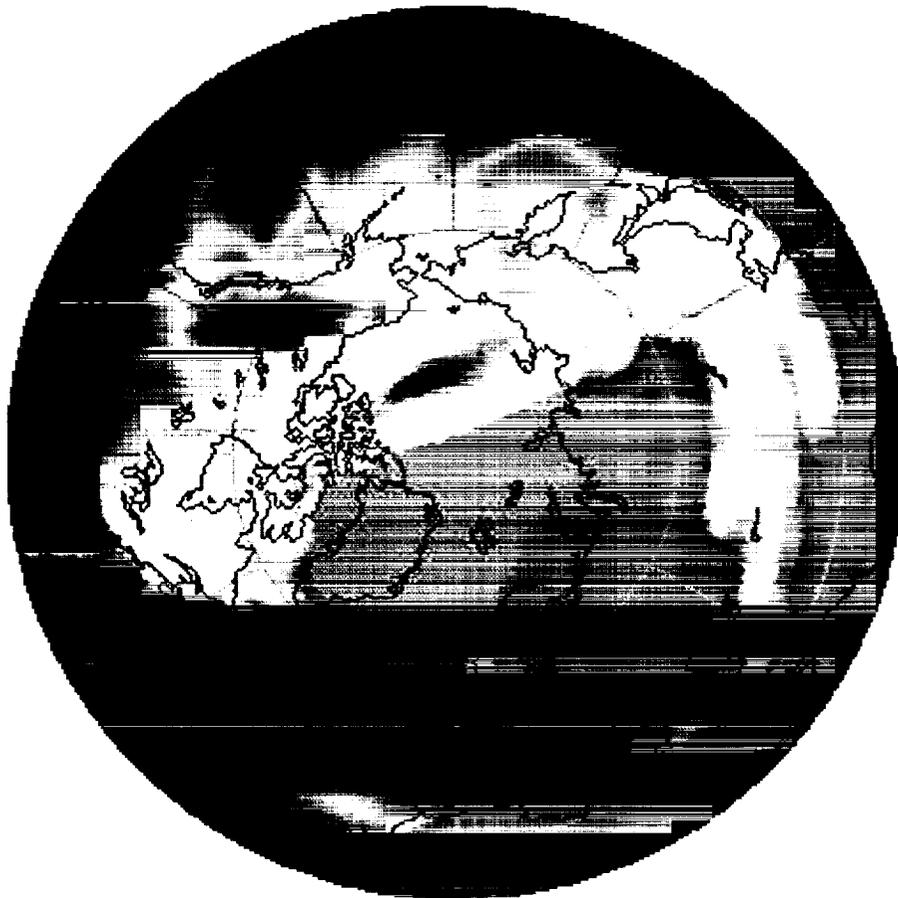
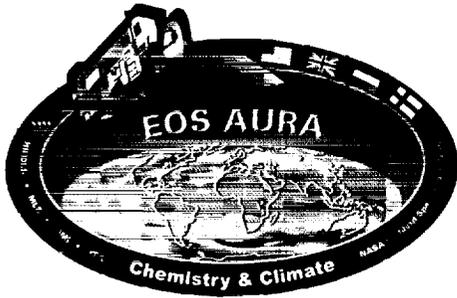


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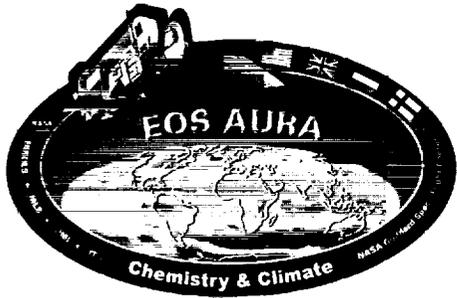
Science Requirements Document for OMI-EOS



RS-OMIE-KNMI-001
VERSION 2

7 December 2000

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This report has been prepared from contributions by members of the International OMI Science Team and experts in relevant fields:

Contributors

R. van der A	KNMI	The Netherlands
P.K. Bhartia	GSFC	United States
F. Boersma	KNMI	The Netherlands
E. Brinksma	KNMI	The Netherlands
J. Carpay	NIVR	The Netherlands
K. Chance	SAO	United States
J. de Haan	KNMI	The Netherlands
E. Hilsenrath (co-PI)	GSFC	United States
I. Isaksen	UiO	Norway
H. Kelder	KNMI	The Netherlands
G.W. Leppelmeier (co-PI)	FMI	Finland
P.F. Levelt (PI)	KNMI	The Netherlands
A. Mälkki	FMI	Finland
R.D. McPeters	GSFC	United States
R. Noordhoek (scientific secretary)	KNMI	The Netherlands
G.H.J. van den Oord (deputy PI)	KNMI	The Netherlands
R. van Oss	KNMI	The Netherlands
A. PETERS	KNMI	The Netherlands
R. Snel	SRON	The Netherlands
P. Stammes	KNMI	The Netherlands
P. Valks	KNMI	The Netherlands
J.P. Veefkind	KNMI	The Netherlands
P. van Velthoven	KNMI	The Netherlands
R. Voors	KNMI	The Netherlands
M. van Weele	KNMI	The Netherlands

Checked and approved by P.F. Levelt,
Principal Investigator of the Ozone Monitoring Instrument (OMI)

De Bilt, 7 December 2000

Front cover: Ozone “mini hole” above Europe on 30 November 1999, retrieved in Near Real Time at KNMI from ESA-GOME data.
(Figure with courtesy from P. Valks, KNMI)

Executive summary

Introduction

A Dutch-Finnish scientific and industrial consortium is supplying the Ozone Monitoring Instrument (OMI) for EOS-Aura. EOS-Aura is the next NASA mission to study the Earth's atmosphere extensively, and successor to the highly successful UARS (Upper Atmospheric Research Satellite) mission. The "*Science Requirements Document for OMI-EOS*" presents an overview of the Aura and OMI mission objectives. It describes how OMI fits into the Aura mission and it reviews the synergy with the other instruments onboard Aura to fulfil the mission. This evolves in the Scientific Requirements for OMI (Chapter 3), stating which trace gases have to be measured with what necessary accuracy, in order for OMI to meet Aura's objectives.

The most important data product of OMI, the ozone vertical column, densities shall have a better accuracy and an improved global coverage than the predecessor instruments TOMS (Total Ozone Monitoring Spectrometer) and GOME (Global Ozone Monitoring Experiment), which is a.o. achieved by a better signal to noise ratio, improved calibration and a wide field-of-view. Moreover, in order to meet its role on Aura, OMI shall measure trace gases, such as NO₂, OCIO, BrO, HCHO and SO₂, aerosols, cloud top height and cloud coverage. Improved accuracy, better coverage, and finer ground grid than has been done in the past are goals for OMI.

After the scientific requirements are defined, three sets of subordinate requirements are derived. These are: the algorithm requirements, i.e. what do the algorithms need in order to meet the scientific requirements; the instrument and calibration requirements, i.e. what has to be measured and how accurately in order to provide the quality of data necessary for deriving the data products; and the validation requirements, i.e. a strategy of how the OMI program will assure that its data products are valid in the atmosphere, at least to the required accuracy.

EOS Aura and OMI Mission Objectives

As the member of the EOS series that is aimed at the atmosphere, Aura addresses three fundamental questions:

- 1) Is the Earth's ozone layer recovering?
- 2) Is air quality changing? and
- 3) How is the Earth's climate changing?

The four instruments on Aura are matched to measure the dominant parameters of the troposphere and the stratosphere (temperature, density, humidity, aerosols and ozone), along with cloud scattering pressure and cloud coverage, and the most relevant molecules involved in the catalytic destruction of ozone, e.g. BrO, OCIO. Finally, pollutants such as NO₂, HCHO and SO₂ are monitored. The emphasis is on global monitoring, in order to understand the processes affecting the global atmospheric composition and climate.

As the Ozone Monitoring Instrument on Aura, OMI's first task is to continue the monitoring of ozone column amounts in the atmosphere over the entire globe as has been carried out by TOMS. Secondly, it shall contribute to improve our understanding of the ozone distribution by supplying ozone vertical profiles. Moreover, it shall contribute to the understanding of ozone production and destruction by measuring relevant trace species (e.g. BrO, OCIO, NO₂) in the same air mass as the ozone. In combination with the EOS-Aura instruments MLS (Microwave Limb Sounder) and HIRDLS (High Resolution Dynamic Limb Sounder), OMI will provide, for the first time, daily maps of tropospheric ozone and NO₂ with global coverage and very high spatial resolution, thus providing direct monitoring of industrial pollution and biomass burning, which both play an important role in air quality control. Therefore, OMI shall measure total O₃ and total NO₂ and perform these measurements with daily global coverage and a grid size finer than previous missions. Finally, OMI shall contribute to climate monitoring by measuring ozone, cloud characteristics and aerosols.

Note that while many of these objectives are stated as related to monitoring, (e.g. "Is the Earth's protective ozone shield recovering?"), they are at the same time essential to understanding many aspects of global climate change.

In addition to fulfil these primary needs, OMI data can be used for special purposes. In particular, OMI measurements can be used directly as input for Numerical Weather Prediction (NWP) models and regional Very Fast Delivery (VFD) products. Here, the requirements on the accuracy of the measurements are much the same, but the timing and location of the measurements are more demanding. In the case of input to NWP, in order for the results to be useful they shall be global and delivered within 3 hours of measurement. In the case of VFD, the Direct Broadcast mode of Aura will be used to receive OMI data in real time while the satellite is passing over Europe.

Scientific Requirements

In order to fulfil the mission objectives of EOS-Aura, OMI shall measure with high accuracy, high spatial sampling, and a global coverage within a day. OMI shall also measure a minimal set of required data products. These products which have the highest priority (A-priority products) are: radiance and irradiance, O₃ column and profile, NO₂ column, aerosol optical thickness, aerosol single scattering albedo, surface UV-B flux, cloud scattering pressure and cloud fraction. In addition, OMI should also be able to retrieve the following desired products (B-priority products): OCIO, BrO, HCHO, SO₂, surface reflectance and UV spectra. The requirements on measurement accuracy and spatial resolution, in order for the OMI data products to meet the OMI objectives, are given in Chapter 3.

Algorithm Requirements

The algorithms needed for retrieving the OMI data products with the accuracy and spatial resolution described in Chapter 3, specify requirements on the Earth radiance and Solar irradiance spectra as measured by OMI and on the instrument design. In Chapter 4 the algorithms that are going to be used to retrieve the data products in Chapter 3 are described with the resulting high level requirements on the Earth radiance and Solar irradiance spectra. These algorithms are mainly based on GOME-type of retrieval or TOMS/SBUV type of retrieval, although some new algorithms are also discussed.

Instrument Requirements

Instrument requirements are derived from the scientific requirements and the algorithms for each product. Clearly, the instrument must cover the spectral range that a particular algorithm uses for retrieval of the trace gas distribution in question, i.e. the wavelength range for the molecule where absorption is largest and/or has the most pronounced spectral structure. The instrument's spectral resolution in the wavelength range of interest shall be able to resolve the structure in the absorption cross section. Given a requirement for a specific ground pixel size, the instrument shall have sufficient effective aperture to collect enough light during the time that specific pixel is in the field of view to meet the signal-to-noise requirement of the algorithm. The instrument's optical field of view shall be large enough to eliminate gaps between successive passes and obtain daily global coverage. Since the viewing and solar geometry varies widely both over an orbit and over the year, strict requirements on polarisation sensitivity are needed.

In addition there are derivative requirements. In order to meet the requirement for radiometric accuracy, there must be a reliable method for in-flight calibration, as no instrument is stable to 1% over the 5-year lifetime of the mission. Similarly, the algorithms for ozone retrieval (as well as other trace gases) have very stringent requirements for wavelength knowledge and stability.

Careful consideration of the scientific requirements and the algorithms leads to a very extensive specification of instrument requirements, which can be found in Chapter 5.

Validation Requirements

The objective of OMI validation is to establish the validity and accuracy of the OMI products. By comparing OMI results with independent, well-calibrated measurements, the quality of the science products can be assured.

The strategy of validation has two aspects: the methodology and the timing. Data for validation shall be preferably obtained from different sources, i.e. in situ measurements from balloons or aircraft, ground-based measurements and measurements from other satellite instruments, and by applying different measurement techniques.

The time schedule of validation can be split up in three phases:

The Commissioning Phase: after instrument calibration has taken place, validation measurements are required to make sure that the results retrieved from OMI measurements are believable, and more or less correct.

The Core Phase: normally lasting about a year, during which every single product is validated to the level of accuracy, precision, and coverage stated in the science requirements.

Long-term Phase: lasting throughout the mission, to assure that the retrieved products are still valid to the stated accuracies, independent of changes in the instrument and/or the spacecraft.

Rationale

This “*Science Requirements Document for OMI-EOS*” describes the scientific objectives of the OMI instrument on NASA’s EOS-Aura mission. From the coherent, detailed description of the objectives of the OMI instrument in the Aura mission, the specific tasks OMI shall carry out are described quantitatively and are summarised in the scientific requirements table in Chapter 3. Taking into account the requirements the algorithms put on the measurements taken by OMI (see Chapter 4), the instrument requirements can be derived and these are summarised in Chapter 5. Although requirements concerning calibration, validation, and groundprocessing issues can also be found, this document’s main focus is nonetheless on the scientific and instrument requirements for OMI-EOS.

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Chapter 1 Introduction

1.1 EOS-Aura Mission Objectives

The core of NASA's Earth Observing System (EOS) missions are Terra, Aqua and Aura. Terra (land processes and earth radiation) was launched in late 1999. Aqua (atmospheric hydrological cycle) and Aura (atmospheric chemistry) are scheduled for launch in late 2000 and mid-2003, respectively. Aura's specific mission objectives are to observe the atmosphere in order to answer the following three high priority environmental questions:

- 1) Is the Earth's ozone layer recovering?
- 2) Is air quality changing? and
- 3) How is the Earth's climate changing?

The mission will continue the observations made by NASA's Upper Atmospheric Research Satellite (UARS) which uncovered key processes that resulted in ozone depletion and the TOMS series of measurements which accurately tracked ozone change on a global scale over the last 22 years.

The Aura satellite is an international platform with significant contributions from the United Kingdom, the Netherlands and Finland.

1.2 EOS-Aura Mission Characteristics

The Aura spacecraft will circulate in a sun-synchronous polar orbit with a local afternoon equator crossing time at 13:45, providing global coverage in one day. The mission has a design lifetime of five years once in orbit. A polar orbit provides a perspective to collect high vertical resolution data of atmospheric constituents and temperature throughout the stratosphere on a daily basis. The Microwave Limb Sounder (MLS) and the High Resolution Dynamics Limb Sounder (HIRDLS) are limb sounding instruments. The Ozone Monitoring Instrument (OMI) is a nadir sounder, and the Tropospheric Emission Spectrometer (TES) has both limb sounding and nadir sounding modes and can also point to targets of opportunity such as pollution sources and volcanic eruptions. MLS is on the front of the spacecraft while HIRDLS, TES and OMI are mounted on the nadir side. These locations were chosen so that the instruments could observe in the orbit plane, and thus could sample the same air mass within minutes. When the high vertical and horizontal resolution measurements from Aura are combined they will provide unprecedented insights into the chemical and dynamical processes in the stratosphere and upper troposphere. The Aura instruments balance new capabilities with proven technological heritage, covering wavelengths in the ultraviolet, visible, throughout the infrared, and sub-millimeter and microwave ranges.

The mission is designed to synergistically collect data to answer the key questions of ozone depletion and recovery, the global change in air quality, and the changing climate. Key constituents (all important radical, reservoir, and source gases including first time ever global surveys of OH) in the ozone destroying catalytic NO_x , ClO_x and HO_x cycles will be measured using HIRDLS, MLS and OMI. Monitoring of global ozone trends, with TOMS precision, will be continued using OMI. Air quality on urban-to-continental scales will have unprecedented coverage because of the mapping capabilities of OMI and the target gases measured by TES. These two instruments will measure most of the precursors to tropospheric ozone. Breakthrough research on climate will be conducted from measurements of all four of EOS-Aura's instruments of dynamics, water vapour, clouds, and aerosols, where each are important components of climate forcing.

