

Study - GOME-2 Error Assessment

Executive Summary

Version 1 December 2002 EUMETSAT Contract No EUM/CO/01/901/DK





Executive Summary of Final Report

Version 1

Study Team

Dr Brian Kerridge (Science Coordinator) Dr Richard Siddans Mr Barry Latter

Space Science Department Rutherford Appleton Laboratory Chilton, Didcot Oxfordshire OX11 0QX UK

Eumetsat Technical Officer:

Dr R Munro

EUMETSAT · Am Kavalleriesand 31 Postfach 10 05 55 · D-64295 Darmstadt Germany Prof. Dr Ilse Aben Dr C. Tanzi Dr W. Hartmann

SRON Earth Oriented Science Division Sorbonnelaan 2 NL-3584 CA Utrecht The Netherlands Prof. Dr. J. P. Burrows Dr Mark Weber Dr Ruediger de Beek Dr Vladimir Rozanov Dr Andreas Richter

FB1 Institute for Environmental Physics (IUP) University of Bremen Postfach 33 04 40 D-28334 Bremen Germany

Study Manager

Mr M.G. Wickett

Serco Europe Ltd Kempton Point 68 Staines Road West Sunbury-on-Thames Middlesex TW16 7AX UK

Date: December 2001





serco



List of Contents

1	I	Introdu	iction I	
2		Approc	ach I	
3	3.1 3.2 3.3	Error De Gene Ozone Trace	efinitions and Baseline Error Budgets ral e profiles gas columns	
4		Analys	is of Instrument Parameters and Specified Errors	IV
	4.1 4.2	Samp Spatic	ling Options for Band 1 al Aliassing and Static Scene Inhomogeneities	IV V
	4.3	4.2.1 4.2.2 4.2.3 Spect 4.3.1 4.3.2 4.3.3	General Ozone profiles Trace gas columns tral Resolution and Slit-Function Shape General Ozone profiles Trace Gas Columns.	VV VVI VIVI VI VI
	4.4	Pseuc 4.4.1 4.4.2 4.4.3	do-Spherical Approximation and Earth's Curvature General Ozone Profiles Trace Gas Columns	VII VII VIII VIII
	4.5	Non-L 4.5.1 4.5.2 4.5.3	ambertian Surface BRDF General Ozone profiles Trace gas columns	VIII VIII VIII VIII
	4.6	Clouc	d Obscuration and Horizontal RI Gradients	IV
		4.6.1 4.6.2 4.6.3	General Cloud obscuration Horizontal gradient in RI	IX IX IX IX IX IX
	4.7	Pointii 4.7.1 4.7.2 4.7.3	ng and Geolocation General Ozone profiles Trace gas columns	IX IX IX IX
	4.8	Error E 4.8.1 4.8.2 4.8.3 4.8.4 4.8.5 4.8.6	Budget Summaries Ozone Profiles Trace gas columns Total ozone Nitrogen dioxide Bromine oxide Chlorine dioxide	X X XI XI XI XI



5	Recommendations and Further Work	XII	
5.1	Background to the Recommendations	XII	
5.2	Band 1 sampling	XII	
	5.2.1 Long-wave limit	XII	
	5.2.2 Spatial/temporal	XIII	
5.3	Diffuser	XIII	
5.4	Pre-flight characterisation of slit-function shape	XIII	
5.5	Slit-function widthX		
	5.5.1 Defocusing	XIV	
	5.5.2 Slit opening	XV	
5.6	Detector read-out time	XV	
5.7	Selection of swath width and ground-pixel size	XVI	
5.8	Summary of Recommendations	XVIII	





EXECUTIVE SUMMARY

1 Introduction

The GOME-2 Error Assessment Study was commissioned by Eumetsat with the following scope:

- > To identify through quantitative simulations the factors which will limit the accuracies of *trace gas column* and *ozone profile* retrievals from GOME-2.
- On the basis of this quantitative assessment, to recommend operational settings for GOME-2 and, if necessary, algorithmic approaches to mitigate errors.

The study was conducted by the following consortium:

- Serco Europe Ltd (Prime Contractor; Study Administrator)
- > RAL (Technical Coordinator; Ozone Profile Analysis)
- > IUP (Trace Gas Column Analysis; Radiative Transfer Model Calculations)
- SRON (Assessment of Instrumental Errors)

2 Approach

The schemes employed in simulations for ozone profiles and trace gas columns are based very closely on those applied to real GOME-1 measurements by RAL and IUP, respectively. Both these schemes are the result of nearly a decade of development work, so are now mature and have been demonstrated to be among the most reliable of their kind. Although the magnitudes of simulated errors are specific to the detailed formulations of these two particular algorithms, the conclusions and recommendations arising from this study are expected to prove quite robust and to be applicable also to other schemes, which might be adopted for operational processing of GOME-2 data.

For ozone profiles, the sensitivity of the *optimal estimation* retrieval scheme to wavelength ranges and *a priori* constraints was explored before embarking on the investigation of instrumental parameters and errors.

The initial review of instrumental error sources and magnitudes was conducted by SRON and benefited from SRON's extensive knowledge of instrumental issues for GOME-1 and GOME-2. An issue of key importance for GOME-2 is the extent to which its improved design for measuring and correcting for polarisation will benefit data quality. The review drew directly on findings from SRON's recent study for ESA/Eumetsat, which covered this topic in depth (H.W. Hartmann and I. Aben, Final Report, GOME-2 Phase-B Polarisation Study, RP-GOME2-002SR/00, January 2001).

Another very important element of this study was the availability of state-of-the-art radiative transfer models at University of Bremen, which permitted:

- a) Calculations to be performed for a fully-spherical atmosphere using the CDI radiative transfer model¹
- b) Calculations with a pseudo-spherical version of CDI, which apart from numerical differences is equivalent to GOMETRAN that is commonly used in the GOME-1 retrievals.

¹ Another spherical radiative transfer code exists, which is named CDIPI. This model is specifically designed for limb viewing LOS. CDI is equivalent to CDIPI without Picard iterations (PI).



Pseudo-spherical and spherical versions of CDI were used to assess errors arising from (a) the pseudo-spherical approximation² and (b) the assumption of Lambertian surface BRDFs.

Most simulations in the GOME-2 Error Assessment Study 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) and a variety of view-angles spanning two of the GOME-2 swath-width options: 960 km and 1920 km. The conclusions and recommendations from this study are therefore expected to be applicable to GOME-2 observing conditions generally (though not universally).

Except for errors, which were sufficiently large to necessitate iterative, non-linear simulations, *linear mapping* was employed throughout this study. In this approach, the impact of a given error on sun-normalised radiances was calculated by perturbing the forward model, and the spectral signature of this perturbation was then mapped onto the retrieved ozone profile or trace gas column using the matrix algebra of optimal estimation.

