- a. Ideally, to improve the spectral resolution of the PMDs in the Huggins bands. A resolution of order 1 nm (c.f. PMD pixel sampling in this region of 0.7 nm) would be expected to largely remove these errors. However, it is recognised that neither an across-the-board increase in PMD spectral resolution nor a preferential focusing in this spectral range of the PMDs would be practical at this time.
- b. Shifting the 1920 km swath to the west would reduce the occurrence of the largest errors<sup>9</sup>. Further work would be required to model fully the across-track dependence of this error<sup>10</sup>, in order to define

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<sup>7</sup> Q/I is the ratio of Stokes parameters defining the linearly-polarised and total intensities.

<sup>8</sup> This is because, when Q/I tends to zero, the Stokes parameter U and FPA and PMD sensitivities to this component become important. Although the FPA and PMD responses to U have been measured, there are uncertainties in these key data.

<sup>9</sup> Selecting a (symmetric) 960km swath instead of the 1920km swath could also alleviate this problem at tropical latitudes, though not at middle and high latitudes where scattering angles ~ 90° are not confined to the most easterly pixels.

<sup>10</sup> Across-track scanning strategy should also consider recommendations from the main study to alleviate scan-angle dependent errors from sun-glint (low latitudes) and the pseudo-spherical approximation (high latitudes).



an optimum across-track scan, which would be asymmetric about the nadir point and would vary around the orbit and the annual cycle.

- c. Low Q:I ratio occurs in at least 1 across-track ground pixel throughout most of the orbit. It is important to implement a polarisation correction algorithm which can cope with this specific condition.
- d. A more sophisticated polarisation correction scheme can be envisaged, which would make use of knowledge of the ozone profile<sup>11</sup> to model the wavelength dependence of polarised radiation at finer scales than can be captured by the PMDs. It would require significant further work to assess whether such an approach might be feasible.

**Recommendation V5:** *The base-line polarisation correction scheme for Level 1 processing should be improved to accommodate low Q:I cases.*

**Recommendation V6:** *To mitigate residual polarisation errors correlated with the Huggins absorption features, the following strategies should be investigated: (a) devise across-track scan pattern to avoid 90° scattering angle, (b) devise scheme to correct for fine structure in polarisation.*

## 5 Spatial aliasing via polarisation monitoring detectors

Because spectral pixels in the GOME-2 detector arrays are read-out sequentially, and this takes a finite time, the scene over which each spectral pixel integrates is slightly different. The possibility therefore exists for spatial variability in the scene to be aliased into the measured spectrum. The most extreme difference in scene is between spectral pixels at the ends of the arrays, which causes spectral discontinuities at band boundaries. This had provided clear evidence of spatial aliasing in GOME-1 flight data. The ratio of integration time to read-out time is smaller for GOME-2 than for GOME-1, so GOME-2 is more susceptible to this phenomenon.

During the main part of the study (Phase I to Phase IV), this error source had been assessed by mapping the impact on FPA signals of spatial variations in surface reflectance (derived from a limited number of LANDSAT images) onto the constituent retrieval. An important finding from this work, which had not previously been appreciated, was that the GOME-2 instantaneous fields of view (IFOV: 0.29° ~ 4 km across-track on ground) will effectively filter out structure at high spatial frequencies in the scene (i.e. spatially-aliased noise). In Phase V, the investigation of spatial aliasing has been extended to the PMD detectors.

The realistic simulation of spatial-aliasing via the PMDs was complicated and involved a number of steps. The first step was to generate time-series of the Stokes parameters I(t), Q(t) and U(t) from a set of five LANDSAT images using a polarised radiative transfer model. The second step was to calculate PMD and FPA signal time-series, integrating and sampling in time as appropriate and applying time and wavelength interpolation as necessary to synchronise FPA and PMD signals as closely as possible. The polarisation correction algorithm was then applied to the time series of FPA signals.