1.3 OMI and Aura in Relation to Envisat and other Atmospheric Chemistry Missions

1.3.1 Introduction

Aura and Envisat are major upcoming space missions by NASA and ESA, respectively, that will collect an unprecedented amount of data on the Earth's atmosphere. Envisat will collect data on several Earth science issues while Aura will make measurements exclusively of the atmosphere. Both missions will perform a variety of atmospheric observations including gas constituents, aerosols, clouds, temperature and pressure in both the stratosphere and upper troposphere. Measurements of the column amounts of certain gases will also be measured. The Envisat mission will be launched in August 2001 with planned operation of five years. The Aura launch is planned for June 2003 with six years of operations (design lifetime 5 years). The two missions will cover nearly a decade and will significantly enhance our knowledge of atmospheric chemical processes that are highly relevant to ozone depletion, air quality, and climate. The following briefly compares what each of the two missions brings to understanding these three environmental issues. The issues and the science questions themselves are discussed in detail in Chapter 2 of this document.

1.3.2 Mission Description and Instruments

The Aura mission was described in detail in Section 1.2 and is only summarised here. Aura carries four instruments, HIRDLS, MLS, OMI and TES. The first two instruments are limb-viewing radiometers observing in the mid-infrared and microwave regions respectively. TES is an interferometer, which views middle infrared emission in both the limb and nadir. OMI measures backscattered radiances in the nadir in the UV and visible ranges.

Envisat carries three instruments for atmospheric observations: GOMOS, MIPAS, and SCIAMACHY. GOMOS measures stellar occultation in the UV, visible, and near infrared; MIPAS is a mid-infrared interferometer and measures limb emission; SCIAMACHY measures backscattered Solar radiation in the UV, visible and near infrared in both the limb and nadir. In addition it will measure both lunar and solar occultations.

Aura and Envisat therefore have many overlapping measurements. However, there are significant differences that make these missions highly synergistic. These synergisms will be realised by the different viewing configurations, fields of view, and the satellites' different orbits. Aura will be placed in a polar orbit with an *ascending* equator crossing time of about 1:45 pm. Envisat is also in a polar orbit, but with a *descending* equator crossing time of 10:00 am.

1.3.3 Atmospheric Measurements

Figures 1.1 and 1.2 illustrate the atmospheric parameters measured by Aura and Envisat. The parameters illustrated represent the standard data products but additional special products are planned. The exact altitude range particularly at the lower end is still to be determined since algorithms are still under development. For the overlapping gases the accuracy is roughly the same. Both missions observe atmospheric parameters relevant to the three major atmospheric chemistry issues: ozone depletion, air quality, and climate. The differences are described in the following.

Ozone Depletion

In order to understand ozone trends, it is important to track and to measure simultaneously key gas radicals, the sources and reservoirs for each of the catalytic cycles as well as ozone itself. The catalytic cycles operating in the stratosphere and their more important constituents are listed in the Table 1.1.

Comparing Table 1.1 to Figures 1.1 and 1.2, it is clear that Aura has an advantage over Envisat in that more of the key gases in the catalytic cycles are measured. HCl is a critical reservoir for active chlorine and has been monitored in the upper stratosphere from NASA's UARS mission since 1991. Recent data has shown

that its amount is levelling off, consistent with the Montreal and subsequent protocols. This record will be continued by MLS on Aura.

Table 1.1 Catalytic cycles of the key gas radicals, the sources and reservoirs in the stratosphere

Cycle	Source	Radical	Reservoir
ClO _x	CFC ⁻¹¹ , CFC ⁻¹²	ClO	HCl, ClONO ₂
NO _x	N ₂ O	NO ₂ , NO,	ClONO ₂
HO _x	CH ₄ , H ₂ O	OH, HO ₂	HNO ₃

BrO in the stratosphere is an extremely potent catalytic radical for ozone destruction. Aura and Envisat measurements are highly complementary for profile measurements. Envisat's and Aura's column measurements of BrO will allow separation of tropospheric and stratospheric sources for this active molecule.

Both Aura and Envisat will measure total column ozone. However, a priority for OMI is the continuation of the TOMS highly precise, long-term column ozone record. Tracking global column amounts of ozone is critical for verifying model predictions and is relevant for climate studies. Envisat to date has not explicitly included long term trends in column ozone as a mission objective, although long term stratospheric ozone is the primary objective for GOMOS.

Climate Change

Chemistry of the atmosphere is now recognised to have a profound effect on the climate and it is now established that there is feedback between climate change and ozone depletion. Ozone is a greenhouse gas and will be adequately measured for this purpose by both missions. Both GOMOS and HIRDLS have excellent vertical resolution (1.0 – 1.5 km) and should provide more comprehensive information on transport in the lower stratosphere and across the tropopause. Nonetheless, because of differences between the stellar occultation and emission techniques, HIRDLS will produce about twice as many profiles per day (~1000 vs. ~500) and may go somewhat lower down in altitude. Water vapour in the upper troposphere and lower stratosphere is also a contributor to the greenhouse effect. MLS' ability to measure water vapour by observing microwave emissions in the presence of clouds has distinct advantage over the Envisat water vapour measurements, particularly in the tropics. Both Envisat and Aura will measure CH₄, another important greenhouse gas. Only Envisat will measure CO₂, and with sufficient analysis Envisat may provide first ever data on global scale of its sources and sinks.

Air Quality

Sources and regional and intercontinental transport of trace gases must be measured in order to formulate policy regulating anthropogenically (industrial and agricultural) produced toxic gases. Both Aura and Envisat represents first efforts to view air quality from a global perspective. Aura will measure tropospheric ozone using three techniques: subtraction of stratospheric column from total column, cloud slicing and directly from profiles. In principle, Envisat can accomplish the same, but the better spatial coverage by Aura over Envisat (see below) will provide better mapping of this crucial pollutant. CO and NO₂ are important precursors to ozone. NO₂, smoke and dust are also pollutants. The mentioned gas constituents and aerosols will be measured by both missions but the better coverage and spatial resolution of Aura (see below) will allow better identification of sources and mapping of these constituents. Sulphur dioxide will be observable by both Aura and Envisat under volcanic conditions. Averaging over time will allow mapping of SO₂ resulting from coal burning. Aura potentially will provide better coverage and spatial resolution for SO₂ measurements.

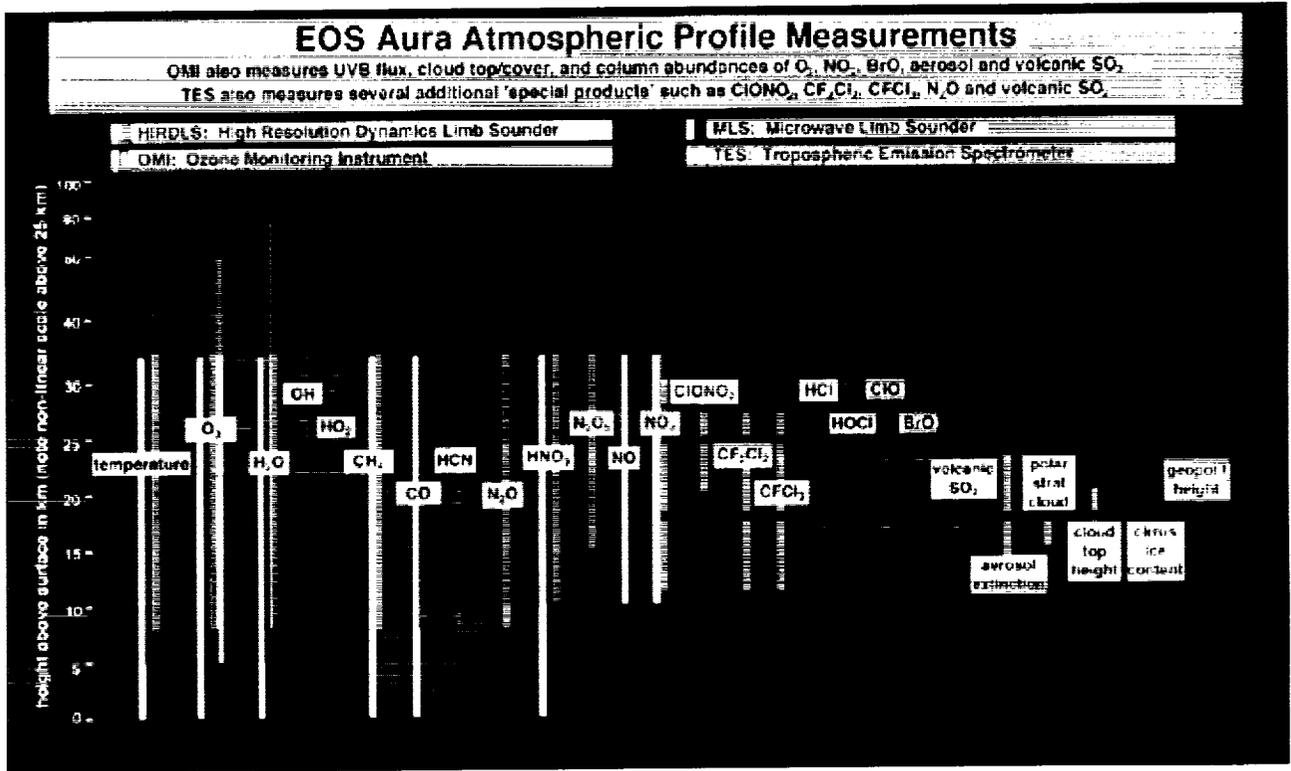


Fig 1.1 EOS-Aura (profile) measurements
 (© EOS-Aura website: <http://eos-aura.gsfc.nasa.gov/>)

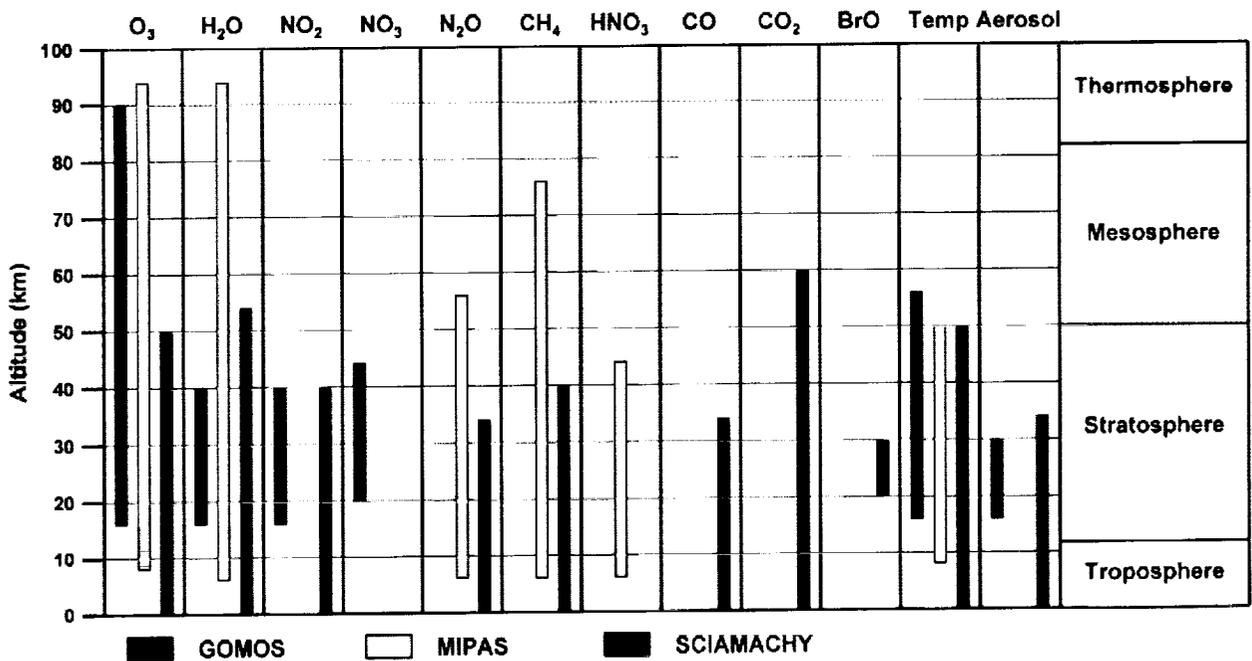


Fig 1.2 Envisat measurements
 (© Envisat MIPAS, An Instrument for Atmospheric Chemistry and Climate Research, SP-1229, ESA, March 2000)

Aerosols

Aerosols play a role on all three of the atmospheric chemistry issues described above. Aura and Envisat will derive aerosol characteristics from both limb and nadir measurements. Aura has an advantage in the stratosphere because of the better altitude resolution and coverage, and broader wavelength range of its instruments over Envisat. Nadir measurements in the ultraviolet are used to distinguish aerosol types such as smoke and dust over land. Aura has an advantage with OMI's better spatial resolution, while SCIAMACHY covers a broader wavelength range, which could give better particle size distributions. However, the combination of MERIS and AATSR on Envisat with their ultrahigh spatial resolution and broad wavelength range in the visible and infrared will provide important complementary data to Envisat's chemistry instruments.

1.3.4 Coverage and Spatial Resolution

All instruments that view in the limb (or occultation) have horizontal resolutions along the line sight of about 200-300 km. This limits the ability to observe transport process in detail. However, this can be improved by incorporating nadir measurements. Aura's OMI spatial resolution ranges from $20 \times 20 \text{ km}^2$ to about $40 \times 40 \text{ km}^2$ depending on data product type, with daily global mapping. TES has a spatial resolution in the nadir of $5 \times 9 \text{ km}^2$, which will be excellent for tropospheric observations, but global coverage will take some time. Envisat's nadir measurements, made only by SCIAMACHY, will have $30 \times 60 \text{ km}^2$ pixels for most products and will require six days for global coverage. The higher spatial resolution affords better identification of sources and mapping plumes and also substantially improves the ability to observe between clouds.

Aura is designed such that measurements are made in the same air mass by two or more instruments within 10 minutes. (While SCIAMACHY obtains the same in its normal operating mode by synchronising nadir- and limb-viewing.) This will allow a better assessment of process studies in the stratosphere and perhaps in the troposphere. HIRDLS vertical resolution is about 1 km and will provide an enormous source of data on stratospheric/tropospheric exchange. The ability of Aura to measure geopotential height as well as temperature will enable the derivation of winds concurrent with the gas measurements. In addition to the high vertical resolution, HIRDLS will scan in the azimuth (cross track) direction and will provide full latitudinal coverage in one day at 600 km intervals. This will enable observations of transport across the tropopause and outflows from the tropics using N_2O as tracer. This high spatial resolution in the stratosphere is well matched with OMI, which also has better (than SCIAMACHY) mapping resolution. In addition OMI

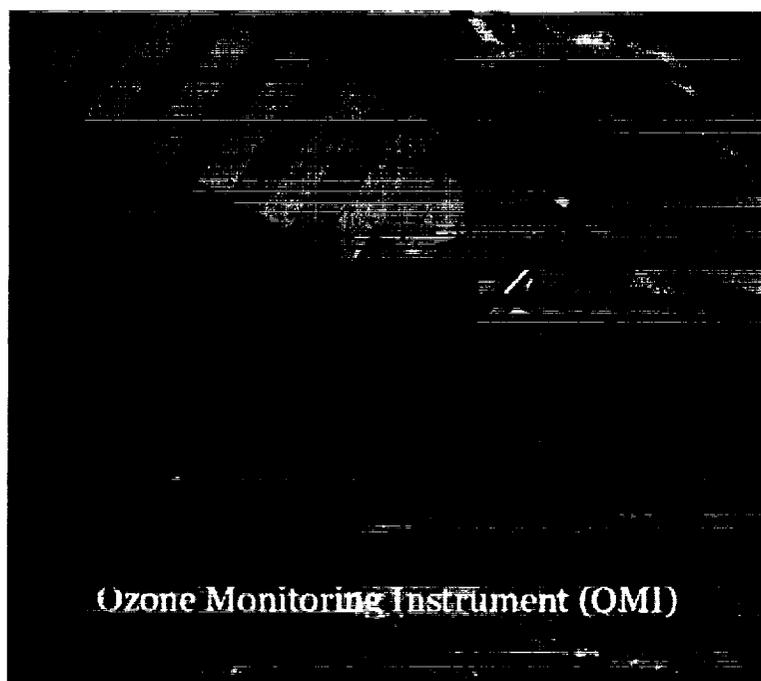


Fig. 1.3 Artist impression of OMI on EOS-Aura showing OMI's the wide swath

stratospheric profiles has significantly more coverage and spatial resolution than SCIAMACHY's nadir mode. Aura's TES will have an off nadir pointing capability which will allow direct observations of point source pollution episodes. Measurements of key air quality and green housegases will have much better resolution from Aura over Envisat.