3 Error Definitions and Baseline Error Budgets

3.1 General

In order to gauge the importance of error sources specifically identified for attention in this study, errors known to have affected GOME-1 retrievals were reviewed and a *baseline error* budget compiled. The components of the *baseline error* budgets for ozone profiles and trace gas columns are described below.³

3.2 Ozone profiles

The baseline *precision* of GOME-2 was defined as the *estimated standard deviation* (*ESD*) at each retrieval level, evaluated from the diagonal elements of the solution error covariance matrix (S_x) for the retrieval. The ESDs were based solely on linear propagation of *measurement noise* through the optimal estimation retrieval equations, adopting an *a priori* uncertainty of 100% on ozone at each level (with vertical Gaussian correlation lengths as described in the final report). Measurement noise is estimated from a GOME-2 noise model, which combines *photon noise* with *read-out* noise. Based on GOME-1 experience, measurement precision from this model is better than can realistically be achieved in fitting simulated to measured spectra (due to forward model errors and/or unaccounted for instrumental errors). "*Noise-floors*" corresponding to 1% and 0.05% of sun-normalised radiance were therefore imposed in Bands 1 and 2, respectively. Other errors were handled by *linear mapping*.

For retrieval levels at 20 km and above, the ESD is markedly lower than the *a priori* uncertainty. For retrieval levels below 20 km (i.e. at 0, 6, 12 and 16 km), however, the ESDs are often >50% of the *a priori* uncertainties, so the a priori constraint is quite significant. It should be borne in mind that the error estimates obtained by linear mapping will also have been influenced by this *a priori* constraint⁴.

The sources and magnitudes of errors included in the *baseline error* budget by linear mapping are as specified in Table 1.

 $^{^{2}}$ The term pseudo-spherical approximation is applied to models in which attenuation of the incoming solar beam is calculated for a spherical atmosphere but the intensity of scattered radiation is calculated for a plane-parallel atmosphere.

³ It should be noted that the baseline error budgets did not include clouds, spectroscopic or instrumental errors other than those described.

⁴ In the limit in which there is no reduction in the *a priori* uncertainty at a given altitude, due to absence of information in the measurements, the retrieved ozone mixing ratio at that altitude will not deviate from the *a priori* value, and linearly mapped errors will be identically zero.



Error Source	Magnitude
Radiometry	2% of sun-normalised radiance
Wavelength-dependent degradation of scan-mirror UV reflectance.	Equivalent to uncorrected GOME-1 degradation after 3-years (excl. from RSS)
Residual error from polarisation correction	SRON prescription for GOME-2
Surface pressure uncertainty	10hPa
Temperature profile uncertainty	Error covariance matrix from IASI retrieval
Aerosol profile uncertainty	LOWTRAN "high" - "background" cases

Table 1: Components of baseline error budget for O₃ profiles

Linearly mapped *baseline errors* were combined in a root-sum-squared (RSS) way for comparison with the ESDs and with the specific errors addressed in this study.

It should be noted that, although a realistic *wavelength-independent* error in sun-normalised radiance was included in the RSS (in accordance with the error budget for pre-flight radiometric calibration), *wavelength-dependent* error in sun-normalised UV radiance arising from degradation in the UV reflectivity of the scan mirror was quantified (for a case equivalent to GOME-1 after three-years operation) but was not incorporated into the RSS. The reason for this is two-fold: firstly, it is very difficult to predict the character (e.g. wavelength and time dependencies) that such degradation will exhibit for GOME-2 and, secondly, if similar to GOME-1 Band 1, this would dominate over all other errors after several years of operation, unless corrected for.

Aerosol is highly variable in the troposphere, especially in the boundary layer, and also in the lower stratosphere following volcanic eruption. In this study, the aerosol profile was fixed in the GOME-2 FM to be the LOWTRAN "*background*" profile (as it is in the RAL GOME-1 ozone profile retrieval scheme) and enhancements to aerosol loading were treated as a potential source of error. As discussed in the final report, this error has been estimated by linear mapping of the spectral difference between LOWTRAN "*background*" and "*high*" cases. Aerosol loading in the LOWTRAN "*high*" case makes this a conservative estimate in many circumstances. However, it was beyond the scope of this study to investigate and account for errors in the FM due to neglect of cloud, and the nature of such errors is somewhat similar to that of a large tropospheric aerosol excursion. RSS *baseline errors* were therefore calculated both with and without inclusion of the mapped aerosol error. The latter can be considered to be a lower limit, applicable to a cloud-free, background aerosol situation⁵. The former can be considered to be representative of an extreme aerosol event and also indicative of pervasive, thin cloud.

In considering the specified errors and their importance in relation to the baseline GOME-2 error budget, it is useful to distinguish between those, which vary in a quasi-random way with time and location, and those, which vary in a non-random way. The former affect precision but can be reduced by averaging, whereas the latter give rise to systematic biases, which cannot be reduced by averaging but can in certain conditions be amenable to *a posteriori* correction. The more relevant comparisons for the quasi-random and non-random errors are therefore with the ESD and RSS, respectively. In the following sections, quasi-random errors are deemed to be significant if comparable to the ESD and non-random errors are deemed significant if comparable to the RSS. The RSS is typically <5% at 20 km and above and $\sim10-20\%$ at 16 km and below.

⁵ This lower limit would also apply if accurate independent information on aerosol/cloud scattering properties within the GOME-2 pixel could be derived either from other GOME-2 measurements (e.g. O₂ A-band and/or PMDs) or from co-located AVHRR3 images.



EXECUTIVE SUMMARY

3.3 Trace gas columns

The standard DOAS approach, as investigated in this study and used in operational GOME-1 retrieval, consists of a two-step procedure. Firstly, a slant column density is retrieved from spectral fitting. Secondly, airmass factors are calculated using a multiple scattering radiative transfer model (RTM), assuming *a-priori* knowledge of the profile shape. Division of the slant column density by the airmass factor results in the vertical column density (total column). Both steps involve errors, which can be combined into an overall error budget. In the application to real data, the error sources from both steps can be distinguished. In this study, however, perfect *a-priori* knowledge has been assumed, so a distinction between AMF and slant column errors for a given error source is not always clear-cut.⁶.

Attribution of the error sources to AMF and/or slant column has important implications for strategies of error mitigation. Slant column errors tend to be instrument related and improvable only by operational settings or hardware changes. On the other hand, errors assigned to AMF can be reduced by algorithm improvements.

For trace gas columns, photon noise and read-out noise were combined using the GOME-2 measurement noise model and ESDs were calculated by fitting the Ring cross-section in addition to trace gas columns. Residual errors following the application of the polarisation correction were linearly mapped but found to be negligible. Errors potentially arising from spectral structures in the diffuser plate BRDF were imported directly from a study on GOME-1 (see annex to Final Report), where they had been shown to be dominant for trace gases other than ozone.

In the following sections, the specified error sources analysed as part of this study are referenced to the basic ESDs for an integration time of 0.1875 sec. This corresponds to a 40x 80 km² ground pixel area at nominal swath width of 1920 km across-track. In general, error sources are considered significant if they are of same order of magnitude or higher than the baseline ESD.