At wavelengths < 310 nm, ozone absorption hides clouds and other sources of scene inhomogeneity, so spatial aliasing via the PMDs (as well as directly via the FPAs) is only seen in the signatures at longer wavelengths. So the O<sub>3</sub> profile retrieval is affected exclusively through Band 2, except when the selected interval of Band 1 is extended from 306 nm to 314 nm.

Key points arising specifically from the exercise to linearly-map signatures of additional spatial-aliasing via the PMDs (i.e. additional to residual errors from the PCA reported in preceding section) were:

1. The signature of aliasing via PMDs has little impact over and above that of error in the polarisation correction algorithm itself (see preceding section).
2. Results from the main study on the direct impact of spatial aliasing via the FPAs are therefore still considered representative of the spatial-aliasing problem as a whole (subject to the limited number of cases represented by the chosen LANDSAT images).

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<sup>11</sup> It might be desirable to incorporate a correction for polarisation fine structure into the L2 processor since this could exploit real-time O<sub>3</sub> information rather than depend on an O<sub>3</sub> climatology, as would be necessary in the L1 processor.



In summary, the consequences for ozone profile retrieval of perturbations to the polarisation correction caused by spatial aliasing are minor compared to: (i) direct impact of spatial aliasing on the signals recorded by the FPAs and (ii) other errors from the PCA. It should, however, be recalled that although (i) was found not to be a source of significant additional random error, this would not be true for a profile algorithm which used composite spectra from Bands 1 and 2. Inhomogeneity within the scene is also known to cause two problems in addition to spatial aliasing: (a) radiative transfer non-linearity means that significant retrieval errors are inevitable for a mixed scene comprising both high and low intensities, as shown in the main study, (b) variation in instantaneous pattern of illumination along the cross-dispersion axis of the slit (i.e. the along-track direction) will cause GOME-2's true response to differ subtly from that characterised on the ground with uniform illumination, e.g. spatial inhomogeneity in detector pixel sensitivity and/or slit-function shape.

## 6 Requirements for measurement of slit-Function shape

The main study had demonstrated unequivocally that characterisation of the slit-function shape in the relevant wavelength interval of Band 2 was of critical importance to ozone profile retrieval, in order to avoid errors in excess of 100% in the troposphere which would otherwise occur. Pre-flight measurements of slit-function shape were therefore recommended so as to meet User Requirements on the accuracy of GOME-2 ozone profile retrieval. Such measurements would also offer a major advance on GOME-1, for which errors in knowledge of slit-function shape can now be identified to be a limiting factor on accuracy.

In Phase V, trace gas column retrieval was considered in addition to ozone profile retrieval and requirements have been defined for laboratory measurements of slit-function to satisfy both applications.

### 6.1 Approach

The approach employed in this part of Phase V was based on a development of the linear-mapping methodology used elsewhere in the study. In summary, this involved propagating errors associated with the laboratory set-up for measuring the slit-function onto retrieved ozone profiles and trace gas columns. By exploiting the matrix algebra for linear mapping, the following three steps were conveniently combined into a single mathematical step:

1. Propagation of errors in laboratory set-up onto errors in retrieved slit-function shape
2. Propagation of errors in slit-function shape onto errors in calculated, sun-normalised spectra
3. Propagation of error signatures in sun-normalised radiance onto retrieved O<sub>3</sub> profiles and trace gas columns

The representation of the slit-function was, of course, a critical issue in this analysis. A piece-wise linear representation was used on a wavelength grid with 0.01 nm spacing, since this offered the degree of flexibility which would be needed in practice to analyse laboratory measurements of slit function and avoided pre-selection of a particular functional form<sup>12</sup>. Of equal importance was the degree of spectral correlation permitted in the representation. A *spectral correlation length* was defined from measurements of the GOME-2 slit-function width, which was assumed to result from the convolution of three functions:

1. The detector pixel spatial response
2. The image of the slit on the detector array if perfectly focused
3. A Gaussian spot function

The width of the spot function was adjusted until the convolution of the three functions gave the measured FWHM for the FM2 slit function (~ 0.3 nm).