1.3.5 Other Atmospheric Chemistry Missions

Aura's and Envisat's atmospheric chemistry measurements will be complemented by other international research and operational meteorological missions. In general, these research missions are more limited than Aura and Envisat with regard to science objective and coverage. The other research missions have less sophisticated (and much less costly) suites of instruments. The operational meteorological missions have much fewer measurements relevant to chemistry. These missions are briefly discussed here.

OSIRIS and SMR (Sub-Millimeter Radiometer) will fly on Odin (launch early 2001), a Swedish-led mission with Canadian, Finnish, and French participation. The mission is shared with an astronomy mission. The OSIRIS is similar to SCIAMACHY's limb scattering measurement but will have limited coverage because of its long vertical scan time and its orbit is near the terminator. Co-aligned with OSIRIS, the SMR will produce vertical profiles of ozone and a number of related molecules. ACE flying on SciSAT, to be launched about 2003, is a solar occultation measurement flying in inclined orbit, which allow nearly global mapping over a month or more. Measurements will be made by an FTIR and will enable observation of a large array of chemical species in the stratosphere. GCOM, to be flown by the Japanese space agency in 2006, will carry two instruments for chemistry observations. The first is ODUS, an ozone column mapper, will have capabilities similar to GOME-1; however its ability to map gases absorbing in the visible, e.g. NO₂, is uncertain at this time. The second instrument is an FTIR solar occultation measurement, which also measures many gases in the stratosphere. The orbit is non-Solar-synchronous providing about monthly global coverage for the occultation measurement.

The United States and Europe will fly ozone instruments (OMPS and GOME-2, respectively) on their next generation operational polar orbiting meteorological satellites, NPOESS and METOP respectively. METOP will begin in 2005 and NPOESS in 2010. METOP has been designed to provide data for operational meteorological applications for 15 years from 2005 on, and this will be valuable for meteorological and climate research. GOME-2 has a slightly better spatial resolution and coverage than its predecessor, GOME. Also onboard METOP is IASI, whose primary objectives are temperature and water vapour profiles, with cloud parameters and trace gases as secondary objectives. OMPS has two instruments consisting of an ozone mapper and a profiler. The mapper has spatial resolution similar to TOMS and the profiler employs limb scattering similar to SCIAMACHY, however its products will be limited to ozone columns and profiles.

1.3.6 Synergism

Clearly there is a great deal of synergism between Aura and Envisat. A major benefit is the timing of the missions. The combined data record is likely to be about ten years between the missions with three years of overlap. This will enable very accurate determination of trends. The different local observing times will be highly synergistic for studies of diurnal variations of both troposphere and stratosphere. For the troposphere, Envisat's morning crossing will have an advantage because of less cloudiness. On the other hand, for studying pollution, Aura's afternoon crossing will be more advantageous since chemical production advances during the course of the day.

Several measurements from Envisat and Aura are highly complementary since the altitude range is extended when the measurements are combined, e.g. BrO. The overlap regions will allow highly valuable validation data. Overlapping measurements using the same measurement technique (MIPAS and TES) will provide a cross-check of the algorithms. On the other hand, comparison of data products derived using different techniques (SCIAMACHY and HIRDLS), will allow some assessment of measurement calibration. Profile measurements combined with column measurements of the same species will provide a cross-check of tropospheric amounts.

The different equator crossing time of OMI on EOS-Aura (afternoon) and GOME-2 on METOP (morning) potentially provides valuable information on the daily cycle of tropospheric chemistry. Moreover, with the different overpass times of EOS-Aura (afternoon) and METOP (morning) the ozone information in the Numerical Weather Prediction (NWP) models can be updated at least twice a day.

1.4 Structure of the report

The main purpose of this “Science Requirements Document for OMI-EOS” is to formulate Science and Instrument requirements which shall be fulfilled by the OMI instrument on NASA’s EOS-Aura satellite. Starting from the Mission Objectives of the EOS-Aura satellite, the role OMI plays on EOS-Aura in order to achieve those mission objectives is described. This logically results in the Science Objectives of the OMI-instrument (Chapter 2).

These Science Objectives lead to a number of data products which will be measured by OMI. The list of OMI data products and the requirements put on those data products to ensure their quality fulfils the OMI Science Objectives, is discussed in Chapter 3.

The OMI data products are obtained by applying several retrieval techniques on the OMI measurements. Since the retrieval techniques require a certain quality of the OMI spectra this results in high level requirements on the radiance and irradiance spectra provided by OMI (Chapter 4).

The detailed and specific Instrument Requirements, which follow from the Science and Algorithm Requirements as derived in Chapters 3 and 4, are listed in Chapter 5. In order to specify Instrument Requirements, knowledge on the specific instrument design is however inevitable. Therefore a reference is given in Chapter 5 to the document written by industry, in which the OMI instrument is described (“*Instrument Specification Document*”). Some Instrument Requirements can only be achieved after applying correction algorithms in the level 0 → 1b software which are based on on-ground or in-flight characterisation and calibration activities. In Chapter 5 the key Calibration Requirements are given.

Another essential aspect to guarantee the quality of the OMI data products is validation. Chapter 6 gives an overview of the required Validation Strategy for OMI-EOS.

It should be clear that this document is focused on the Scientific and Instrument Requirements for OMI-EOS. Requirements on Earth radiance and solar irradiance spectra which are not on the instrument, but have to do with ground processing facilities, etc., can be found in the “*User Requirements Document for level 0 → 1b processing*”. Concerning calibration requirements, only the requirements which have a large impact on instrument design or have a considerable financial or schedule impact are listed (Chapter 5). The complete list of requirements concerning calibration can be found the “*Calibration Requirements Document*” and the “*In-flight Calibration Requirement Document*”. Specific Validation Requirements can be found in the “*OMI Validation Requirements Document*”. All Science and Instrument Requirements put on OMI-EOS are listed according to the following rule: **SR w.x.y.z**, in which **SR** stands for Science Requirement and **wxyz** stand for respectively chapter (**w**), section (**x**), subsection (**y**) and number of the requirement (**z**) (see Annex I and II).

Chapter 2 The OMI contribution to the EOS-Aura Mission Objectives

2.1 Introduction

The Ozone Monitoring Instrument (OMI) should contribute to the EOS-Aura mission objectives by measuring ozone and other minor atmospheric constituents, aerosols, surface UV, and cloud parameters. The Mission Objectives of the EOS-Aura mission are:

- (i) To measure ozone and other trace gases in order to monitor the ozone layer and its predicted recovery following from the Montreal Protocol and its subsequent Amendments and Adjustments.
- (ii) To monitor tropospheric pollutants worldwide.
- (iii) To monitor atmospheric constituents that are important for climate change.

For mission objectives (i) and (iii) OMI provides the continuation of the TOMS total ozone data record. Besides the provision of data for the three primary EOS-Aura objectives, OMI aims

- (iv) To deliver near-real time ozone observations for assimilation in numerical weather prediction (NWP) models.

Therefore OMI contributes to several of the most important science questions in atmospheric research concerning the role of ozone in the climate system. In the remaining of this chapter these possible contributions are shortly evaluated, and this is done such that scientific and instrument requirements for OMI can be based on these evaluations in Chapter 3, 4 etc.

2.2 Science Questions for OMI on EOS-Aura

This section details the possible contributions of OMI to the science questions underlying the EOS-Aura mission objectives and it also details the OMI contribution to the area of operational meteorology. The synergy with the other EOS-Aura instruments, and with GOME-2 on METOP-1 is explored for the various science questions. OMI should provide daily high-resolution global maps of ozone and other constituents. The daily ozone profiles around the globe allow detailed studies on the ozone layer and the physical and chemical processes underlying its possible recovery. Especially the continuation of the TOMS data record is invaluable for ozone trend studies (see Figure 2.1). Section 2.2.1 gives more details on the role of OMI for monitoring the ozone layer and for ozone trend studies.

The combination of ozone, nitrogen dioxide and aerosol measurements in the troposphere by OMI should provide unique, worldwide information on tropospheric pollution events that are connected with industrial, agricultural, traffic emissions and biomass burning. The combination of column ozone and column nitrogen dioxide with stratospheric profiles should lead to high-resolution determination of tropospheric columns of ozone and NO₂ with daily global coverage. The distinction between the stratospheric and tropospheric columns will likely benefit from combination with limb measurements, such as made by HIRDLS and/or MLS on EOS-Aura. In so-called “zoom modes”, OMI should be able to study the troposphere with a horizontal resolution of the order of 10 × 10 km². These zoom modes are well adapted to monitor pollution events in partially cloudy regions, e.g., the industrial regions at mid-latitudes. The zoom modes will also improve the evaluation of the surface UV-B radiation intensity. Section 2.2.2 explores the role of OMI for the important science questions related to the tropospheric composition.

The connections between ozone change and climate change can be studied by assimilation of OMI ozone data in climate-chemistry models. In this respect OMI can, for example, help to distinguish between stratospheric cooling that results from chemical ozone loss and stratospheric cooling that is linked with

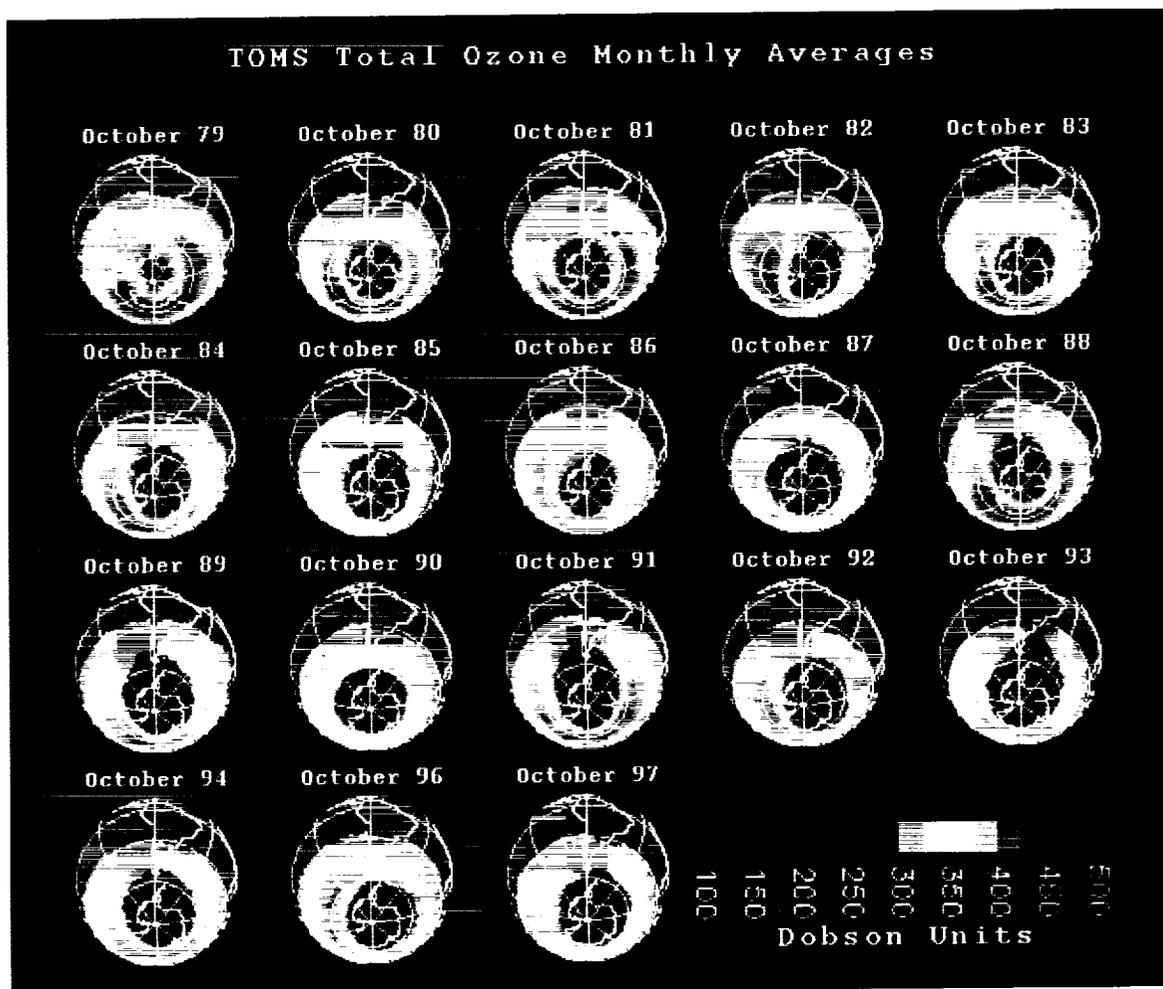


Fig 2.1 Occurrence of the Antarctic ozone hole, as detected by TOMS instruments in the period 1979 – 1997.
(© <http://toms.gsfc.nasa.gov/multi/multi.html>)

tropospheric warming and climate change (WMO, 1999; Shindell, 1998). In general, the OMI ozone measurements should further improve our knowledge on the general circulation in the upper troposphere, stratosphere and mesosphere and the possible changes therein. Section 2.2.3 details the possible role of OMI for the science questions at the interface of ozone research and climate change studies.

Finally, the development of fast-delivery ozone algorithms in recent years gives the unique possibility to use OMI ozone products in the area of operational meteorology. The dynamics in the upper layers of numerical weather prediction models (NWP), and also in data sparse regions, are currently still insufficiently constrained. Therefore, data assimilation of OMI ozone measurements into NWP promises to significantly improve the NWP model performance (see Section 2.2.4).

2.2.1 The ozone layer and its possible recovery

During the last decades a depletion of stratospheric ozone due to anthropogenically emitted substances has been observed (WMO, 1999). The first studies that indicated that there were close connections between observed ozone decreases and increasing chlorine levels in the lower stratosphere, were observations made over Antarctica about 15 years ago (Farman et al., 1985). More recently, similar relations between chlorine loading and reductions in ozone have been found at high northern latitudes (von der Gathen et al., 1995, Braathen et al., 1994). The strongest ozone loss at middle and high northern latitudes occurs during the period February – April. The observed trend in total ozone is of the order of -3 to -6 % per decade (WMO, 1999). During summer and fall seasons the trend is less, of the order of -1 to -3 % per decade. The observed

ozone trends also vary with height in the stratosphere, with the largest decreases in the lower stratosphere below 20 km.

Several chemical processes have been identified to be of importance for the chemical ozone loss in the stratosphere. These include the chemistry of chlorine (ClO/Cl), bromine (BrO/Br), hydrogen (HO₂/OH) and nitrogen (NO₂/NO). In addition, heterogeneous processes occurring on aerosol/PSC (Polar Stratospheric Cloud) surfaces lead to enhanced levels of active HO_x and ClO_x components and explain the pronounced ozone depletion at high latitudes (Solomon et al., 1996). Sulphate aerosols are present all over the global stratosphere, while PSCs are confined to high latitudes of the winter hemisphere. Hydrolysis of N₂O₅ on sulphate aerosols indirectly enhances ozone loss by increasing the level of active chlorine compounds and contributes significantly to mid-latitude ozone depletion. The ozone loss by the HO_x, NO_x and Br_x cycles is also affected by the presence of aerosol particles in the lower stratosphere. The mid-latitude ozone chemistry is thus in many ways similar to the polar ozone chemistry.

A characteristic of the ozone changes during the last decade is that there has been significant variability on different time scales. Year-to-year variations can be linked to a large extent to variations in dynamics and volcanic eruptions. It is often difficult, in particular on a time scale of a few years, to separate man-made impacts from natural variability. Therefore, continuity in satellite missions dedicated to ozone observations is essential for the detection of trends in the ozone layer. In order to obtain this, long-term calibration of satellite instruments like TOMS, GOME and OMI is an essential aspect of satellite missions.

Since the decrease in stratospheric ozone is so clearly linked to changes in chlorine and bromine loadings in the stratosphere, future changes in stratospheric ozone will to a large degree be determined by future changes in the emissions of the chlorine and bromine source gases. Observations over the last few years have shown that the tropospheric burden of chlorine is leveling off due to the phase out of key chlorine compounds included in the Montreal Protocol (WMO, 1999). The reductions in emissions have been large for F¹¹ and methylchloroform (MCF) which contribute significantly to lower stratospheric ozone destruction. Emissions of F¹², of importance to chlorine loading in the upper stratosphere, are also reduced. It is expected that due to the highly different lifetimes of the individual chlorine and bromine compounds, the future reduction in their atmospheric concentrations, and therefore also their contributions to stratospheric chlorine and bromine levels, will be highly different in the course of time (WMO, 1999).