4 Analysis of Instrument Parameters and Specified Errors

4.1 Sampling Options for Band 1

The baseline integration times for GOME-2 going into the study were: 12s for Band 1A and 0.1875s for Band 1B, with the 1A/1B boundary being set at 283 nm. For Band 1A, a 12s integration time would give rise to a ground pixel of 1920 km x 80 km, for the 1920 km swath option. However, there are known to be several disadvantages to such a large ground pixel, e.g.:

- > Non-linear dependence of radiative transfer on view angle over the range $\pm 45^{\circ}$
- Errors (e.g. pseudo-spherical approximation) in modelling radiative transfer at large view angles
- ▶ Horizontal variability of the stratospheric O₃ profile

For GOME-2, the flexibility exists to read out Band 1A at 1.5s (640 km x 40 km) and co-add spectra to recover signal to noise, and this co-addition could be performed in the along-track direction as well as the across-track direction, thereby alleviating the above-mentioned problems. However, more frequent read-out of detector arrays would result in increased read-out noise. This was quantified for ozone profile retrieval in the frame of a 1% noise floor.

⁶ An extensive study of possible AMF errors due to assumptions made in RTM and imperfect *a-priori* knowledge was beyond the scope of this study.



EXECUTIVE SUMMARY

Co-addition of 1.5s Band 1A pixels to 12s (640 km x 320 km) or 24s (640 km x 640 km) was found to yield similar ESDs to those for a single 12s Band 1A pixel. Additional read-out noise associated with more frequent read-out was also found to be insignificant for co-addition of 0.1875s Band 1B pixels to 1.5s.

It was therefore concluded that there would be no impediment to reading out Band 1A at 1.5s and Band 1B at 0.1875s.

4.2 Spatial Aliassing and Static Scene Inhomogeneities

4.2.1 General

Because spectral pixels in the GOME-2 detector array 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, and spectral discontinuities at Band boundaries 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. An important component of the study was therefore to quantify spatial aliasing as realistically as possible for GOME-2 and to determine its impact on trace gas columns and ozone profiles.

Several Landsat ETM+ images were acquired (\sim 180 km x 180 km at 1 m resolution) for this purpose. From these, an ensemble of >350 spatially-aliased signatures were calculated (in terms of dependent surface albedos) for each of the 12 geo-temporal scenarios. Spatially-aliased signatures were then linearly mapped and the ensemble error extremes, mean (bias) and RMS were examined.

An important finding from this work, which had not previously been appreciated, was that the GOME-2 IFOV (0.29° ~4 km on ground) will effectively filter out high-frequency structure (i.e. spatially-aliased noise)⁷.

4.2.2 Ozone profiles

For O_3 profile retrieval, the impact of spatial-aliasing was determined separately for the Band 1 and 2 steps. Band 1 can see down to the surface and can therefore detect low-frequency spectral structure from spatial aliasing only at the longest wavelengths. Spatially aliased errors were found to be less than ESDs when the Band 1 wavelength range was restricted to 265-307 nm but to exceed ESDs in extreme cases when the range was extended to 265-314 nm. By shortening the read-out time sufficiently, spatially-aliassed errors could be reduced below the ESD levels, even for these extreme cases.

From the point of view of O_3 profile retrieval, it was therefore concluded that a reduction in the Band 1B detector readout time would be desirable.

It was found from simulations in which detector read-out time was reduced to a negligible value by comparison to integration time that errors still arise if surface albedo varies spatially within a scene between high and low values (eg cloud/sea, land/sea). Such errors were ~10-20% in the troposphere, and could therefore exceed the RSS and sometimes approach the ESD. Such (static) errors are inherent to *scene inhomogeneity* and are due to the non-linear dependence of radiative transfer on surface albedo. Because their occurrence is related to geography and meteorology, it will not be random. Such errors are therefore significant even though they fall below the ESD.

Because only a small spectral interval (~100 of 1024 detector pixels) of Band 2 is used and a 2nd order polynomial is fitted to log(sun-normalised radiance), the Band 2 retrieval step is insensitive to *low-frequency* structure from spatial aliasing. However, alternative algorithms which attempt to use (a) sun-normalised

⁷ This means that images with much coarser resolution than Landsat ETM (e.g. ATSR-2, 1 km x 1 km) would suffice for a future, more comprehensive study of spatial-aliasing.



Band 2 radiances directly and/or (b) extensive intervals of Bands 1 and 2 simultaneously would be more vulnerable.

4.2.3 Trace gas columns

Windows used in spectral fitting of trace gas columns are very narrow in comparison to the widths of the GOME-2 bands (n.b. Bands 2 and 3). Trace gas column retrievals were therefore found to be insensitive to low-frequency structure in the spatially-aliased signatures. The maximum errors from spatial aliasing were: $0.02\% O_3$, $2\% NO_2$, 1% BrO, 10% OClO), all of which were below the ESDs

From the point of view of trace gas column retrieval, it was therefore concluded that no further reduction in detector read-out time would be necessary.

4.3 Spectral Resolution and Slit-Function Shape

4.3.1 General

The ability to resolve absorption signatures of target gases in sun-normalised spectra is fundamental to the GOME-class of measurement. As resolution is degraded, the ability to retrieve information on trace gases tends to decrease. However, spectral resolution had been deliberately decreased in the optical design of GOME-2 in comparison to GOME-1, in order to reduce the degree to which fine structure in the solar spectrum is undersampled. This undersampling had resulted in artificial spectral structure in sun-normalised GOME-1 spectra, due to minute changes in the wavelength registration of detector pixels between the measurements of direct-sun and backscattered spectra. An issue for the GOME-2 study was to assess the extent to which a further decrease in spectral resolution might be beneficial.

At the initiative of the study-team, this topic was broadened to also consider the impact of errors in knowledge of slit-function shape and how these would vary with spectral resolution (i.e. slit-function FWHM).

4.3.2 Ozone profiles

(a) Slit-function FWHM

Although undersampling errors are controlled to a satisfactory level by the RAL algorithm, accounting for them in the retrieval is a source of non-linearity which limits computational efficiency and which it might be possible to avoid if the slit width was increased. The trade-off between *increasing ESD* and *decreasing undersampling error* was examined in simulations of defocusing, in which the slit function FWHM was increased, redistributing but conserving the total photon flux on the detector array. In a *worst case* estimate, in which no attempt was made to retrieve wavelength misregistration between direct-sun and backscattered spectrum using the high-resolution solar reference spectrum, the undersampling error was found to be comparable to and sometimes exceed the ESD for the nominal slit width, but to be substantially reduced when the slit width was increased from 2 to 3 px. The corresponding increase in ESD from defocusing from 2 to 3 px was found to be very modest. So, for ozone profile retrieval with the RAL algorithm, the net *direct* impact of such an increase in slit width would be positive. It can be anticipated that such an increase would also facilitate alternative algorithms, which do not attempt to retrieve wavelength misregistration parameters using a high-resolution solar reference spectrum. However, consideration of the *indirect* impact of an increase in slit width (see below) complicates this picture.