The laboratory set-up assumed to apply for GOME-2 was similar in concept to that used recently for OMI: a quasi-monochromatic source with Gaussian spectral shape was scanned in wavelength at steps of 0.005 nm. The FWHM of this source was varied from 0.005 nm to 0.500 nm to assess sensitivity to this parameter.

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<sup>12</sup> The primary reason for laboratory measurements is that the GOME-2 slit-function shape cannot be specified from theoretical considerations alone and is unlikely to follow a simple functional form.



Four sources of error on laboratory measurements, each with four different assumptions regarding their spectral correlation, were propagated onto trace gas columns and ozone profiles.

Propagated errors were found to be large for a source whose width was comparable to or larger than the slit function itself. Errors were found to decrease as source width was reduced from 0.1 nm to 0.01 nm (the resolution at which monochromatic radiance/irradiance spectra had been simulated).

## 6.2 Derivation of requirements

### (a) O<sub>3</sub> profile analysis

The propagated errors were translated into stability / knowledge requirements on the lab set-up, taking into account the observation time required to achieve the necessary signal to noise. This translation was done by scaling propagated errors such that the End User Requirements on O<sub>3</sub> profile were satisfied at all altitudes, for both albedos and for all three geo-temporal scenarios. The table below presents requirements for the case of errors which are uncorrelated over a GOME-2 detector pixel but fully correlated from one detector pixel to the next (worst case of the four simulated). Assumptions common to all derived requirements in the table are: (1) that the source width is 0.04 nm (comparable to the OMI stimulus) and (2) that observations are scanned across the detector array in 0.005 nm steps<sup>13</sup>.

It is important to note that requirements in the table apply to a GOME-2 spot width of 0.21 nm, which corresponds to a GOME-2 slit-function width of 0.3 nm, as pertains to FM2 after defocusing. Calculations performed within the study show that more stringent requirements would have to be imposed for a more focused instrument. It is therefore recommended that FM1 and FM3 be defocused to at least 0.3 nm slit-width for this reason, in addition to those given in the main study.

### (b) Trace gas column analysis

For retrieval of trace gas columns using the DOAS algorithm, the slit-function enters explicitly into the so-called under-sampling correction. This allows structure in the sun-normalised spectrum, which originates from fine structure in the solar spectrum together with wavelength misregistration between backscattered and direct-sun spectra, to be compensated using calculations from a high-resolution solar reference spectrum convolved with the slit-function. Doppler shift of the solar irradiance spectrum incident at GOME-2 ensures that there is typically a misregistration of ~ 0.007 nm, as has been simulated here.

Slit-function convolution can also enter explicitly into the trace gas column retrieval, if high-resolution laboratory measurements of absorption cross-section are used instead of absorption cross-section measurements by the GOME-2 instrument itself. Using the proper slit-function will permit the assessment of the error from using an under-sampling correction scheme as proposed for GOME-1.

On the trace gas column side, requirements on the slit-function measurement set-up were driven by the End User Requirement on O<sub>3</sub> accuracy, which is quite strict (< 4%). They were found to be comparable to those derived from the O<sub>3</sub> profile retrieval side, which were driven by an End User Requirement of < 30% accuracy in troposphere.

Table 2 below also refers to information supplied by ESA in regard to the OMI slit-function measurement set-up. Quantitative requirements derived for GOME-2 appear to be reachable with a set-up of this kind.

**Recommendation V7:** *The slit function of GOME-2 (all flight models) should be determined according to the quantitative requirements specified in this study, with particular attention to the Huggins bands (315 - 335 nm).*

**Recommendation V8:** *FM1 and FM3 should be defocused to at least the level implemented in FM2 (slit width of 0.3 nm in Huggins bands), with the same physical slit dimension.*

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<sup>13</sup> A larger step size could be used instead. However, the S/N requirement would then need to be increased by the square root of the ratio of the new step size to 0.005nm.