A major scientific issue for EOS-Aura is to check whether the stratospheric ozone layer is recovering as predicted by current models. In particular, it is presently under debate to what extent climate change may interfere with the recovery. Changes in the stratospheric circulation and cooling of the lower stratosphere may alter the ozone trends. It is anticipated that assimilation of the daily, global ozone observations of OMI contributes to a better quantification of the transport and mixing processes in the stratosphere. In this way OMI can help to distinguish between dynamical and chemical causes of the breakdown of the ozone layer. Apart from the ozone distribution, OMI and the other instruments on EOS-Aura should observe several components that play a role in the chemical ozone depletion processes, in particular BrO, OCIO, ClO, NO₂, aerosols and PSCs. Therefore, it will be possible to compare the observed ozone changes with the trends in the ozone destroying gases.

The main contributions of OMI to the monitoring of the ozone layer, its variability, and its possible recovery are:

- Continuation of the TOMS and GOME total ozone records for monitoring the thickness of the ozone layer and to detect trends.
- Continuation of the SBUV and GOME ozone profile measurements for monitoring the ozone-hole and the global ozone distribution and to detect trends.
- BrO, OCIO distribution and NO₂ column measurements similar to those from GOME.
- Stratospheric volcanic aerosol and volcanic SO₂ monitoring.

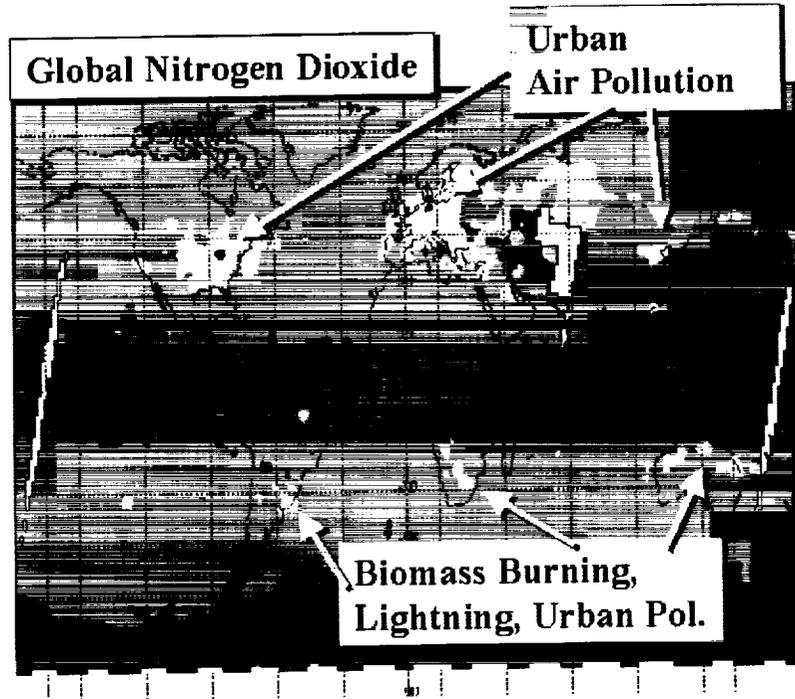


Fig. 2.2 Total column NO_2 showing effects of urban areas in Northern Hemisphere and biomass burning in Southern Hemisphere. Measurements made by the Global Ozone Monitoring Experiment (GOME) on ERS-2. Figure with courtesy of A. Richter and J.P. Burrows, Institute of Environmental Physics and Remote Sensing, University of Bremen.

The first two bullets imply that long-term calibration over several years of the OMI instrument is an essential requirement to fulfil the OMI mission objectives for EOS-Aura.

Synergy exists with the other instruments on EOS-Aura, and also with GOME-2 on METOP-1. OMI will measure with daily global coverage and a $20 \times 20 \text{ km}^2$ resolution, while GOME-2 will either measure with a $40 \times 40 \text{ km}^2$ resolution and a global coverage of three days or with a $40 \times 80 \text{ km}^2$ resolution and a global coverage of two days. The different equator-crossing time of EOS-Aura (afternoon) and METOP (morning) will provide valuable information on the daily cycle of the stratospheric chemistry. HIRDLS, MLS and TES on EOS-Aura will provide additional information on longer-lived reservoir species such as HNO_3 , ClONO_2 , N_2O_5 , HCl, and CFCs, which will also help to better quantify the chemical ozone loss processes.

2.2.2 Monitoring of tropospheric pollution

Anthropogenic emissions to the atmosphere are growing continuously due to increasing human activities. Consequently, the atmospheric concentrations of some species are increasing dramatically (Brasseur et al, 1998). Major contributions to the anthropogenic emissions are from fossil fuel burning, biomass burning, and agricultural activities. The factors that determine these anthropogenic sources are many and complicated, including population increase, economic development, and numerous other economical and sociological factors. Changes in land-use constitute one of the major forcings affecting atmospheric composition. Furthermore, recent emission controls in the developed countries and the increasing economical activities in the developing countries may result in major geographical redistributions of the anthropogenic emissions. Due to the increasing emissions of CO, hydrocarbons, and NO_x , substantial increases in tropospheric O_3 concentrations are foreseen in the developing countries in the tropics and subtropics. Increasing emissions of nitrogen and sulphur oxides will intensify acid deposition and particle formation. Effects of photochemical air pollution and acid deposition include health effects, acidification of surface waters and subsequent damage to aquatic ecosystems, damage to forests and vegetation, and damage to materials and structures. Furthermore, tropospheric ozone is an efficient greenhouse gas whose global increase contributes significantly to the total radiative forcing by climate gases (IPCC, 1996).

Pollution (see Figures 2.2 & 2.3) exported from the emission regions to remote regions affects the background level of ozone and its precursors (CO, HCHO, NO_x, etc.), and of aerosols on the global scale. More particularly, transport of pollutants from North America and Europe may have a major impact on tropospheric chemistry over the Atlantic Ocean. Similarly, export of pollutants from Asia has an impact on the pollutant levels over the Pacific Ocean, and possibly North America.

Biomass burning is much more extensive and widespread than previously thought. Biomass burning refers to the burning of the world's forests, grasslands and agricultural lands following the harvest for land clearing and land conversion. Biomass burning occurs in the tropics (tropical rainforests and savanna grasslands), in the temperate zone, and in the boreal forest, and is a truly global phenomenon. A considerable part of the biomass burning is human-initiated and such burning is increasing with time. There may also be an increase in forest fire induced by global warming. Deforestation plays an important role in releasing large amounts of CO₂ into the atmosphere. Biomass burning is also a significant source of ozone precursors. Plumes of elevated tropospheric ozone concentration emanating from South America and Africa have been identified during the biomass-burning season. These pollution events occurring during the dry season are similar in magnitude to those observed in industrialised regions. Convection is efficient in taking the pollutants to higher levels in the troposphere, and plumes of lifted pollutants may be detected far away from the source regions.

OMI will be able to monitor pollutants such as ozone, nitrogen dioxide, and aerosols in the troposphere, as well as their transport away from the source regions. Further, OMI should be able to observe plumes of SO₂ (see Figure 2.4), HCHO. The determination by OMI of surface UV radiation in polluted areas is relevant, because elevated UV-B radiation levels increase the photochemical smog formation.

OMI will have a small instantaneous field-of-view to be able to look between the clouds, and to detect tropospheric pollution (including aerosols) down to the surface. In this way OMI will be a step forward in atmospheric chemistry instrumentation with respect to sensitivity for clouds.

In summary, the main contributions of OMI for the measurement of pollution in the troposphere include:

- O₃ and NO₂ tropospheric (column) measurements
- Aerosol optical thickness and aerosol single scattering albedo
- Observation of HCHO, SO₂, and dust column densities in plumes
- surface UV radiation measurements

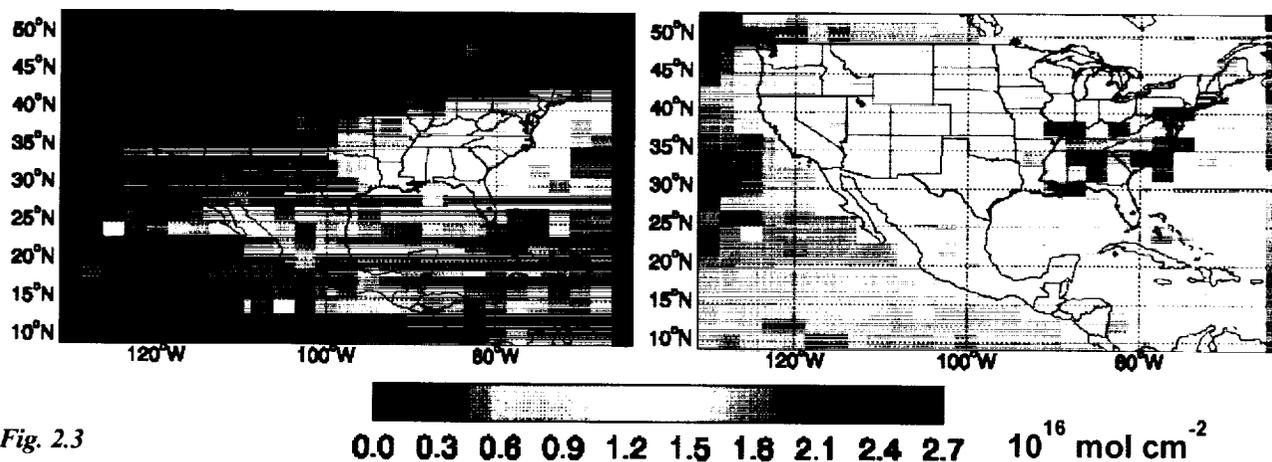


Fig. 2.3

HCHO columns retrieved from GOME spectra over the U.S. for July 1996. Observations are for 10:26-11:54 local solar time and for cloud cover less than 40%. The left figure shows the "geometric" total vertical columns and the right figure shows the total vertical columns where Rayleigh scattering was taken into account (Chance et al., 2000).

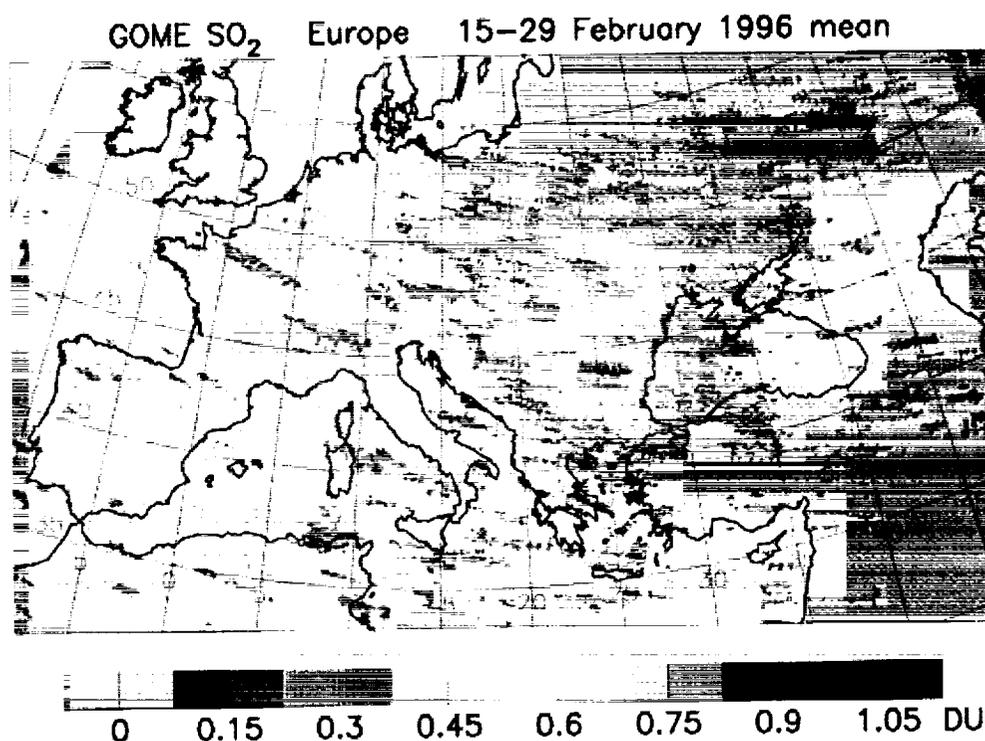


Fig. 2.4 GOME SO₂ total columns above Europe averaged over the period 15-29 February 1996. Enhanced SO₂ levels observed in Eastern Europe are most likely emissions from coal power plants. During this period surface temperatures were extremely low so that private household may also have contributed to the high SO₂ values (Courtesy Eisinger and Burrows, 1999, © <http://www.iup.physik.uni-bremen.de/gome/gallery.html>).

Cloud detection is important for the tropospheric measurements of polluted air masses by OMI. The pollution events that will be detected by OMI are either in cloud-free areas, or in pollution layers that are situated above clouds. Most (severe) pollution events occur in situations with limited cloud cover, but some type of events are notoriously cloudy. Ideas about cloud detection by OMI are given in Chapter 3.

The OMI tropospheric measurements are synergistic with those from HIRDLS, MLS and TES on EOS-Aura. TES will benefit from the cloud-detection capabilities of OMI. The determination of tropospheric columns of ozone and nitrogen dioxide from OMI should benefit from the stratospheric measurements by HIRDLS and MLS observations. The TES measurements of, e.g., CO will allow more detailed analyses of the specific pollution events that are seen by OMI. Studies of pollution events may also benefit from combinations of TES measurements and the OMI measurements made in zoom-in mode.

2.2.3 Coupling of Chemistry with Climate

Ozone plays different roles in the climate system. Ozone is radiatively active, absorbing both ultraviolet and infrared radiation. Secondly, ozone distributions are effected by the temperature and circulation in the upper troposphere and stratosphere. Up till present, the most important source of data used to study height resolved ozone trends and variability has been the global network of ozone soundings, from which various climatologies have been constructed (e.g. Fortuin and Kelder, 1998; Logan, 1999 (1+2); Randel and Wu, 1995). OMI and the limb viewing instruments on EOS-Aura should improve on this by improving the accuracy and vertical resolution of satellite derived ozone profiles with global coverage.

Ozone is an important climate gas as an absorber of UV radiation, heating the stratosphere, and protecting the Earth's surface and its inhabitants against the highly damaging part of the solar UV spectrum. Moreover, ozone is also a climate gas, because it absorbs infrared radiation. Hence, changes in the ozone abundances have consequences for the radiative balance of the atmosphere. In particular, ozone changes in the stratosphere are likely to induce changes in the temperature structure and the dynamics of the stratosphere.

With the ozone profile observations from OMI it should be possible to improve our knowledge of the general stratospheric circulation and its variability.

As remarked earlier, changes in the stratospheric circulation may result from stratospheric cooling. Such cooling may be a result of ozone loss, but also of increasing greenhouse abundances, i.e., a global warming of the troposphere due to the increase in climate gases (mainly CO₂) will be accompanied by a cooling of the stratosphere (Shindell, 1998). In fact, a cooling of the stratosphere and mesosphere has been observed during the last decades, which is most probably due to the observed ozone depletion (WMO, 1999). A positive feedback related to this is the formation of PSCs at low temperatures in the lower stratosphere, which enhances the ozone loss further via heterogeneous reactions. Temperature-ozone feedbacks may also exist in the troposphere. However, the coupling between ozone changes and climate changes are only beginning to be studied with current chemistry-climate models.

Another science question is how much of the observed ozone loss at mid-latitudes is a local phenomenon, and how much can be attributed to the observed polar ozone loss? To answer this question the amount of leakage of the polar vortex as a function of height needs to be quantified. Above approximately 16 km the polar vortex is probably relatively well isolated, so that only a relatively small fraction of ozone depleted air is transported to mid-latitudes before the break up of the polar vortex. There are also model studies that indicate significant leakage of the vortex (e.g. Wauben et al., 1997). Below 16 km the vortex structure is much less pronounced and significant mixing of polar and mid-latitude air takes place. Therefore, polar ozone depletion could affect the mid-latitude trend at these heights significantly.

The large-scale mixing of mid-latitude and polar air after the break-up of the polar vortex, has a dilution effect on the ozone distribution in both hemispheres. Estimates of the amount of leakage could be improved by accurate determination of the rate of descent in the vortex and by quantification of the erosion of the vortex by breaking planetary waves that peel off filamentary structures from the vortex. The filaments have widely varying widths and depths. Typical depths are of the order of a km and typical widths are a few hundred km. The filaments often stretch into the sunlit part of the atmosphere while the vortex itself may still be in the polar night. It is expected that OMI may detect the (larger) filaments because the ozone concentrations in these filaments should be distinctively different from the surroundings. HIRDLS and MLS should contribute by measuring the vertical profile of ozone with a high resolution of a few kilometers. Data assimilation of satellite data into chemistry transport models should strongly improve the description of the parameters.