(b) Slit-function shape

In the ozone profile retrieval scheme, the slit-function shape is assumed to be Gaussian. However, analysis by Officine Galileo of the GOME-2 EQM had indicated: (i) the true shape to be non-Gaussian and asymmetric and (ii) to be broader and more strongly wavelength-dependent (though more Gaussian) in the *defocused* case than in the *focused case*.



Errors from assuming the slit-function shape to be Gaussian were simulated explicitly and found frequently to exceed not only the baseline RSS but also the ESD, making this the dominant error simulated for ozone profile retrieval (exceeding 100% in the troposphere). Although such errors in retrieved ozone will not be random and have a characteristic height-dependence, they will adversely affect *precision* as well as *bias*.

It was found that, if the true shape of the slit function is that appropriate to defocusing (by a factor of ~1.3 to ~1.5, depending on wavelength, as in the Officine Galileo analysis), then sensitivity to the error of assuming a Gaussian shape in the retrieval scheme increases dramatically, despite the fact that the true shape then more closely resembles a Gaussian⁸.

Because undersampling errors are controlled quite well by explicitly retrieving misregistration parameters, errors in knowledge of slit-function shape are of paramount importance for the RAL ozone profile algorithm. It is also very likely that errors in knowledge of shape would be crucial for alternative algorithms. To meet user requirements on the accuracy of ozone profile retrievals from GOME-2, it is clear from this study that great attention will have to be paid to characterising slit-function shape in the relevant wavelength interval of Band 2 (<340 nm). It is also clear that the only opportunity to measure the slit-function shape adequately will be during pre-flight characterisation of the FM. Moreover, the increase in sensitivity to shape errors from increasing the width of the slit-function is a strong argument against defocusing (or physically opening the slit) unless pre-flight characterisation of slit-function shape will be undertaken.

4.3.3 Trace Gas Columns

For trace gas columns, simulations were performed of an increase in slit-function FWHM due to defocusing from 2px to 5 px (0.24-0.6 nm Band 2 and 0.5-1.25 nm Band 3). The ESDs for O₃ (<1%) and BrO (<60%) were found to increase by only a factor ~1.1, whereas that for NO₂ (<20% at 2 px) was found to increase by a factor ~1.24 by 3 px. Undersampling errors were found to be small for O₃ (<0.5%) and NO₂ (<2%), but substantial for BrO (\leq 100%). The variation of undersampling error with FHWM was found to be complicated and to differ greatly from one trace gas to another, i.e. it did not simply decrease monotonically with increasing FWHM.

At the initiative of the study team, an initial assessment was also made of *slit opening*. This potentially offers an alternative means to reduce undersampling errors, and the increased photon flux could also permit: (a) reduction in integration time, hence ground pixel size, or (b) increased S/N (by 30% for NO₂ from doubling the slit width). Small ground pixel sizes are particularly beneficial to tropospheric column retrieval due to the enhanced probability of cloud-free scene occurrences It is, however, recognised that the fixed GOME-2 data rate and detector saturation would provide practical constraints on (a) and (b), respectively, and that the other consequences and implications of slit opening also need to be evaluated.

4.4 Pseudo-Spherical Approximation and Earth's Curvature

4.4.1 General

Radiative transfer models (RTMs) in current usage for GOME-1 data processing employ the pseudo-spherical approximation and also neglect the curvature of Earth's surface. More sophisticated models are now becoming available which dispense with the pseudo-spherical approximation and account for Earth's curvature. However, because the CPU power required for a fully-spherical calculation would be prohibitive for GOME-2 data processing on contemporary computers and might still be too expensive in 2006, when GOME-2 will first deliver data, the accuracy of these approximations was examined.

Calculations by the fully-spherical model, CDIPI, demonstrated the less-rigorous model, CDI, to be sufficiently accurate for the viewing geometry of GOME-2. By differencing calculations by the CDI model,

 $^{^{8}}$ This is because, although its amplitude is smaller, the spectral signature of the error in the defocused case is actually closer in structure to the O₃ Huggins bands than that in the focussed case.



with and without the pseudo-spherical approximation, the spectral signature of this approximation was derived for all geo-temporal scenarios and these were then linearly mapped.

4.4.2 Ozone Profiles

For the 960km swath-width (i.e. view angles $\pm 29^{\circ}$), errors from the pseudo-spherical approximation (as implemented in CDI) were found always to be <10%, and therefore only rarely to exceed the RSS, and never to exceed the ESD. For the 1920km swath-width western extreme (+46°) pixel, however, errors were found always to exceed the RSS and to exceed the ESD for the three geo-temporal scenarios in which solar zenith angle was largest (Jan 55°N, Oct 75°N and Oct 75°S). It would therefore be necessary to avoid the pseudo-spherical approximation if the accuracy of ozone profile retrieval is not to be compromised at high solar zenith angles near the western edge of the 1920 km swath.

4.4.3 Trace Gas Columns

Errors on O_3 , NO_2 and BrO slant-columns were found to be negligible (<1%), provided that solar geometry for the ground rather than the top-of-atmosphere was used by the pseudo-spherical calculation.

4.5 Non-Lambertian Surface BRDF

4.5.1 General

Another approximation of radiative transfer models in contemporary use for GOME-1 is to neglect the angular dependence of surface BRDF, i.e. to assume that surfaces are all Lambertian. The error due to this approximation was quantified in the study for comparison to those arising from other sources. The CDI model was used to calculate spectra as a function of view-angle for a variety of surface-types (dark land, bright land, ocean and snow (April 55°N) and sunglint (April 5°N), employing angle-dependent BRDFs and their Lambertian equivalents.

4.5.2 Ozone profiles

For ozone profiles, a quasi non-linear simulation was employed in which gross deviations between the angledependent and Lambertian equivalent BRDFs were accommodated through retrieval of a (Lambertian) surface albedo. Errors from the Lambertian assumption were found to be <5%, except for sunglint where they were sometimes as high as 30%.

The extent to which sunglint will affect a given GOME-2 spectrum will depend upon the fraction of cloud obscuring the ocean, which is quasi-random, but in the absence of cloud the impact of sunglint is predictable. Such errors are therefore more usefully compared with the RSS than with the ESD. Errors of >10% (comparable to the RSS) were found for sunglint in the troposphere at tropical and mid-latitudes. For GOME-2 on METOP, sunglint will occur in eastward views, peaking near the 960 km swath edge. It will affect a substantial fraction of data in tropics south of the equator. The peak intensity and affected geographical area were shown to depend on surface wind-speed.

Because its occurrence is predictable, it would be feasible to adapt the ozone profile retrieval algorithm to utilise an angularly-dependent BRDF at sunglint locations, with surface wind-speed being either taken from met service analysis or retrieved from the GOME-2 measurements themselves. It can be anticipated that this should reduce errors on ozone profiles caused by sunglint to levels below the RSS.