Source error type	O <sub>3</sub> Profile	Trace gas column	OMI Source
Signal:Noise	700	100	~ 1000 <sup>14</sup>
Power	1%	2 %	0.5-1% <sup>15</sup>
Shift	3% of width (0.0012 nm)	8% of width (0.0032 nm)	0.003nm <sup>16</sup>
Width	40%	20%	~ 10's% <sup>17</sup>

**Table 2: Requirements for laboratory measurements derived from O<sub>3</sub> profile and trace gas column analyses assuming defocused slit and FM2 spot size**

## 7 Recommendations from Phase V and from the Main Study

### 7.1 Summary

The eight new specific recommendations for operational settings and error mitigation arising from Phase V are listed in the table below (V1 – V8):

New recommendations from Phase V of study	
V1	The quasi volume diffuser should be used for GOME-2.
V2	Measurements of NO <sub>2</sub> , BrO, OClO, H <sub>2</sub> CO and SO <sub>2</sub> columns should be made regularly for several years by ground-based instruments to characterise the <i>seasonal-dependence</i> of errors arising from diffuser spectral structures for each FM in flight.
V3	Realistic error budgets should be defined for FM1, FM2 and FM3 diffuser BSDF, paying particular attention to fine-spectral scales.
V4	Zenith-sky and direct-sun measurements should be made with flight models on ground to verify BSDF calibration and to test the Level-1 algorithm
V5	The base-line L1 polarisation correction scheme should be improved to accommodate low Q:I cases.
V6	To mitigate residual polarisation errors correlated with the Huggins absorption features, the following strategies should be investigated: (a) devise cross-track scan pattern to avoid 90° scattering angle; (b) devise scheme to correct for fine structure in polarisation.
V7	The slit function of GOME-2 (all flight models) should be determined according to the quantitative requirements specified in this study, with particular attention to the Huggins bands (315 - 335 nm).
V8	FM1 and FM3 should be defocused to at least the level implemented in FM2 (slit width of 0.3 nm in Huggins bands), with the same physical slit dimension.

<sup>14</sup> A basic S/N of ~ 1000 can be achieved at the stimulus central wavelength.

<sup>15</sup> For sufficiently long integration times, and Echelle angles within 1° of the nominal angle (at 75° angle of incidence)

<sup>16</sup> Relative accuracy near 335 nm arising from motor drive. Bias of ~ 0.01 nm is also expected from the alignment procedure, but is not important to derivation of slit-width since it would apply to all wavelengths.

<sup>17</sup> Uncertainty in knowledge of stimulus width has been inferred indirectly by comparison of measured and predicted OMI slit-function widths to be ~ 10's %.



## Executive Summary

The specific recommendations from the original study (Phases I to IV) were reviewed in the context of the new findings from Phase V. As a result of this review, the following have been retained in their original or modified form:

Retained recommendations from Phases I to IV of study	
A1	For O <sub>3</sub> profile retrieval, it is recommended to not use Band 1B wavelengths above 307 nm.
A2	For O <sub>3</sub> profile retrieval, it is recommended that the integration times for Bands 1A and 1B be 1.5 sec and 0.1875 sec, respectively.
A4	It is recommended that the impact of spatial aliasing be assessed more thoroughly: <ul style="list-style-type: none"> <li>a) Global statistical analysis of O<sub>3</sub> profiles and trace gas columns using ATSR-2 images</li> <li>b) Impact on geophysical products retrieved directly from PMD measurements</li> <li>c) Impact on multi-wavelength aerosol retrieval.</li> </ul>
A5	It is recommended that an Observing System Simulation Experiment (OSSE) be undertaken for GOME-2 to decide on optimum ground-pixel size and swath width <sup>18</sup> .
B2/C3	It is recommended to review the feasibility of doubling the number of ground pixels sampled across-track, so as to halve ground pixel size for a given swath-width, in order to maximize the number of cloud-free scenes observed and hence the quality of O <sub>3</sub> and minor trace gas distributions in the troposphere <sup>19</sup> .
C2	It is recommended to quantify the impacts of: (a) scene inhomogeneity on radiometric response and slit-function shape <sup>20</sup> and (b) errors in knowledge of slit-function shape on aerosol and cloud retrievals using the O <sub>2</sub> A-band.
C5	Assess possible use of onboard white light source to monitor wavelength-dependent degradation in UV
C6	Implement and quantify the benefits to ozone profile and trace gas column retrievals of algorithm improvements to mitigate errors due to sun-glint.
C7	Quantify errors arising from non-linear radiative transfer in conjunction with static scene inhomogeneities in cloud and surface reflectance.
C8	Assess errors on ozone profiles from the assumed vertical distribution of aerosol more thoroughly, in order to better gauge instrumental errors
C9	Assess the impact on ozone profile and ozone column error budgets of adding visible wavelengths
C10	Assess errors from uncertainties in absorption cross-sections of ozone and other trace gases, the high-resolution solar reference spectrum and polarised atmospheric radiative transfer, in order to better gauge instrumental errors