The distribution and variability of upper tropospheric and lower stratospheric ozone is an important question in climate research. Due to the long chemical lifetime, most of the variability in the ozone distribution observed directly above and below the tropopause can be attributed to dynamical causes. Much variability is caused by the up- and downward movements of the tropopause, following the passage of low- and high-pressure systems in the extratropical troposphere. Since the tropopause marks the boundary above which ozone concentrations increase, the vertical movement of the tropopause translates into huge variations in ozone and temperature lapse rate. Studies of the stratosphere-troposphere exchange and tropospheric chemistry of ozone need to take into account these movements. Estimates of the global transport of ozone from the stratosphere to the troposphere still vary by almost a factor of five. The transport of ozone across the tropopause in the extra-tropics is amongst others accomplished by tropopause foldings, which occur along local wind maxima (jet streaks) of the polar, mid-latitude and subtropical jet streams. The persistence of elevated ozone layers in the troposphere due to folds can be quite long and may be observed by OMI. Part of the variability of tropospheric ozone is due to upward transport of boundary layer air into the upper troposphere. This transport can be induced by deep convection or by extratropical cyclones. In the tropical upper troposphere intrusions of subtropical stratospheric air have been observed by in situ measurements, but the quantification of their global contributions is still needed.

In the coupling between chemistry and climate, aerosols and clouds play an important role. Clouds have a large radiative effect in both the shortwave and longwave range. Aerosols affect mainly the shortwave radiation balance in a direct and indirect way. The direct aerosol effect is the increased shortwave reflection due to anthropogenic aerosols, which may partly offset the increased greenhouse effect due to increased concentrations of CO₂, methane, and other greenhouse gases. The indirect aerosol effect is the process in

which tropospheric pollution yields small aerosols, which may act as cloud condensation nuclei. In this way, clouds become optically thicker and reflect more sunlight, which cools the Earth's atmosphere system. On the other hand, tropical clouds may bring up absorbing aerosols from anthropogenic origin to high tropospheric altitudes, where these aerosols may heat the atmosphere, thereby reducing the amount of clouds. Recent results of chemistry, cloud, and aerosol field campaigns (e.g. ACE-2 and INDOEX) demonstrate the link between the chemical and physical processes in the atmosphere, which contribute to climate change. In spite of the importance of aerosols for the Earth's radiation balance, the uncertainties in the estimates of the aerosol forcing are large (IPCC, 1995). These large uncertainties are caused by the complexity of the aerosol-climate coupling processes as compared to the forcing by the well-mixed greenhouse gases, and the sparseness of data on a global scale. Because of the short lifetimes of aerosols in the troposphere, the aerosol is highly variable in both space and time. Only satellite remote sensing has the potential to measure the highly variable aerosol field (see Figure 2.5) on global scales during longer periods (IPCC, 1995), which are needed to quantify the effects of aerosols on climate.

In summary, the most important contributions of OMI to the study of climate change include:

- Continuation of the TOMS total ozone data record.
- Ozone profiles for the study of dynamical, chemical, and radiative processes in the upper troposphere and stratosphere.
- Aerosol and cloud detection.

Other important climate parameters that are measured by the other instruments on EOS-Aura include temperature and the water vapour content, besides ozone, aerosol and cloud information. In combination with the data from OMI a very complete data set should be obtained that can be used for comparison with chemistry-climate models. Thus, for such climate studies synergy exists between all EOS-Aura instruments. The study of stratosphere-troposphere exchange processes may especially benefit from the combination of OMI ozone profiles, with the water vapour, ozone and temperature profiles that are obtained with limb viewing instruments on EOS-Aura. The study of dynamical processes may further benefit from observations of tracers, such as the measurements of nitrous oxide by HIRDLS and MLS. The advantage of the ozone data from OMI, compared to the limb viewing instruments on EOS-Aura is the high horizontal resolution of $20 \times 20 \text{ km}^2$, which is required for a number of process studies.

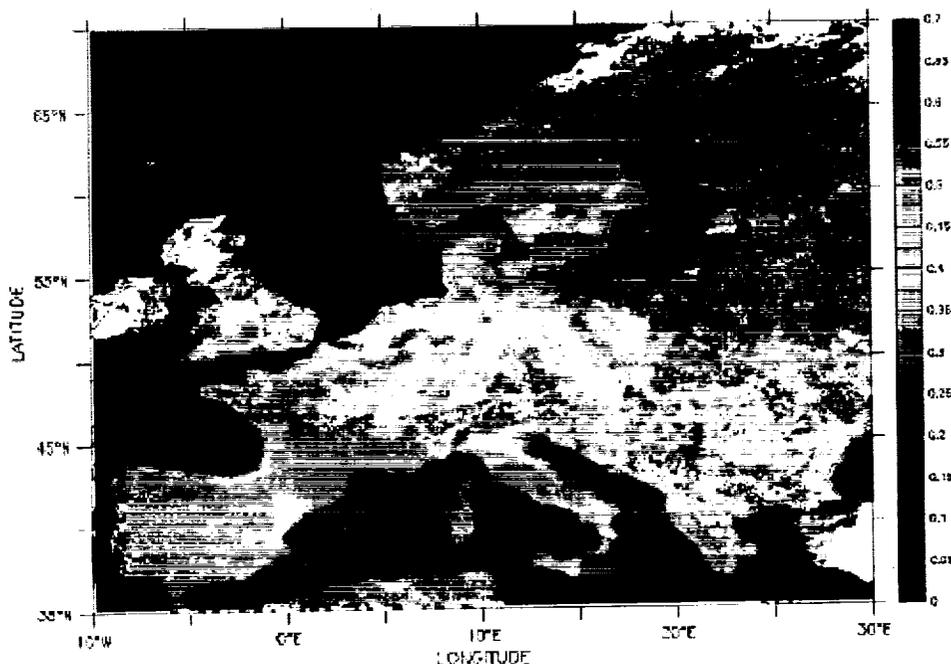


Fig. 2.5 Mean aerosol optical depth in August 1997 (monthly average). OMI will achieve a similar spatial resolution. Retrieved from ATSR-2 image (see Gonzalez et al., 2000).

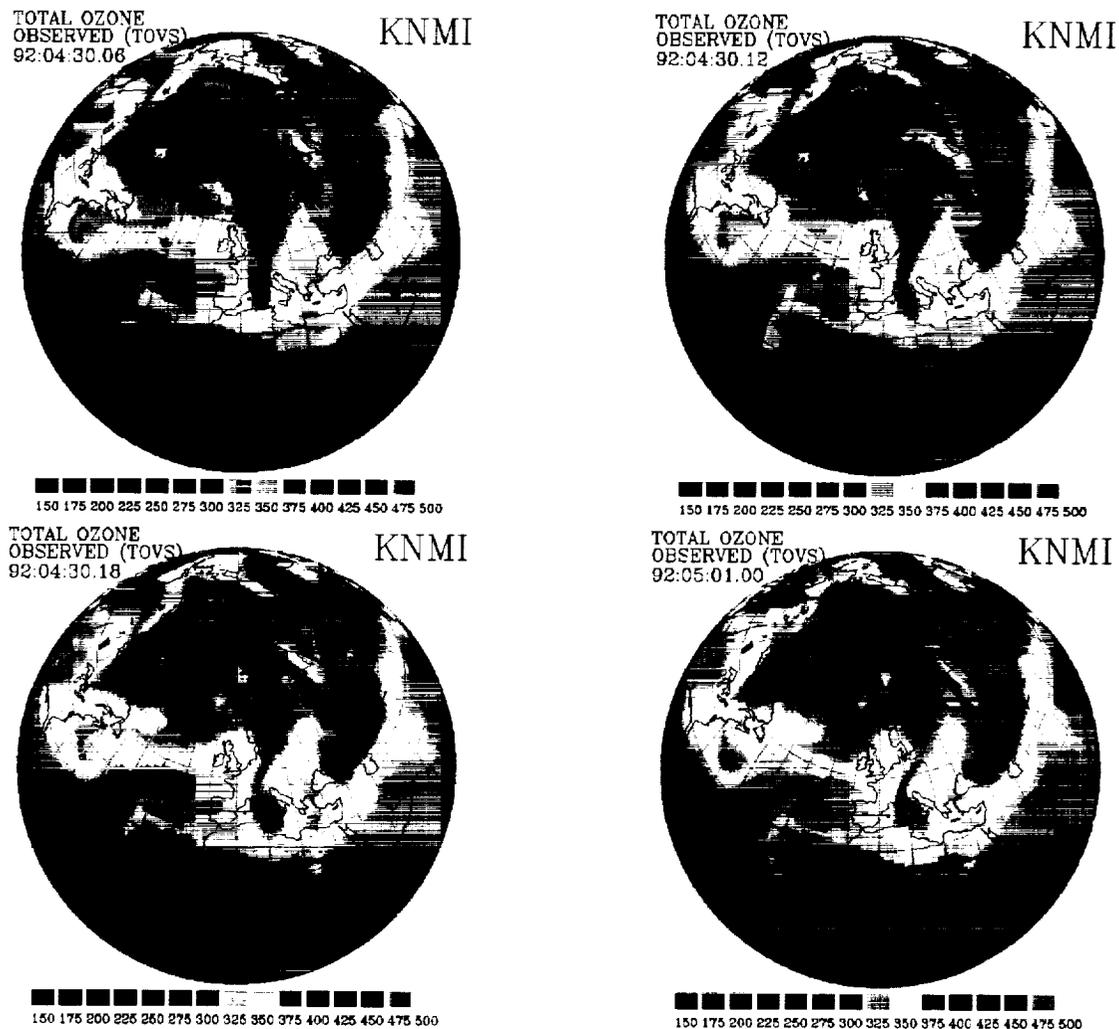


Fig. 2.6 *Development of depressions above Europe and Atlantic Ocean near the USA can be seen in the ozone field (a low pressure field corresponds with high total ozone and a high pressure field corresponds with low total ozone). Figure with courtesy of M. Allaart, KNMI.*

2.2.4 OMI Observations for Operational Applications

The term operational meteorology covers all the activities that lead to the regular provision of reliable weather forecasts by meteorological institutes. Measurements from a global weather observation network are assimilated to produce the initial state of the atmosphere (the “analysis”) which forms the basis of the weather forecasts calculated by Numerical Weather Prediction (NWP) models.

Ozone measurements from OMI should be of significant value when assimilated into NWP models, as they should improve the determination of wind fields in the stratosphere, in particular near the tropopause. These measurements should have an impact on the quality of the analysis, as there are very few other observations of this important altitude region over large parts of the globe. Since fluctuations in observed ozone fields are dominated by horizontal and vertical transport processes, the changes in these fields may be used to derive information about the wind fields (see Figure 2.6). It has been shown, for instance, that the total ozone field can fairly well be predicted up to a week by simply advecting it with winds at tropopause height (Levelt et al., 1996). Horizontal wind fields derived with pattern recognition techniques are mainly representative for the wind component along the horizontal gradient in the total ozone column. Better wind information can be obtained when using data-assimilation techniques in three-dimensional models (e.g. Jeuken et al. 1999). Considering ozone as a passive tracer is a good approximation on time scales of a few days to weeks in the upper troposphere and lower stratosphere. Even in ozone hole conditions the destruction of ozone in the

lower stratosphere is at most a few percent per day. In this case, parameterisation of the chemistry in the data-assimilation model should be sufficient to derive wind fields.

The fact that ozone concentrations generally increase sharply above the tropopause can be used to observe the tropopause dynamics on a global scale, including the detection of tropopause breaks in the surface due to baroclinic activity. The changes in the structure of the tropopause surface provides insights into the locations of jet streams and vorticity zones, improving the interpretation of the NWP analyses and forecasts.

The ozone measurements from OMI, along with the “classical” meteorological parameters, i.e., pressure, temperature, wind, humidity, clouds, etc.) have to be assimilated into the NWP model to derive the analysis. Current operational assimilation schemes are usually three-dimensional, taking “snapshots” of observed three-dimensional fields. Four-dimensional assimilation methods have recently been implemented which take into account the temporal evolution of the observations. They combine in an iterative way forecast steps with the assimilation cycle, accounting in this manner for the actual time when the observations were made (e.g. Eskes et al, 1999).

A current subject of study in NWP is using retrieved atmospheric parameters (in case of OMI ozone columns and ozone profiles) instead of directly assimilate measured radiances which contain implicit information about ozone (and other parameters). These assimilation methods involve the use of radiative transfer models to calculate simulated radiances of model states of the atmosphere, which are then adapted according to observed radiances. It is anticipated that both types of NWP models, those assimilating radiances directly and those using retrieved products, will exist in parallel for some time in the future. Two other forecasting applications from OMI include surface UV predictions and volcanic cloud detection.

At present, predictions of the amount of ultraviolet radiation reaching the Earth's surface form part of the daily weather forecast in several countries. These predictions can be valuable for, e.g., agricultural purposes, but the main interest stems from the fact that an excess of ultraviolet radiation is related with an increased risk of skin cancer and other health problems, and also poses a potential threat to many of the Earth's life

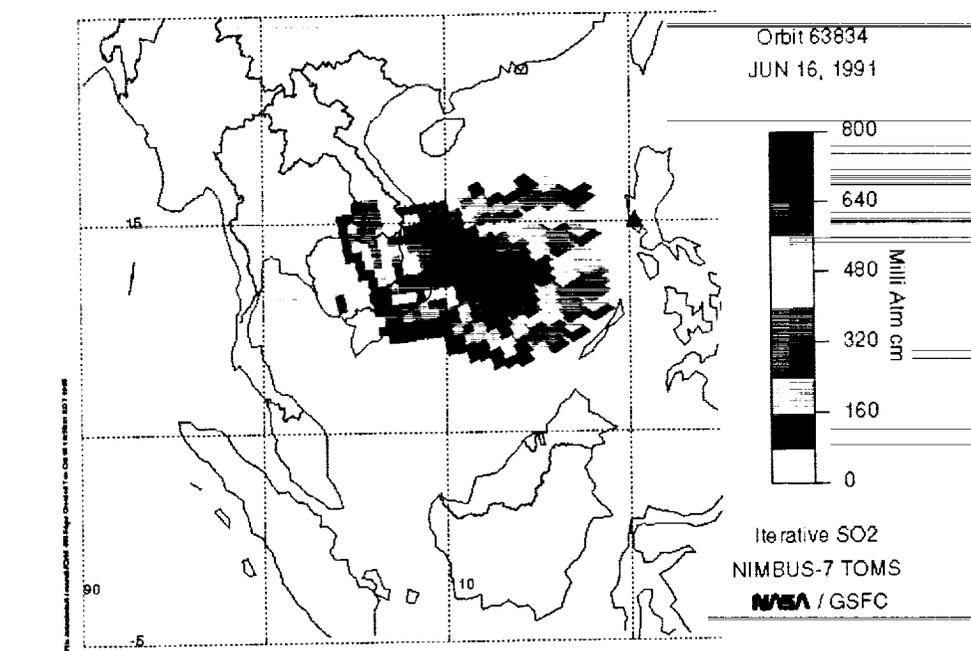


Fig 2.7 This false-color image is from the 16 June 1991 eruption of Mt. Pinatubo, Philippines, showing the released SO_2 . The gas and ash clouds were tracked by TOMS for several weeks as they encircled the Earth. These satellite observations demonstrate the enormous amounts of gas and ash emitted, as well as details such as differences in peak concentrations and geographic extent.
© TOMS Volcanic sulphur dioxide and ash homepage <http://skye.gsfc.nasa.gov/> (Courtesy A. Krueger et al.)

forms. When weighting the ultraviolet frequency spectrum with the sensitivity curve of the human skin, one can obtain a quantity called the “Damaging Ultraviolet”, which serves as an estimate of the risk of skin cancer. UV radiation also degrades certain materials. The amount of ultraviolet radiation reaching the Earth's surface is a function of, among other, the distributions of ozone, aerosols and the cloud coverage. Measurements of these parameters by OMI, can be used to estimate the actual UV flux at the surface. Currently, the quality of the prediction of ultraviolet radiation levels depends on the validity of the assumption that ozone can be treated as a passive tracer within the prediction time range and on the quality of the cloud forecast. Using OMI ozone and aerosol data a short-range UV forecast for the next 2 to 3 days can be undertaken.