4.5.3 Trace gas columns

Errors on O_3 , NO_2 and BrO slant-columns were found to be <1%, except for sunglint, where they were up to 3% for all gases. It was noted that these errors would arise via airmass factors, and could be reduced via retrieval of (Lambertian equivalent) surface albedo directly from the spectra.





4.6 Cloud Obscuration and Horizontal RI Gradients at Edge of Swath

4.6.1 General

The extent to which cloud obscuration and/or horizontal gradients in refractive index at the swath edge were likely to be more for important for a 1920 km swath than for a 960 km swath was another issue addressed by the study.

4.6.2 Cloud obscuration

The ATSR-2 forward view (~46° from nadir) is a good surrogate for the GOME-2 extreme across-track views in the 1920 km swath (\pm 46° from nadir). The statistics of cloud occurrence for a ground pixel size of 80 km x 40 km (appropriate to the 1920 km GOME-2 swath) were analysed for the forward and nadir-views of ATSR-2 for one year. Forward/nadir differences were found not to be significant, even for the occurrence of totally cloud-free scenes: 12% vs. 14%. Ground pixel *size* is a separate issue though.

4.6.3 Horizontal gradient in RI

Line-of-sight path-lengths were calculated with a ray-tracing model for a non-refracting atmosphere and for a refracting atmosphere with and without a horizontal temperature gradient of 0.14K/km (at all altitudes from 0-40 km). Differences were found to be negligible, even for the extreme view angles of the 1920 km swath.

4.7 Pointing and Geolocation

4.7.1 General

Errors were specified according to the EPS Geolocation and Co-registration Budget

- Nadir: 1.6 km along-track, 1.2 km across-track
- > 1920 km swath edge: 3.1 km along-track, 3.6 km across-track

Spectra were calculated with and without these errors and the resulting spectral signatures were linearly mapped.

4.7.2 Ozone profiles

Across-track errors were found to be generally <2% (even at 1920 km swath edge) and along-track errors were found to be <<1%. The direct impact of pointing errors at the levels specified is therefore negligible by comparison to other sources of error⁹.

4.7.3 Trace gas columns

Errors were found to be always <1% and generally <0.5%

⁹ The direct impact is the error in view-angle adopted in radiative transfer modelling. Indirect impacts associated with errors in geolocation (data bases on coastline, land surface type and topography) and co-location with AVHRR images (cloud fields) could also result, but were outside the scope of this study.





4.8 Error Budget Summaries

4.8.1 Ozone Profiles

The significance of individual errors in relation to the baseline ESDs and RSS errors was described in preceding sections and illustrated in an extensive series of plots in an annex to the Final Report. The four most salient points to be recalled here are that:

- Error from assuming an incorrect (Gaussian) slit-function shape is pervasive, and dominates over other the RSS and ESD.
- > Error from the pseudo-spherical approximation in extreme westerly views of the 1920km swath exceeds the ESD at large solar zenith angles and always exceeds the RSS.
- > Error from sunglint exceeds the RSS in easterly views at tropical and mid-latitudes.
- > Error from static scene inhomogeneity is often significant in comparison to the RSS.

4.8.2 Trace gas columns

Table 2 summarizes the various error sources discussed in this study. Error estimates in most cases are precision estimates for 1σ . Errors cited for undersampling (interpolation) and RTM assumptions are systematic errors and introduce biases in the retrieval results. Numbers given in that table present average numbers from all scenarios and may be higher for specific atmospheric conditions. Maximum errors are indicated by the "< smaller" sign. In light yellow those errors are indicated which are on the same order of magnitude as the basic ESD, while orange marks errors which exceed the ESD. It is difficult to assess the combined effect of all errors. In cases of precision estimates, one can assume that the overall errors are obtained by the square root of summed squares. Before detailing the individual error sources and trace gases two general remarks can be made here:

- The various errors for UV total ozone are generally quite small, but they are in many cases significant because of the small baseline error due to SNR.
- For all trace gases other than ozone, by far the most dominant error comes from the differential spectral structure caused by the diffuser plate.

Table 2: Trace gas column error budgets for GOME-2

COMEL HALL GAL	s column error budget	03	O3 VIS	NO2	BrO	OCIO O3 hole, alb=0.8
Basic SNR (IT=0.1875	s)	<0.5% (~0.3%)	<5% (~3%)	<30% (~15%)	<60% (~30%)	>100% (~100%)
polarisation error diffuser plate		<0.4% ~0.3%	? (larger than UV)	50%	70%	2
diffusion plato		0.070	· (larger than ev)	0070		
Spatial aliassing WP210		0.2%		<2%	<1%	<15%
Spectral Resolution	Defocusing (1/2)*	0.3%	3%	18%	35%	
WP 230	Open slit (1/2)*	0.2%	2%	11%	25%	
	usampl./defoc(2.2px. FWHM)*	0.2%±0.3%	19691357	2%±15%	80%±30%	
*basic SNR included						
RTM assumption	PS vs Spherical w/ refraction	<1%	<1%	<1%	<1%	1
WP250	Spherical w/o refraction	<0.3%	<0.2%	<0.5%	<1%	
00220-000-0020	Spherical vs. PS GRD	<1%	124.03106.0310.04	<1%	<1%	
	Spherical vs PS TOA	<4%		<6%	<5%	
BRDF	1	< 0.3%	<3%	<2%	<3%	1
WP260						
Pointing accuracy	1	<0.5%	r r	<1%	<0.5%	1
WP270				2018/19/22		

GOME2 trace gas column error budget



The impact of the diffuser plate spectral characteristics on the NO_2 and BrO column retrieval was taken directly from the technical note for GOME-1 by Richter and Wagner, given in Appendix D of the Final Report.

For a fixed wavelength shift between measurements of backscattered and direct-sun spectra (ie for a fixed Doppler shift), undersampling gives rise to a systematic error. Combining the basic ESD and undersampling error is not possible, thus the bias can only be added to the ESD (ie bias $\pm 1\sigma$ shown in Table 2). Here the undersampling error is given as an error resulting from correcting a 0.008 nm shift (characteristic Doppler shift for GOME-1) by back interpolation. For the particular case of a 0.008nm shift, the undersampling error was found to vary in a highly non-linear way (even in terms of sign) with slit-function FWHM and in a different way for different trace gases. Although a suitable undersampling correction may suffice for most trace gases, systematic errors due to undersampling were observed to be important for BrO. In the following, each trace gas is discussed individually.

4.8.3 Total ozone

In the UV (Band 2), ozone absorption is strong and this results in a very small baseline ESD for the nominal integration time of 0.1875s. Spatial aliasing¹⁰ and geolocation/ pointing errors have negligible impact on total ozone. All other error sources are non-negligible, though still fairly small¹¹.

Interference from other trace gases, notably water vapour, and the angular dependence of sunglint BRDF have more severe impacts on the VIS retrieval¹². Slant column errors in the visible are higher than in the UV, however, the advantage lies in the negligible wavelength dependence of the AMF in this spectral region. The influence of the diffuser plate on the retrieved total ozone column is still unknown, but may be on the order of few tenths of a percent (higher in the visible) and may be non-negligible.