<sup>18</sup> It is envisaged that although such an OSSE might be conducted using the O<sub>3</sub> assimilation scheme of an NWP centre, the “figure of merit” should be the 4D O<sub>3</sub> field itself, and possibly the surface UV flux, rather than the usual NWP forecast variables. I.e ground-pixel size and swath would be optimised by minimizing (time-evolving) deviations between assimilated and true O<sub>3</sub> fields, taking into account the likelihood of cloud obscuration for different ground pixel sizes and known variations with integration time and scan-angle of random and systematic errors on retrieved O<sub>3</sub>.

<sup>19</sup> This would require Band 2B, 3 and 4 integration times to be halved from 0.1875 sec to 0.09375 sec. Onboard data compression could offer a practical means to double the number of ground-pixels without doubling the GOME-2 data downlink capacity. If not, an alternative would be to halve the integration times and downlink alternate ground-pixels across the swath. This would still permit the frequency of cloud-free pixels to be increased substantially, although at the expense of losing half the total measurement time. In the redesign of a future UV/VIS satellite-borne spectrometer, it would benefit photometric S/N on trace gas column retrievals for individual ground pixels to have a slit-function wider than that of GOME-2: ~ 0.5 nm in Band 2 and ~ 1 nm in Band 3.

<sup>20</sup> Non-uniform illumination of the entrance slit in conjunction with non-uniform detector pixel spatial response will modify signal level and variation in illumination along the cross-dispersion axis (i.e. along-track direction) will modify slit-function shape.



## 7.2 Selection of swath and ground-pixel size

In Phases I – IV and V of this study a number of factors have been identified which, for one of two reasons, need to be taken into account in selecting an operational swath and ground-pixel size:

- A number of significant errors vary in an asymmetric way with view-angle across-track (and therefore on swath width), as well as solar geometry (latitude and season)
  1. Residual error from the polarisation correction algorithm
  2. Error from Lambertian surface approximation in presence of sun-glint
  3. Error from pseudo-spherical approximation at high solar zenith angles
- Other key factors depend upon ground-pixel size (and therefore on swath width).
  1. Frequency of cloud-free scenes
  2. Non-linearity error for a scene of mixed (i.e. high and low) albedo

A simple recommendation concerning the operational swath and ground-pixel size is not forthcoming on the basis of information from this study. Further work is therefore needed to support this selection, as indicated in preceding sections:

1. View-angle dependence of the residual error from the polarisation correction algorithm (PCA) should be quantified in detail (i.e. at angles in addition to the three assessed so far: nadir plus the two extreme view angles of the 1920 km swath)
2. The alternative option, to mitigate residual PCA errors by modifying Level 2 algorithms, should be investigated
3. Investigate the feasibility to double downlink data rate (e.g. by onboard data compression) or to downlink alternate ground-pixels, so as to halve the ground-pixel size for a given swath width
4. An OSSE with realistic prescription of cloud statistics and retrieval errors as functions of view angle, latitude, season and ground pixel size is recommended in order to select an operational swath and ground-pixel size in an objective manner.

## 7.3 References

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