It has been shown that satellite observations of SO₂ and sulphate can be used to identify the presence and evolution of volcanic clouds (Stowe et al.; 1992, Krueger et al., 1995, Figure 2.7). In the weeks after a volcanic eruption the emitted SO₂ gas gradually turns into sulphate aerosols. The capability of OMI to detect SO₂ as well as aerosols, i.e., initial and later stages of an eruption, could therefore provide a valuable contribution to the detection of volcanic clouds, which is especially important for the safety of the aviation sector. Some aviation routes pass over a string of volcanoes (viz. the Pacific Rim). It is important that the aviation authorities are warned when eruptions occur and that they are kept informed on the advection and evolution of the volcanic clouds. This application requires a warning system based on SO₂ and aerosol data, as well as the implementation of SO₂ and aerosols as additional prediction parameters in NWP models, thus enabling predictions of the evolution and advection of volcanic clouds. In this way OMI measurements can contribute to the optimisation of route planning for aircraft in such circumstances.

In summary, the main contributions of OMI to the area of operational applications include:

- Daily global ozone columns and daily global ozone profiles in near-real time for use in numerical weather prediction models.
- UV flux forecasts using near-real time ozone columns and aerosol information.
- Detection of volcanic events and evolution of volcanic plumes.

2.3 References

- Braathen, G.O., M. Rummukainen, E. Kyrö, U. Schmidt, A. Dahlback, T. Jørgensen, R. Fabian, V. Rudakov, M. Gil, and R. Borchers, *Temporal development of ozone within the arctic vortex during the winter of 1991/92*, Geophys. Res. Lett., 21, 1407-1410, 1994.
- Brasseur, G.P., J.J. Orlando, and G.S. Tyndell, (eds), *Atmospheric Chemistry and Global Change*, Oxford Univ. Press, New York, USA, 1999.
- Chance, K., P.I. Palmer, R.J.D. Spurr, R.V. Martin, T.P. Kurosu, and D.J. Jacob, *Satellite observations of formaldehyde over North America from GOME*, Geophys. Res. Lett., 27, 3461-3464, 2000.
- Eisinger, M. and J.P. Burrows, *GOME observations of tropospheric sulfur dioxide*, in proceedings ESAMS'99 European Symposium on Atmospheric Measurements from Space, ESTEC, Noordwijk, The Netherlands 18-22 January 1999, ESA WPP 161 ISSN 1022-6656, p. 415-419, March 1999.
- Eskes, H.J., A.J.M. Piters, P.F. Levelt, M.A.F. Allaart and H.M. Kelder, *Variational assimilation of total-column ozone satellite data in a 2D lat-lon tracer-transport model*, J. Atmos. Sci., 56, 3560-3572, 1999.
- Farman, J.C., B.G. Gardiner and J.D. Shanklin, *Large losses of total ozone in Antarctica reveal seasonal seasonal ClO_x/NO_x interaction*, Nature, 315, 207-210, 1985.
- Fortuin, J.P.F. and H.M. Kelder, *An ozone climatology based on ozonesonde and satellite measurements*, J. Geophys. Res., 103, 31709-31734, 1998.
- von der Gathen, P., M. Rex, N. R. P. Harris, D. Lucic, B. M. Knudsen, G. O. Braathen, H. De Backer, R. Fabian, H. Fast, M. Gil, E. Kyrö, I. St. Mikkelsen, M. Rummukainen, J. Stähelin and C. Varotsos, *Observational evidence for chemical ozone depletion over the Arctic in winter 1991-92*, Nature, 375, 131-134, 1995.
- Gonzalez, C.R., J.P. Veefkind and G. de Leeuw, *Aerosol optical depth over Europe in August 1997 derived from ATSR-2 data*, Geophys. Res. Lett., 27, 955-958, 2000
- Intergovernmental Panel on Climate Change (IPCC), *Climate change 1994 - Radiative forcing of climate change*, edited by Houghton, J., Filho, L. G. M., Bruce, J., Lee, H., Haites, E., Harris, N. and Maskell, K., p. 1-231. Cambridge Univ. Press, 1995.
- Intergovernmental Panel on Climate Change (IPCC), *Climate Change 1995 - The Science of Climate Change*, edited by Houghton et al., Camb. Univ Press, 1996.
- Jeuken, A.B.M., H.J. Eskes, P.F.J. van Velthoven, H. M. Kelder and E.V. Hólm, *Assimilation of total ozone satellite measurements in a three-dimensional tracer transport model*, J. Geophys. Res., 104, 5551-5563, 1999.
- Krueger, A.J., L.S. Walter, P.K. Bharthia, C.C. Schnetzler, N.A. Krotkov, I. Sprod and G.J.S. Bluth, *Volcanic sulfur dioxide measurements from the total ozone mapping spectrometer instruments*, J. Geophys. Res., 100, 14057-14076, 1995
- Levelt, P.F., M.A.F. Allaart and H. Kelder, *On the assimilation of total ozone satellite data*, Ann. Geophys., 14, 1111-1118, 1996.
- Logan, J. A. (1), *An analysis of ozonesonde data for the troposphere: Recommendations for testing three-dimensional models and development of a gridded climatology for tropospheric ozone*, J. Geophys. Res. Vol. 104, No. D13, p. 16-115, 1999.
- Logan, J. A. (2), *An analysis of ozonesonde data for the lower stratosphere: Recommendations for testing models*, J. Geophys. Res. Vol. 104, No. D13, p. 16-151, 1999.
- Randel, J.W. and F. Wu, *Climatology of stratospheric ozone based on SBUV and SBUV/2 data: 1978-1994*, NCAR Techn. Note 412+STR, 137 pp., Nat'l Cent. For Atm. Res. Boulder Colo., 1995
- Shindell, D.T., D. Rind and P. Lonergan, *Increased polar stratospheric ozone losses and delayed eventual recovery due to increasing greenhouse gas concentrations*, Nature, 392, 1998.
- Stowe, L.L., R.M. Carey, and P.P. Pellegrino, *Monitoring of the Mt. Pinatubo aerosol layer with NOAA/11 AVHRR data*, Geophys. Res. Lett., 19, 159-162, 1992.
- Wauben, W.M.F., R. Bintanja, P.J.F. van Velthoven and H. Kelder, *On the magnitude of transport out of the Antarctic polar vortex*, J. Geophys. Res., 102, 1229-1238, 1997.
- World Meteorological Organisation (WMO), *Scientific Assessment of Ozone Depletion*, 1999.

Chapter 3 Scientific Requirements

3.1 Introduction

In this chapter the scientific requirements for OMI are identified. Requirements on accuracy, frequency of observation, coverage, horizontal resolution and, where relevant, vertical resolution are specified for each OMI data product. A summary of these requirements for each OMI data product is given in Table 3.1.

The requirements have been derived from the OMI mission objectives as described in Chapter 2. One of the objectives of the OMI mission requires a continuation of the TOMS data record. It is therefore necessary that ozone columns are retrieved using the TOMS algorithm (McPeters et al, 1996).

The products, which shall be retrieved by OMI (SR 3.1.1 – SR 3.1.14) to fulfil the OMI mission objectives and which shall be available directly after launch (priority ‘A’ products) (**Definition 3.1.1**), are:

- Earth radiance and solar irradiance
- Ozone (total column and profile, Near Real Time (NRT) total column and profile and Very Fast Delivery (VFD) total column)
- Aerosol optical thickness and aerosol single scattering albedo
- NO₂ total column
- Cloud scattering pressure and cloud fraction
- Surface UV-B flux and VFD Surface UV-B flux

Desirable products from OMI (SR 3.1.15 – SR 3.1.23), aiding in the studies mentioned in Chapter 2, but which are not necessarily available directly after launch (priority ‘B’ products) (**Definition 3.1.2**), are:

- SO₂ total column
- BrO total column
- HCHO total column and VFD HCHO total column
- OCIO total column
- UV spectra and VFD UV spectra
- VFD Ozone profile
- Surface reflectance

Furthermore, it appears to be feasible to retrieve tropospheric columns of O₃ and NO₂ by (among others) synergetic use of HIRDLS, TES, MLS and OMI. This possible use of OMI data should be kept in mind in the definition of the requirements (SR 3.1.24 and SR 3.1.25).

In the subsequent sections the scientific requirements for all products are defined.

3.2 Requirements for the data products of OMI

The next sections include the scientific requirements for the OMI data products, derived from the OMI Mission Objectives formulated in Chapter 2. Requirements are defined on accuracy, frequency of observation, coverage, horizontal resolution and, where relevant, vertical resolution. The accuracy is defined, roughly, as the combination of all random and systematic errors with *known* magnitude. The reason for this is that it should be possible to test whether the requirements given here will be met.

The pragmatic definition of the accuracy therefore is: the RMS difference between 1) product values retrieved from simulated (“measured” and calibrated) theoretical Earth radiance spectra generated with a state of the art radiative transfer model (including well-defined atmospheres) and 2) the input product values used for the generation of these spectra. The theoretical spectra should be fed into instrument simulation

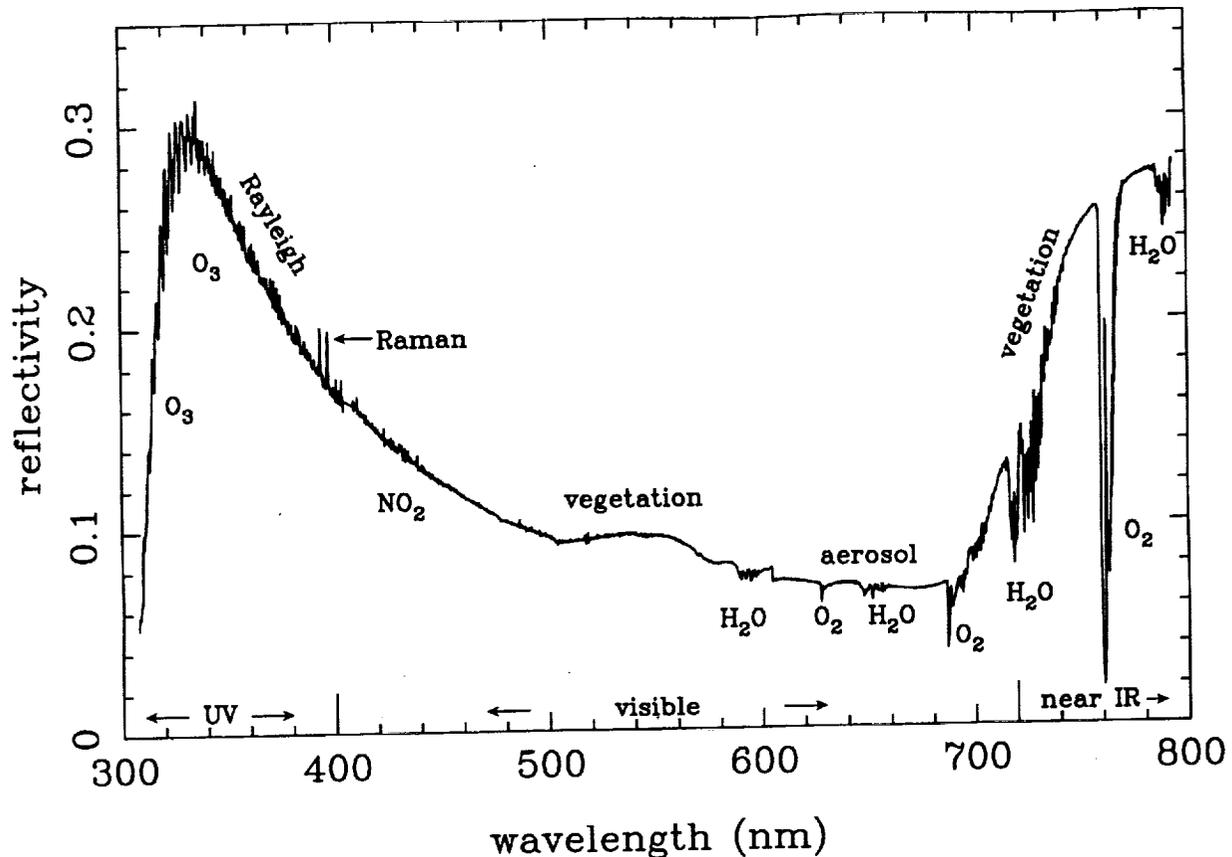


Fig. 3.1 A cloud free reflectivity spectrum observed with GOME on 25 July 1995 above The Netherlands (Stammes and Piters, 1996)

software (“measured”), with all known error sources included; and calibrated with level 0-1b available directly after launch software (**Definition 3.2.1**).

Hence the accuracy is determined by systematic and random errors in the retrieval and calibration algorithms, and by systematic and random errors associated with the measurement technique. Note that this definition of accuracy is different from the usual definition (i.e. the average difference between the retrieved value and the “true” value). Many known systematic and random error sources with unknown magnitude, such as interference due to partially cloudy scenes, are not included in the present definition (i.e. **Definition 3.2.1**) of the accuracy.

All requirements will be summarised in Table 3.1.

3.2.1 Requirements for ozone

Below, the scientific requirements for ozone are identified from the OMI mission objectives (see Chapter 2). For each of the three objectives the requirements on ozone are derived separately. These are combined afterwards to produce overall requirements for ozone.

3.2.1.1 The ozone layer and its possible recovery

In order to extend the TOMS & GOME ozone record, the accuracy of the ozone column measurement should be better than 2%. Long-term ozone trend analysis can then benefit from earlier global ozone measuring instruments such as TOMS, GOME and SCIAMACHY. Since the ozone trend will be analysed on a global scale, or on different parts of the Earth, the OMI column measurements have to cover the whole globe. Requirements on the spatial and temporal resolution of ozone measurements are set by the analysis of correlations with circulation, stratospheric particle loading, PSC occurrence and temperature. A horizontal resolution of $50 \times 50 \text{ km}^2$ for the ozone column is useful for this. Since the ozone decrease in the polar

regions are most pronounced between 15 and 25 km, the ozone profile from OMI shall be able to discern the ozone in this range from ozone above and below it. This sets a requirement on the vertical resolution of better than 10 km in this altitude region. In the upper stratosphere, between 40 and 45 km, a global scale reduction occurs. To be able to measure this decrease a vertical resolution of about 5 km is minimally required in this region. The required accuracy for the mixing-ratio of ozone in the stratosphere amount 10%. The temporal resolution shall be daily to be able to follow the course of the relevant meteorological processes.

3.2.1.2 Tropospheric pollution

Information on the tropospheric ozone is contained in the ozone profile product and also in the ozone column. Ozone column measurements can be useful for studies of plumes from areas of biomass burning and industrial activities, and following the development over years in regions of large increases in emissions (developing countries). The ozone profile shall have a vertical resolution of at least 10 km in the lowest part of the atmosphere to deliver a reliable tropospheric column.

The ozone column measurements can be useful for tropospheric studies due to the larger spatial variability of the tropospheric column compared to the column in the stratosphere. Hot spots of pollution can be distinguished from a map of column measurements if the hot-spot tropospheric column is a high-enough fraction of the total column and the spatial extension of the polluted area is large enough. A typical difference in tropospheric column between a polluted and an unpolluted region is 30 DU, with a horizontal extension of typically $40 \times 40 \text{ km}^2$. This sets a combined requirement on accuracy and horizontal resolution of 10 DU and $40 \times 40 \text{ km}^2$ respectively.

Large cloud-cover impedes the detection of ozone below the cloud deck. This part of the tropospheric column is, for pollution events, the principal part. Using smaller ground pixels increases the probability of a small enough cloud fraction for tropospheric studies. A ground-pixel size of $20 \times 20 \text{ km}^2$ for the column measurements is small enough to greatly improve presently available data on tropospheric ozone (Kerridge et al., 2000).

3.2.1.3 Climate Change

Since ozone is an important climate gas its spatial and temporal variability needs to be established on a global scale. Measured ozone profiles assimilated in dynamical models will improve on this knowledge if the vertical resolution in the stratosphere is good enough to resolve the vertical structure of ozone, which is typically 5 km. The required accuracy of the mixing-ratio of ozone in the stratosphere amounts to 10%. The requirement on horizontal resolution is not strict: $100 \times 100 \text{ km}^2$ is enough. Daily measurements are required to be able to follow the dynamical processes. Global coverage is essential.