4.8.4 Nitrogen dioxide

In case of nitrogen dioxide, the error is clearly dominated by diffuser plate signatures (50%) and photon noise (30%). ESDs can be improved by co-adding. This leads, however, to larger ground pixel areas, which is unfavourable for tropospheric retrieval. The latter is hampered by reduction of the clear-sky occurrences with larger pixel areas. Opening the slit leads to a net reduction in ESD. (The increase in photon flux outweighs the information loss from reduced spectral resolution). Defocusing, by contrast, leads to an increased ESD. (There is no increase in photon flux to compensate the decreased spectral resolution.) For some scenarios, saturation of detectors would occur if the slit was opened. This could be overcome by halving the integration time to 93.75 ms and: (1) co-adding to 0.1875 sec; (2) reading-out every second 93.75ms ground pixel or (3) reading-out every pixel and doubling the data rate. In the second and third cases, ground pixel size would be decreased to 40X40km2 (1920 km swath width) benefiting tropospheric retrieval. The second option leads to gaps in the ground coverage in the across-track scan but keeps the data rate unchanged in comparison to the 0.1875 sec ground pixel observations, as does the first option. It is appreciated by the study team that the increase in GOME-2 data rate associated with the third option would be difficult to accommodate in practice. All other error sources are insignificant against the baseline and diffuser plate error.

4.8.5 Bromine oxide

Similar conclusions to NO₂ can be drawn for bromine oxide retrieval. Largest error sources are diffuser plate spectral interference (70%) and photon noise (<70%). A systematic bias of up to 80% is also estimated due to interpolation error at 2.2 pixels FWHM spectral resolution in combination with defocusing option. One has to keep in mind that BrO is photochemically active, and is near the detection limit at low solar zenith angles

¹⁰ Spatial aliasing was investigated with a few representative Landsat images. Further investigations may be needed to confirm this result.

¹¹ One should note that violation of the weak absorber approximation is not accounted for in this error budget. It may be more appropriate to use either modified or weighting function DOAS in the UV window. Operational GOME-1 retrieval is still based on the standard DOAS approach. The standard two-step DOAS retrieval is more appropriate in the visible (450-497 nm) where absorption is weak.

¹² Because of dichroic features in Channel 3 of GOME-1, the visible window has been only occasionally used for ozone retrieval.



(tropics). Opening the slit could, in principle, improve ESDs significantly for BrO, as for NO₂. However, the reduction in sensitivity to undersampling from this or defocusing appears very sensitive to the precise choice of FWHM, fitting window and jointly retrieved parameters.

4.8.6 Chlorine dioxide

Chlorine dioxide is a photochemically active species and can only be retrieved under twilight condition and under ozone hole condition. The error is dominated by photon noise (~100%). Some co-adding may be required to improve retrieval, however, one should keep in mind that OCIO column amounts have a strong solar zenith angle dependence.

5 Recommendations and Further Work

5.1 Background to the Recommendations

The recommendations made below are based principally, though not exclusively, on quantitative error estimates from GOME-2 retrieval simulations performed in this study. The schemes employed in simulations for ozone profiles and trace gas columns are based very closely on those applied to real GOME-1 measurements by RAL and IUP, respectively. Both these schemes are the result of nearly a decade of development work, so are now mature and have been demonstrated to be among the most reliable of their kind. Although the magnitudes of simulated errors are specific to the detailed formulations of these two particular algorithms, the recommendations made below are expected to prove quite robust and to be applicable also to other schemes, which might be adopted for operational processing of GOME-2 data.

Most simulations in this study have been performed for a set of realistic and representative, geo-temporal scenarios (24 in total), which span a diverse range of observing conditions. The recommendations below are therefore expected to be applicable to GOME-2 observing conditions generally (though not universally).

Although an extensive set of instrumental and geophysical parameters and error sources have been addressed, it should be noted that errors in the high-resolution solar reference spectrum, trace gas absorption cross-sections and atmospheric scattering parameters have not been considered. These are considered likely to contribute significant additional non-random errors.

Recommendations labelled "A" concern instrument operational settings, ground processor settings and instrument pre-flight characterisation. Those labelled "B" concern the instrument itself. Those labelled "C" concern further studies to define instrument settings and mitigate errors.

5.2 Band 1 sampling

5.2.1 Long-wave limit

The sensitivity of ozone profile retrieval to the longwave limit adopted in Band 1B was assessed, in terms of ESD and the other components of the baseline error budget. Although it would be worthwhile in terms of ESD to extend to 314 nm, this would not be desirable in terms of the magnitudes of other simulated errors and their RSS. More decisively though, the sensitivity to static and dynamic (spatial aliasing) scene inhomogeneity is substantially greater, when it is extended to 314 nm.

Recommendation A1

For ozone profile retrieval, the recommended longwave limit in Band 1B is 307 nm.



EXECUTIVE SUMMARY

5.2.2 Spatial/temporal

For simulations with the RAL algorithm in which a "noise floor" of 1%¹³ is imposed on sun-normalised Band 1 radiances, the additional read-out noise associated with reading-out Band 1A spectra at 1.5s intervals and reading out Band 1B spectra at the nominal 0.1875s instead of the nominal for B1A of 12s has a negligible impact on ESDs. Reading-out Band 1A at a higher frequency reduces the range of (across-track) viewing angles in a given ground-pixel. This would be very desirable in order to alleviate forward modelling errors associated with the strongly non-linear view-angle dependencies of (a) atmospheric radiative transfer and (b) GOME-2 instrumental properties (n.b. wavelength-dependent polarisation properties of the scan-mirror). Co-adding 1.5s Band 1A spectra along-track could then yield comparable radiometric precision to a single 12s integration but more easily modelled spectra.

Reading-out Band 1B at the same frequency as Band 2 allows correspondence between their views of the troposphere (n.b. cloud). Retrievals from individual Band 1B ground pixels should therefore provide more consistent a priori estimates in the troposphere for the corresponding Band 2 pixels.

Recommendation A2

For ozone profile retrieval, it is recommended that the integration times for Band 1A and Band 1B be 1.5s and 0.1875s, respectively.

5.3 Diffuser

The impact of spectral structures in the BRDF of the diffuser plate on trace gas column retrieval was reviewed. For GOME-1, such spectral structures had been found to limit the accuracy (and in some cases detectability) of trace gases other than ozone. For GOME-2, it was confirmed that a diffuser plate with much improved spectral characteristics would be needed to measure trace gases other than ozone.

Recommendation B1

For retrieval of trace gases other than ozone, it is strongly recommended to switch to a diffuser plate with peak-to-peak spectral signatures of less than 10^{-4} .