Another dynamical issue is the leakage of the polar vortex. The leakage below 16 km needs to be discerned from the measurements, requiring the profile to distinguish between the region below and above 16 km. The horizontal scale of the filaments, braking-off from the vortex, requires a pixel size of $40 \times 40 \text{ km}^2$ and an accuracy of 10% for the ozone mixing ratio at the altitude of these structures, i.e. in the lower stratosphere.

Stratosphere-troposphere exchange occurs on a global scale, demanding global coverage. The process can be monitored if the vertical resolution and the accuracy of the ozone profile is good enough to distinguish between the ozone column in the tropospheric and the lower stratosphere. This gives a vertical resolution of 5–10 km at the tropopause and a target accuracy of 30% on the tropospheric and lower-stratospheric column amounts.

The duration of dynamical events requires daily measurements.

3.2.1.4 Combined requirements for ozone products

These are the most stringent requirements for ozone following from the previous sections.

Ozone profile

Ground-pixel size	:	$40 \times 40 \text{ km}^2$
Vertical resolution	:	10 km in the troposphere, about 5 km in the stratosphere
Accuracy of mixing ratio	:	30% in the troposphere, 10 % in the stratosphere
Coverage	:	global
Frequency of observation	:	daily

Ozone column

Ground-pixel size	:	20 × 20 km ²
Accuracy of column	:	2% / 4 DU
Coverage	:	global
Frequency of observation:		daily

3.2.2 Requirements for other gases.

Based on the mission objectives, as formulated in Chapter 2, total vertical column densities are needed for the trace gases NO₂, SO₂ and BrO on a global scale and with a daily frequency.

NO₂ plays an important role in ozone chemistry and indicates tropospheric pollution. NO₂ vertical column densities are typically between 10¹⁵ and 10¹⁶ cm⁻² (Mazière et al., 1998; Leue et al., 1999). To be able to detect variations in tropospheric NO₂, the accuracy has to be better than 10¹⁴ cm⁻². To be able to detect NO₂ caused by industrial pollution a ground pixel size of at most 40 × 40 km² is required, with a smaller ground pixel desired. For unpolluted areas an accuracy of 10% is feasible, however, for polluted areas the accuracy will be about 20%, due to difficulties in determining the air mass factor (Leue et al., 1999, see also Figure 3.2).

The observations of SO₂ (an aerosol precursor) are important to monitor volcanic eruptions and industrial pollution. Volcanic eruptions will result in column densities of 2 DU up to 700 DU (Bluth et al., 1997) depending on the size of the eruption. The presence of aerosols and elevated levels of SO₂ can distinguish volcanic clouds from other cloud types.

The tropospheric background column density of SO₂ is usually low, between 0.2 and 0.6 DU, as SO₂ is a very reactive gas and removed within days (Eisinger and Burrows, 1999). It is therefore also highly variable. The industrial pollution can be up to a few DU (Eisinger and Burrows, 1999). In order to distinct variations in the industrial SO₂ pollution, the accuracy for the vertical column should be more than 0.4 DU and the ground pixel size shall be 40 × 40 km² at most.

One of the important purposes of monitoring SO₂ related to volcanic activity is for aircraft routing. For this application the product has to be delivered within 3 hours (Near-Real-Time) and the accuracy has to be at least 2 DU.

BrO is an important trace gas in the chemical cycle of ozone in the stratosphere. The vertical column densities of BrO are typically between 3 and 6 · 10¹³ cm⁻² (Chance, 1998; Hegels et al., 1998) with little

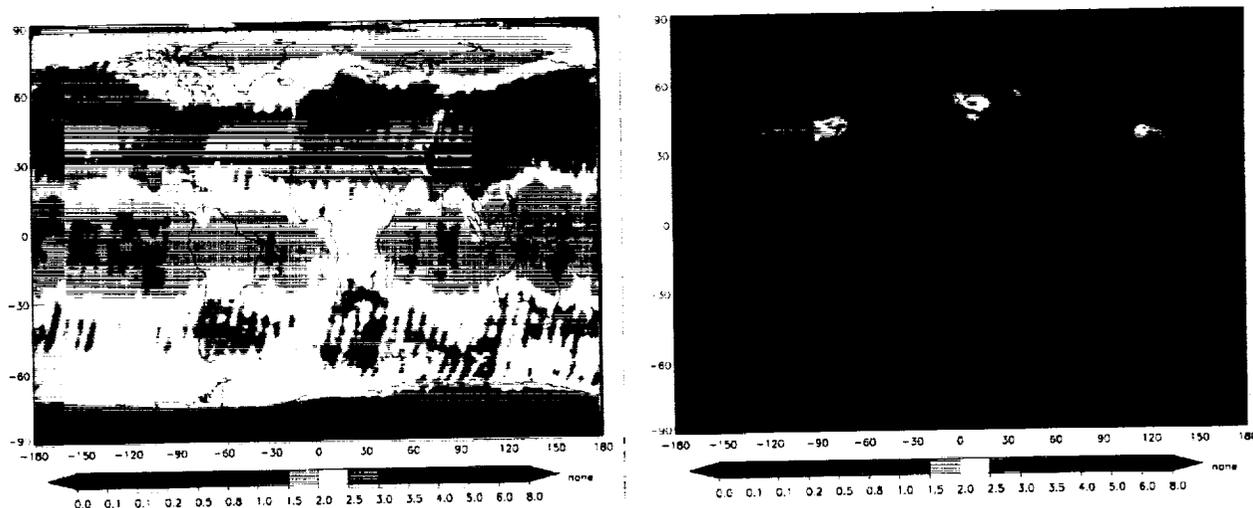


Fig. 3.2 Left figure: monthly average over March 1997 of NO₂ measured by GOME. (in 10¹⁵ molecules / cm²) The tropospheric NO₂ column in the right figure was determined after subtraction of stratospheric NO₂, assuming that the measured NO₂ above the oceans consists only of stratospheric NO₂ and after correction for the reduced sensitivity of GOME in the troposphere (see Leue et al., 1999). With courtesy of M. Wenig, University of Heidelberg and H. Eskes, KNMI

variation, except for tropospheric blooming events in polar springtime where column densities $> 10^{14}$ are observed (Chance, 1998). To monitor BrO an accuracy of 10^{13} cm^{-2} is required for a pixel size of $40 \times 40 \text{ km}^2$.

Other trace gases, which can be measured with OMI, are HCHO and OCIO. OCIO plays an important role in the stratospheric chemistry of the ozone cycle, while HCHO is a tracer of biomass burning and biogenic activity.

Because the absorption features of OCIO have strong overlaps with the ozone absorption bands, OCIO can probably only be observed under ozone hole conditions. Under these conditions the solar zenith angle is usually very high, typically higher than 80° . The OCIO slant column densities are between $2 \cdot 10^{13}$ and $4 \cdot 10^{14} \text{ cm}^{-2}$ for solar zenith angles higher than 80° (Wagner et al., 1999). Therefore, the accuracy has to be at least 10^{13} cm^{-2} for OCIO vertical column density under ozone hole conditions.

HCHO has a vertical column density between 10^{15} and $3 \cdot 10^{16} \text{ cm}^{-2}$ under polluted circumstances (Chance et al., 2000; Thomas et al., 1998; Perner et al., 1997). The accuracy has to be 10^{15} cm^{-2} under these conditions.

3.2.3 Requirements for aerosol optical thickness and aerosol single scattering albedo

The aerosol optical thickness is the extinction by aerosols integrated over a vertical path from the surface to the top-of-the-atmosphere. The aerosol optical thickness is used as a measure of total aerosol load, whereas the spectral variation of the aerosol optical thickness the Ångström exponent, contains information on the aerosol size distribution. The single scattering albedo is the relative contribution of scattering to the aerosol optical thickness and is used as measure for the absorption by aerosols.

Retrieval of aerosol properties is only possible for cloud-free areas. The pixel size for aerosol retrieval should ideally be as small as possible, because of the large spatial variations of aerosol properties and to avoid clouds, but $20 \times 20 \text{ km}^2$ will be sufficient.

To be able to detect trends in the background aerosol, the accuracy has to be smaller than the background level for tropospheric aerosols over the oceans. Therefore, the needed accuracy of the aerosol optical thickness is 0.05 in mid-visible (550 nm), which corresponds to approximately 0.08 at 400 nm. However, because of the difficulties of aerosol retrieval over land, any aerosol information over the continents is valuable. For the single scattering albedo, an accuracy of 0.1 is aimed for. In addition, to the extent possible, it is important that the aerosol size distribution and particle optical properties are retrieved (Penner et al., 1994).

3.2.4 Requirements for clouds

Cloud information is needed in most of the OMI trace gas and aerosol retrieval algorithms. It shall be generated from the OMI level 1 data as an input parameter for OMI level 1-2 processing. Cloud information from OMI is also needed by TES on board EOS-Aura. Furthermore, global cloud information is in itself an important climate parameter. However, the spatial and temporal resolution requirements for the climate aspect would be too restrictive.

The needed cloud information consists of two main parameters: cloud fraction (i.e., fractional coverage by clouds, see Figure 3.3) and cloud scattering pressure. Cloud information shall be retrieved on at least the same scale as the smallest ground pixel of any of the OMI data products (a spatial resolution of $20 \times 20 \text{ km}^2$ will be sufficient) (SR 3.2.4.1). The cloud scattering pressure, defined as the cloud top pressure as determined from scattered light in the UV-visible range, shall have an accuracy better than 100 hPa to be able to estimate "ghost"-column amounts of ozone and to be used in ozone profiles. Several products (e.g. aerosol optical thickness) use cloud free pixels. To be able to create an accurate cloud mask, the cloud fraction should be more accurate than 0.1.



Fig. 3.3 GOME PMD measurements on 2 September 1995 with a $20 \times 40 \text{ km}^2$ resolution. OMI will be able to retrieve clouds and aerosols with a similar resolution, but with daily global coverage. (Figure with courtesy of R. Koelemeijer, KNMI)

3.2.5 Requirements for surface UV-B flux

There is an inverse relationship between ozone and ultraviolet radiation (UV) reaching the surface of the Earth. Photon energies in the UV have an impact the biosphere and are harmful to DNA. UV-B radiation falls in the wavelength range 280 to 315 nm, which is most strongly controlled by overhead ozone. Satellite UV-B data are shown to be highly accurate but comparisons with ground based measurements are dependent on cloud cover. The high spatial resolution of OMI ($\leq 20 \times 20 \text{ km}^2$) will reduce this problem. Global measurements from space will provide UV-B data in locations that are not available from ground based measurements and can more accurately be used for estimating regional and global UV dosages and trends.

Satellite derived UV-B measurements are not sensitive to the ozone profile shape at solar zenith angles less than 70 degrees, but are slightly sensitive to tropospheric ozone. Satellite data has shown a trend in UV-B at mid latitudes consistent with ozone trends. Cloud cover needs to be accounted for in determining trends at any spatial scale. OMI will provide ozone amounts and cloud cover needed to derive UV-B. Absolute accuracy and relative accuracy shall be better than 4% and 2% respectively. Long term trends should be retrievable to better than 0.3%/year.

3.2.6 Requirements for surface reflectance

Surface reflectance is, like cloud information, more or less an auxiliary product that is needed in many OMI level 2 product retrievals, e.g., ozone column, aerosol optical thickness, surface UV-B flux. Also, to determine the cloud fraction the surface reflectance is needed. Furthermore, the surface reflectance is important for the radiation budget of the Earth.

The surface reflectance has to be known with an accuracy of less than 0.01. For surface reflectance values of more than 0.2, the accuracy needs to be less than 5%. In order to avoid cloud contamination the surface reflectance has to be measured with a ground pixel size that will not be more than $20 \times 20 \text{ km}^2$.

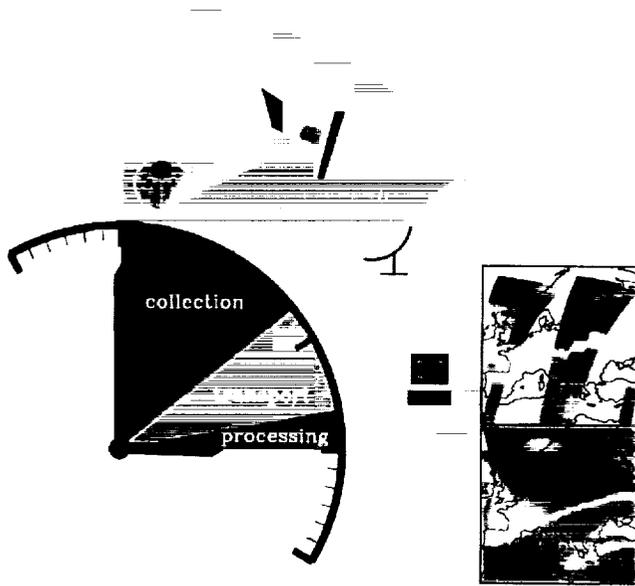


Fig. 3.4 The NRT retrieval time schedule
(Figure with courtesy of A. Piters, KNMI)



Fig. 3.5 Global coverage with the 2600 km wide swath of OMI.
(Figure with courtesy of J.P. Veefkind, KNMI)

3.2.7 Requirements for Near-Real Time (NRT) products

Ozone columns, and stratospheric ozone profiles shall be available within 3 hours after observation (Near-Real Time). SO₂ columns will possibly also be retrieved within 3 hours after observation (Near-Real Time). The ozone columns and profiles shall be accurate enough to be useful in Numerical Weather Prediction. Presently, the estimated needed accuracy is 5% for the ozone columns and 10% for the ozone profiles in the stratosphere (Eskes and Kelder, 1999).

NRT SO₂ columns (with an accuracy of at least 2 DU) can be used for aircraft routing.

Near-Real Time (NRT) products shall be available within 3 hours after observation (SR 3.2.7.1). NRT products shall have the same ground pixel size as the off-line products (SR 3.2.7.2) and also have a global coverage in one day (SR 3.2.7.3). See Figure 3.4 for time schedule of the retrieval of NRT products

3.2.8 Requirements for Very-Fast Delivery (VFD) products

As the VFD products are experimental and not intended to be official products in the NASA sense, the requirements stated here should be taken as guidelines, rather than hard requirements, with the exception of the requirement of a download of OMI data (gathered above Europe and Scandinavia) on one ascending pass per day over Finland (SR 3.2.8.1). In general, since the uses for the products are similar to the off-line products, the requirements are similar. OMI data shall be broadcast to the FMI ground station at Sodankylä on one ascending pass per day, while the spacecraft is in site of the ground station. VFD products shall be available within 30 minutes after the reception of the data (SR 3.2.8.2).

Requirements for the VFD products

Ozone column densities:

Ground pixel size	:	20 × 20 km ² .
Accuracy of column density	:	5% or 10 D.U., whichever is larger.
Coverage	:	2600 km swath above the region from the Alps to the Arctic Ocean.
Frequency	:	daily (Cf. SR 3.2.8.1 and SR 3.2.8.2).

Ozone vertical profiles:

Ground pixel size	:	40 × 40 km ² .
Vertical resolution	:	about 5 km in the stratosphere.
Accuracy of mixing ratio	:	10% in the stratosphere.
Coverage and frequency	:	as for the VFD ozone column densities.

UV radiation (includes Surface UV-B flux and UV spectra)

Ground pixel size	:	20 × 20 km ²
Accuracy (Surface UV-B flux)	:	10%
Accuracy (UV spectra)	:	10-20%, depending on wavelength.
Coverage and frequency	:	as for the VFD ozone column densities.

Formaldehyde (HCHO) column density:

Ground pixel size	:	40 × 40 km ² .
Accuracy	:	20%
Coverage and frequency	:	as for the VFD ozone column densities.

3.3 Requirements for global coverage

OMI shall be able to achieve global coverage in one day (**SR 3.3.1**) (see Figure 3.5). Global coverage means that OMI shall be able to measure the UV/VIS spectrum reflected from every part on Earth within 24 hours, except for regions which are not illuminated by sunlight in 24 hours. (**SR 3.3.2, Definition 3.3.1**) The global coverage shall be possible with the ground pixel sizes as specified in Table 3.1 and a ground pixel sampling equal to the ground pixel sizes (**SR 3.3.3 & SR 3.3.4**).

For solar zenith angles between 85 and 90 degrees, the requirements in Table 3.1 for the ground pixel size for ozone, NO₂, SO₂, HCHO, aerosol, cloud products and the surface reflectance can be slightly relaxed, in order to measure with sufficient S/N while maintaining the same accuracy. In these circumstances, a relaxation of the ground pixel size to 100 × 100 km² can be acceptable (**SR 3.3.5**).