5.4 Pre-flight characterisation of slit-function shape

It has been demonstrated unequivocally in simulations for GOME-2 in this study that characterisation of the slit-function shape in the relevant wavelength interval of Band 2 is of critical importance to ozone profile retrieval. Use of the onboard line-lamp alone to characterise slit-function shape will not suffice because:

a. Absence of suitable lamp lines in the wavelength interval between 307 and 333nm

¹³ The noise floor of 1% is based on typical RMS fitting residuals in Band 1attained in processing of GOME-1 flight data. This noise floor comes into play at long wavelengths in Band 1 (typically 290 nm at Band 1B integration time) where the predictions from a noise model which combines only photon and read-out noise falls below this value. The noise floor therefore represents the combined effects of other noise sources, which are in practice significant at these wavelengths, e.g. errors in the high-resolution solar reference spectrum, slit-function shape and modelling of the Ring effect.



b. Lamp-lines at fixed, discrete wavelengths outside this interval do not permit the slit-function shape to be adequately resolved.

Retrieval of absolute wavelength registration and slit-function width from direct-sun spectra is part of the standard RAL scheme for processing GOME-1 data. However, retrieval of additional parameters to characterise slit-function shape would be a difficult to formulate and ill-posed problem.

Pre-flight measurements of slit-function shape at sub-pixel resolution in the relevant wavelength interval of Band 2 will therefore be necessary 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.

Recommendation A3

For ozone profile retrieval, it is strongly recommended that the slit-function shape in Band 2 below 340nm be accurately determined before flight at sub-pixel resolution.

Recommendation C1

Specify requirements for laboratory measurements of slit-function shape and quantify the benefits for the Band 2 step of O_3 profile retrieval.

The impact on trace gas columns of error in knowledge of slit-function shape was not addressed within this study. However, total column processing options to (a) use absorption cross-sections measured at higher resolution than GOME-2 and (b) correct for wavelength misregistration between direct-sun and backscattered spectra using a high-resolution solar reference spectrum would depend on this¹⁴.

Recommendation C2

Quantify errors in knowledge of slit-function shape for: (a) the Band 1 step of O_3 profile retrieval; (b) trace gas column retrieval and (c) aerosol and cloud retrieval using O_2 A-band.

5.5 Slit-function width

5.5.1 Defocusing

For ozone profile retrieval, simulations in which the slit width was increased while overall photon flux on the detector arrays was held fixed showed that defocusing from 2-3px (0.24 –0.36nm) in Band 2 would not significantly degrade ESDs but would substantially reduce sensitivity to undersampling errors. This could potentially allow a much simpler correction scheme to be applied for wavelength misregistration between backscattered and direct-sun spectra¹⁵, which in turn could substantially improve computational efficiency. Defocusing could therefore offer a potential net gain for ozone profile retrieval.

For trace gas column retrieval, the variation of ESD with FWHM was found to be trace gas specific and the variation of undersampling error with FWHM was found to be highly non-linear and trace gas specific. It was

¹⁴ The alternatives are to use absorption cross-sections measured by the GOME-2 FM itself and to reduce undersampling errors to an insignificant level.

¹⁵ This misregistration is the source of the so-called undersampling error.



therefore not possible on the basis of results from this study to reach a clear-cut conclusion in regard to defocusing.

5.5.2 Slit opening

For trace gas column retrieval, the changes to ESD associated with slit opening have been quantified and compared to those of defocusing and are again trace gas specific. For NO₂, a significant reduction (from 15% to 11%) in basic ESD could be obtained by opening the slit from 0.5nm to 1 nm in Band 3, via the increased photon flux. It is noted that the photon flux in Band 3 could also be increased, in principle, by opening the aperture stop in Band 3/4. Although it is recognised that detector saturation would provide practical constraints and that the other consequences and implications of opening the slit or aperture stop would need to be evaluated.

For ozone profile retrieval, the effects on the ESDs of opening the slit can be qualitatively inferred from those of defocusing to the same slit-function width: ESDs would either increase less than for defocusing or would actually decrease. Sensitivity to undersampling errors would not decrease as much for slit opening as for defocusing to the same slit-function width though, because the opened slit would retain its focused, non-Gaussian shape. Since no ozone profile retrieval simulations were conducted to quantify slit opening¹⁶, it is not possible to conclude what the net gain would be by comparison to defocusing.

Recommendation B2:

For retrieval of trace gas columns other than ozone, it is recommended to open the slit in preference to the defocusing option.

Recommendation C3:

More studies are needed to investigate the impacts of: (a) defocusing, (b) opening the slit and (c) opening the Band 3/4 aperture stop, in particular with respect to hardware implications.

5.6 Detector read-out time

To eliminate susceptibility of ozone profile retrieval to extreme errors from spatial aliasing, it would be desirable to reduce detector read-out time in Band 1B. (*However, the proportion of extreme cases is considered too small to warrant a fully-fledged recommendation*).

Recommendation A4:

It is recommended that the impacts of spatial aliasing be quantified thoroughly:

- (a) Impact on ozone profiles and trace-gas columns via use of PMD measurements to correct polarisation response of detector arrays
- *(b) Global statistical analysis of ozone profiles and trace gas columns using ATSR-2 images*
- (c) Assess impact on geophysical products retrieved from PMD measurements
- (d) Assess impact on multi-wavelength aerosol retrieval

¹⁶ Opening the slit would also impact on PMD measurements, and hence indirectly on ozone profile retrieval via the polarisation correction. However, the impact on PMDs was not assessed either.



along with possible use of PMD measurements at higher spatial resolution to mitigate these impacts.

5.7 Selection of swath width and ground-pixel size

A number of the issues addressed in this study have a bearing on selection of swath-width and/or groundpixel size for GOME-2. Several factors identified from GOME-1 data analysis, though not addressed explicitly in the study, also need to be considered.

- (a) Non-linear Dependencies of Radiative Transfer and GOME-2 Polarisation Response on View-Angle
 - To increase the computational efficiency of the Band 1A retrieval step and to reduce errors associated with non-linear view-angle dependencies, especially in the outer pixels, it would be desirable to limit the pixel size across-track by limiting swath width, as well as the Band 1A integration time.
- (b) Horizontal gradients in RI
 - Temperature-induced horizontal gradients in RI do not affect decisions on swath-width or ground pixel size.
- (c) Pseudo-spherical approximation
 - Selection of the 1920 km swath width would increase the complexity of either the GOME-2 operational timeline or the radiative transfer model used in Level-2 processing for the outer pixels.
- (d) Sunglint occurrence
 - The need to account for sunglint does not significantly influence the decision between 960 km and 1920 km swath widths.
- (e) Dependence of cloud obscuration on view-angle
 - The dependence of cloud obscuration on view-angle is not a significant factor for the choice between 960 km (±29°) and 1920km (±46°) swaths.
- (f) Dependence of cloud-free pixel occurrence on pixel size

In work undertaken outside the scope of this study using ATSR-2 data, the frequency of occurrence of ground pixels containing a given fraction of cloud was determined as a function of ground pixel size. The occurrence of cloud-free pixels was found to be a strong function of ground pixel size:

- ~7% for 80 km x 40 km (nominal for GOME-2 1920 km swath)
- ~10% for 40 km x 40 km. (nominal for GOME-2 960 km swath)
- ~23% for 12 km circular (IASI)
- The rationale for GOME-2 to employ a small ground pixel size is strong, in order to maximize the fraction of cloud-free scenes and facilitate sounding of tropospheric composition.



- (g) Dependence of scene-inhomogeneity on pixel size
 - The rationale for GOME-2 to employ a small ground pixel size is further strengthened by the reduction in ozone profile retrieval errors caused by scene inhomogeneities which this would allow, especially in the troposphere
- (h) Conclusions on swath width and ground pixel size

It can be concluded from the above considerations that:

- 1) The accuracy of individual ozone profile retrievals and
- 2) The fraction and total number of observations of the cloud-free lower troposphere

would both benefit substantially from adopting for GOME-2:

- 1) A ground pixel size smaller than 40 km x 40 km
- 2) A swath-width narrower than 960 km

However, two additional factors, which affect these decisions, are:

- 1) Spatio-temporal sampling of the (4-D) fields of ozone and other trace gases
- 2) Potential use of sub-pixel information on cloud/surface properties from AVHRR3

Although ground-pixel size is intimately linked to swath width for an across-track scanner such as GOME-2, the detector integration time is programmable. So the possibility exists to employ an integration time <0.1875s (i.e. 0.09375s) in Bands 1B, 2, 3 and 4. Even if the overall data-rate (and hence number of across-track pixels) could not be increased from its nominal value, it would therefore still be feasible to combine a pixel of across-track dimension <40 km with a 960 km swath or one of <80 km with a 1920 km swath. If integration time was reduced from 0.1875s to 0.09375s, it would be desirable to also reduce read-out time by a corresponding factor of two, to avoid increasing susceptibility to spatial aliasing.

To decide on the ground-pixel size and swath width to be used operationally, an objective comparison of different options must therefore be made in terms of the fidelity with which structure in the 4-D fields of ozone and other trace gases would be determined. Such an objective comparison could best be performed in the frame of a data assimilation model through an observation system simulation experiment (OSSE) in which the observational errors¹⁷ and the sampling of the lower troposphere took into account cloud and other factors in a realistic way.

Recommendation A5

It is recommended that an OSSE be undertaken for GOME-2 to decide on optimum ground-pixel size and swath width.

¹⁷ Observational errors would need to take into consideration static and *dynamic* (i.e. spatial aliasing) errors from scene inhomogeneity, as well as photon noise and read-out noise.



EXECUTIVE SUMMARY

5.8 Summary of Recommendations

A number of specific recommendations were identified in the previous sections. These are summarised in the tables below. Table 3A concerns instrument operational settings, ground processor settings and instrument pre-flight characterisation.

Table 3A: Recommendations for instrument operational settings, ground processor settings and instrument pre-flight characterisation

A1	For O ₃ profile retrieval, it is recommended to not use Band 1B wavelengths above 307nm.		
A2	For O_3 profile retrieval, it is recommended that the integration times for Bands 1A and 1B be 1.5s and 0.1875s, respectively.		
A3	For O ₃ profile retrieval, it is strongly recommended that the slit-function shape in Band 2 below 340nm be accurately determined before flight at sub-pixel resolution.		
A4	It is recommended that the impact of spatial aliasing be assessed more thoroughly: a. Impact on O ₃ profiles and trace gas columns via use of PMD measurements to correct polarisation response of detector arrays b. Global statistical analysis of O ₃ profiles and trace gas columns using ATSR-2 images c. Impact on geophysical products retrieved from PMD measurements d. Impact on multi-wavelength aerosol retrieval along with possible use of PMD measurements at higher spatial resolution to mitigate these impacts		
A5	It is recommended that an OSSE be undertaken for GOME-2 to decide optimum ground- pixel size and swath width		

Two recommendations identified in previous sections, flowing from the trace gas column analyses performed by University of Bremen in this and other studies, concern the specification of the instrument itself. Eumetsat is therefore invited, in addition, to evaluate possibilities to implement modifications to the GOME-2 instrument in order to mitigate errors, which would otherwise limit the quality of trace gas column retrievals (Table 3B).

Table 3B: Recommendations from trace gas column analysis for error mitigation through instrument modifications

B1	For retrieval of trace gas columns other than ozone, it is strongly recommended to switch to a diffuser plate with peak-to-peak spectral signatures of less than 10^{-4} .	
B2	For retrieval of trace gas columns other than ozone, it is recommended to open the slit in preference to the defocusing option.	

The following further studies are recommended to define GOME-2 instrument settings and to mitigate errors (Table 3C).



Table 3C: Recommendations for further studies to define instrument settings and to mitigate errors

C1	Specify requirements for laboratory measurements of slit-function shape and quantify the benefits for the Band 2 step of O_3 profile retrieval.
C2	Quantify errors in knowledge of slit-function shape for: (a) the Band 1 step of O_3 profile retrieval; (b) trace gas column retrieval and (c) aerosol and cloud retrieval using O_2 A-band.
C3	More studies are needed to investigate the impacts of: (a) defocusing, (b) opening the slit and (c) opening the Band 3/4 aperture stop, in particular with respect to hardware implications.
C4	Investigate and quantify the benefits of algorithm improvements for ozone profile retrieval to mitigate errors from wavelength-dependent degradation in the uv.
C5	Assess possible use of onboard white light source to monitor wavelength-dependent degradation in the UV
C6	Implement and quantify the benefits to ozone profile and trace gas column retrievals of algorithm improvements to mitigate errors due to sunglint.
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
С9	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

To achieve the stringent accuracy in GOME-2 Level-2 processing required for long-term monitoring of ozone, as part of EUMETSAT's remit for climate monitoring, retrieval schemes will need to be more sophisticated than those in contemporary use. Potential advances include the addition of polarization measurements, for ozone profile retrieval, and better (height-resolved) climatologies of trace gases and temperature for AMF data-bases, improved handling of the Ring effect and novel alternatives to the standard DOAS scheme, for trace gas column retrieval. In addition to their relevance to GOME-2 on METOP, studies to improve retrieval schemes could also be relevant to future re-processing of GOME-1 data, and therefore to production of a homogeneous data-set from GOME-1 and GOME-2¹⁸. Further analysis of the degradation to GOME-1 (UV) measurements (principally manifest through changes to scan-mirror reflectivity, and possibly also through changes to diffuser BRDF) will be necessary for this purpose, particularly to utilise height-resolved O₃ data.

High spatial sampling and high accuracy were both confirmed in this study to be important to tropospheric sounding. It would therefore be worthwhile now for ESA to look beyond GOME-2 and identify the *spatial sampling* and *accuracy* requirements of a future mission and begin to evaluate technology developments¹⁹, which might be needed to meet these.

¹⁸ Other UV nadir sounders of a similar class, e.g. SCIAMACHY on Envisat and OMI on Eos Aura, are also expected to contribute to this long-term data set.

¹⁹ For example, to compare the relative merits of (2-D) CCD detectors and conventional diode array detectors.