Note that the data for large solar zenith angles still have a high scientific value. During polar spring the ozone hole is only visible at large solar zenith angles, while it is important to be able to observe the complete polar region in this period. For very large solar zenith angles the ozone column retrieved from the visible spectrum will probably be more accurate than from the UV spectrum. On the other hand, some minor stratospheric trace gases as BrO and OCIO can be retrieved better for large solar zenith angles and low ozone concentrations. For BrO and OCIO the requirements in Table 3.1 are applicable for all solar zenith angles (**SR 3.3.6**).

3.4 Summary of the scientific requirements

In Table 3.1 (**SR 3.4.0**) the scientific requirements for all products are summarised:

SR 3.4.0 *The general product requirements are given in SR 3.1.1 - SR 3.3.6 and SR 4.0.1 (i.e. the priority requirements are given in SR 3.1.1 – SR 3.1.25; the coverage requirements are given in SR 3.2.7.3, SR 3.2.8.1 and in SR 3.3.1 – SR 3.3.6; the product availability requirements are given in SR 3.2.7.1, SR 3.2.8.2 and in SR 4.0.1).*

The product depended requirements are given in SR 3.4.1 – SR 3.4.23 (i.e. the accuracy, ground pixel size at nadir and vertical resolution requirements).

3.5 References

- Bluth G.J.S., W.I. Rose, I.E. Sprod and A.J. Krueger, *Stratospheric loading of sulfur from explosive volcanic eruptions*, *J. of Geology*, 105, 671-683, 1997.
- Chance, K., *Analysis of BrO Measurements from the Global Ozone Monitoring Experiment*, *Geophys. Res. Lett.* Vol. 25, No. 17, 3335-3338, 1998.
- Chance, K., P.I. Palmer, R.J.D. Spurr, R.V. Martin, T.P. Kurosu, and D.J. Jacob, *Satellite Observations of Formaldehyde over North America from GOME*, *Geophys. Res. Lett.* 27, 3461-3464, 2000.
- Eisinger, M. and J.P. Burrows, *GOME observations of tropospheric sulfur dioxide*, in proceedings ESAMS'99 European Symposium on Atmospheric Measurements from Space, ESTEC, Noordwijk, The Netherlands 18-22 January 1999, ESA WPP 161 ISSN 1022-6656, p. 415-419, March 1999.
- Eskes, H.J., and H.M. Kelder, *Proceedings of the SODA workshop on Chemical Data Assimilation KNMI, De Bilt, The Netherlands, 9-10 December 1998*. Edited by A. Stoffelen. KNMI publication 188, 1999.
- Hegels, E., P.J. Crutzen, T. Klüpfel, D. Perner and J.P. Burrows, *Global distribution of atmospheric bromine-monoxide from GOME on earth observing satellite ERS-2*, *Geophys. Res. Lett.* Vol. 25, No. 16, 3127-3130, 1998.
- Kerridge et al, *Final Report on "Definition of Observational Requirements for Support of Future Earth Explorer Atmospheric Chemistry Mission (ACE)"*, ESA contract No.: 1-3379/98/NL/GD, to appear in 2000.
- Leue, C., T. Wagner, M. Wenig, U. Platt and B. Jähne, *Determination of the tropospheric NO_x Source Strength from GOME data*, in proceedings ESAMS'99 European Symposium on Atmospheric Measurements from Space, ESTEC, Noordwijk, The Netherlands 18-22 January 1999, ESA WPP 161 ISSN 1022-6656, p. 385-389, March 1999.
- Mazière, M. de, M. van Roozendaal, C. Hermans, P.C. Simon, P. Demoulin, G. Roland and R. Zander, *Quantitative evaluation of the post-Mount Pinatubo NO₂ reduction and recovery, based on 10 years of Fourier transform infrared and UV-visible spectrometric measurements at Jungfraujoch*, *J. Geophys. Res.*, 103, 10849-10858, 1998.
- McPeters, R.D. et al, *Nimbus-7 Totale Ozone Mapping Spectrometer (TOMS) Data Products User's Guide*, NASA Reference Publication 1384, April 1996.
- Penner, J., et al., *Quantifying and Minimizing Uncertainty of Climate Forcing by Anthropogenic Aerosols*, *Bulletin of the American Meteorological Society* Vol 75, No3, 375-401, 1994.
- Perner, D., T. Klüpfel, Hegels, E., P.J. Crutzen and J.P. Burrows, *First Results on Tropospheric Observations by the Global Ozone Monitoring Experiment, GOME, on ERS 2*, Proceedings of the 3rd ERS-2 Users Conference, Florence, Italy, 1997.
- Stammes, P. and A.J.M. Pijters (Eds), *GOME validation at KNMI and collaborating institutes*, p. 10, Scientific Report WR96-08, KNMI, De Bilt, 1996.
- Thomas, W., E. Hegels, S. Slijkhuis, R. Spurr and K. Chance, *Detection of biomass burning combustion products in Southeast Asia from backscatter data taken by the GOME spectrometer*, *Geophys. Res. Lett.* Vol. 25, No. 9, 1317-1320, 1998.
- Wagner, T., K. Pfeilsticker, C. Leue, U. Platt, *Measurements of Atmospheric BrO and OCIO by GOME*, in proceedings ESAMS'99 European Symposium on Atmospheric Measurements from Space, ESTEC, Noordwijk, The Netherlands 18-22 January 1999, ESA WPP 161 ISSN 1022-6656, p. 415-419, March 1999.

Table 3.1 Overview of the scientific requirements for the priority 'A' and 'B' OMI data products.

In column 2, priorities are listed for each product (in the context of the OMI mission objectives): Priority A indicates highest (at launch availability) priority, priority B is assigned to desired (post launch availability) products. All products are level 2 products, except the (ir)radiance which are level 1b products. Each product has a global coverage of one day, except for the Very Fast Delivery (VFD) products. Product delivery requirements are for Near Real Time (NRT) products less than 3 hours after observation and less than 30 minutes after the data receipt for the VFD products, for other products less than two days after observation. The accuracy is defined in the introduction of section 3.2.

With column 3 is meant the vertical column. (T) stands for "in the troposphere", (S) stands for "in the stratosphere". 1 DU \equiv 2.687 10^{16} mol./cm². mol. stands for molecules.

Data product	Priority status	Accuracy of observations ¹⁾	Ground pixel size at nadir (km x km)	Vertical resolution (km)	Remarks
Irradiances ^{2), 3)}	A	$\leq 2\%$	N/A	N/A	
Radiances ²⁾	A	$\leq 2\%$	$\leq 20 \times 20$	N/A	
Ozone column	A	$\leq 2\% / 4$ DU	$\leq 20 \times 20$	N/A	
Ozone profile	A	$\leq 30\%$ (T) $\leq 10\%$ (S)	$\leq 40 \times 40$	≤ 10 km (T) ≥ 5 km (S)	Vertical range is 0-50 km
Aerosol optical thickness	A	$\leq 10\% / 0.08$	$\leq 20 \times 20$	N/A	At 400 nm
Aerosol single scattering albedo	A	0.1	$\leq 20 \times 20$	N/A	
NO ₂ column ⁴⁾	A	$\leq 10\% / 10^{14}$ mol. cm ⁻²	$\leq 40 \times 40$	N/A	
Cloud scattering pressure	A ⁵⁾	≤ 100 hPa	$\leq 20 \times 20$	N/A	
Cloud fraction	A ⁵⁾	≤ 0.1	$\leq 20 \times 20$	N/A	
Surface UV-B flux	A	$\leq 4\%$	$\leq 20 \times 20$	N/A	
SO ₂ column	B	$\leq 20\% / 0.4$ DU	$\leq 40 \times 40$	N/A	Pollution, volcanic
BrO column	B	$\leq 10\% / 10^{13}$ mol. cm ⁻²	$\leq 40 \times 40$	N/A	
OCIO column	B	$\leq 20\% / 10^{13}$ mol. cm ⁻²	$\leq 40 \times 40$	N/A	Polar vortex
HCHO column	B	$\leq 20\% / 10^{15}$ mol cm ⁻²	$\leq 40 \times 40$	N/A	Pollution
Surface reflectance	B	$\leq 5\% / 0.01$	$\leq 20 \times 20$	N/A	
UV spectra	B	$\leq 10-20\%$ (wavelength dependent)	$\leq 20 \times 20$	N/A	Accuracy is wavelength dependent
Near Real Time Products					
Ozone column	A	$\leq 5\% / 10$ DU	$\leq 20 \times 20$	N/A	
Ozone profile	A	$\leq 10\%$ (S)	$\leq 40 \times 40$	≥ 5 km (S)	Vertical range is 10-50 km

Data product	Priority status	Accuracy of observations ¹⁾	Ground pixel size at nadir (km × km)	Vertical resolution (km)	Remarks
<i>Very Fast Delivery Products</i>					
Ozone column	A	≤ 5 % / 10 DU	≤ 20 × 20	N/A	Over Northern Europe
Surface UV-B flux	A	≤ 10 %	≤ 20 × 20	N/A	Over Northern Europe
Ozone profile	B	≈ 10 % (S)	≤ 40 × 40	≥ 5 km (S)	Vertical range is 10-50 km Over Northern Europe
HCHO column	B	≤ 20 % / 10 ¹⁵ mol. cm ⁻²	≤ 40 × 40	N/A	Over Northern Europe
UV spectra	B	≤ 10-20 % (wavelength dependent)	≤ 20 × 20	N/A	Over Northern Europe Accuracy is wavelength dependent

Note 1)

The valid requirement on accuracy will be the largest of the given percentile or absolute number.

Note 2)

The requirements for radiance and irradiance follow from Chapter 4.

Note 3)

Irradiance is not a separate data product.

Note 4)

The required accuracy for the NO₂ column is about 10% in unpolluted areas, but about 20% in polluted areas.

Note 5)

Cloud scattering pressure and cloud fraction are also needed for the retrieval of other products by OMI and other instruments.

Chapter 4 Algorithm Requirements

In this chapter the requirements are given for Level 1b products, which follow from the retrieval algorithms used to produce the Level 2 products. The definition of Level 0, 1b and 2 data is given in Annex II (**Definition 4.0.1 – 4.0.3**). The algorithms shall produce the Level 1b and Level 2 data products with the accuracy and at the data rate described in chapter 3. For the Level 2 products there are requirements on the time between measurement and availability. The off-line level 2 products shall be available less than two days after observation (**SR 4.0.1**), the Near Real Time product within 3 hours after observation (**SR 3.2.7.1**) and the Very Fast Delivery Products within 30 minutes after the data downlink (**SR 3.2.8.2**). The Level 2 products are derived from the Level 1b and other data. Hence, the Level 2 algorithms put requirements on the accuracy and availability of the Level 1b product, as well as on the other ancillary and auxiliary data (see Annex II, **Definition 4.0.4 and 4.0.5**).

4.1 Level 2 retrieval algorithms

4.1.1 Algorithm description

4.1.1.1 DOAS products (Ozone column, NO₂, BrO, SO₂, OCIO and HCHO)

In the Differential Optical Absorption Spectroscopy (DOAS) method, a differential reference absorption cross-section spectrum of the pertinent trace gas is fitted to the differential Earth's reflectivity spectrum (i.e. the Earth radiance spectrum divided by the solar irradiance spectrum), in a certain wavelength window (see Figure 4.1). This yields the slant column density of the trace gas. This slant column density is divided by an air mass factor (calculated with a radiative transfer model) to obtain the vertical column density. A cloud correction procedure is used to account for the invisible column below the clouds. The fact that only differential spectra are needed in the DOAS method, leads to an insensitivity to absolute calibration of the instrument. Relevant references on DOAS and comparable differential absorption methods for trace gas column detection from scattered light are: Noxon (1975); Noxon et al. (1979); Platt (1994); Diebel et al. (1995); and Burrows (1999).

4.1.1.2 Ozone profile

Singer & Wentworth (1957) were the first to realise that from satellite nadir measurements of backscattered solar UV radiation emerging from the Earth atmosphere information on the vertical distribution of ozone can be deduced. Twomey (1961) showed that the ozone profile from a single nadir earthshine spectrum could be retrieved from radiance measurements at different wavelengths in the near-ultraviolet. The strong increase of the ozone absorption cross section, going from 300 nm to 250 nm, causes the backscattered radiance in this spectral interval to originate from decreasing depths in the atmosphere. The atmospheric radiance spectrum in the near-ultraviolet therefore holds information on the vertical distribution of the constituents that absorb and scatter the radiation: mainly absorption by ozone and scattering by air molecules, respectively.

An operational ozone profile retrieval algorithm based on this principle has been developed for the BUUV, SBUV, SBUV/2 and SSBUV experiments (Bhartia et al. (1996); Munro et al. (1998); Hoogen et al. (1999); van der A et al., (1999)) reported ozone profile retrieval algorithms for GOME. The high spectral resolution of GOME has opened the possibility to extract additional profile information from the Huggins band (320-340 nm) caused by the temperature dependence of the ozone cross sections (Chance et al, 1997).

The algorithms for GOME (see Figure 4.2) and SBUV are based on an iterative sequence of inversions of the linearized forward model. The forward model maps the ozone profile to the radiance spectrum; the linearized model, or weighting function, maps changes in ozone to changes in radiance. The inversion is performed using Optimal Estimation (Rodgers, 1976). This method necessitates the use of a priori information on the profile and regularises the inversion to prevent error amplification. These algorithms are quite laborious and time consuming since many radiance and weighting function computations are necessary.

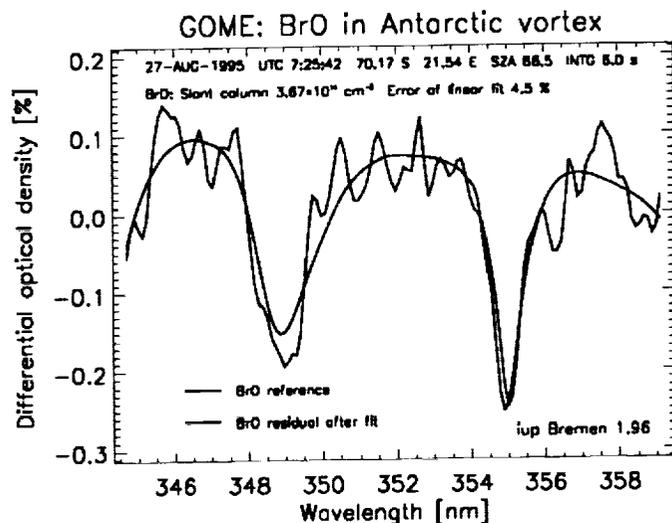
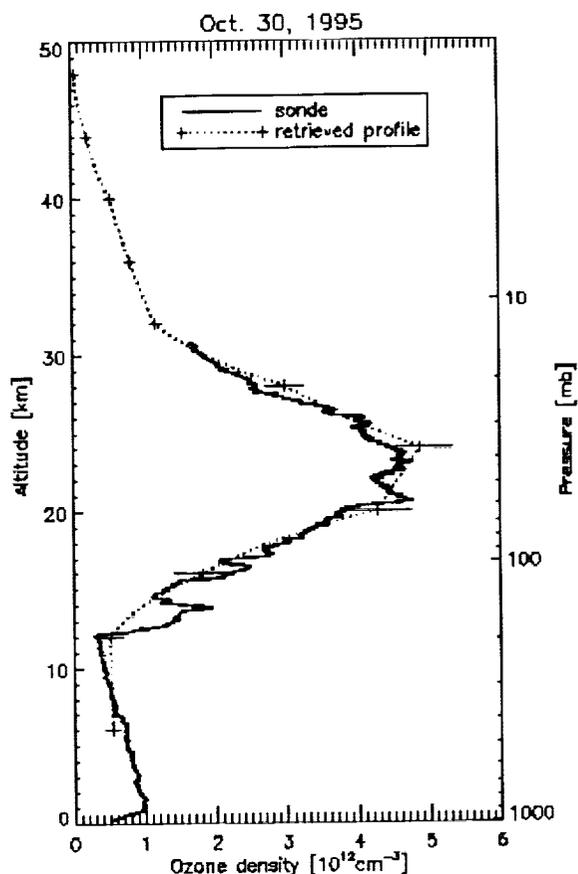


Fig. 4.1 (Above) A slant column retrieval of BrO in the Antarctic vortex on 27 August 1995 from GOME data (Eisinger et al., 1996).

Fig. 4.2 (Right) Retrieved GOME ozone profile (red dotted line) above The Netherlands and ozone sonde measurement (blank line) above KNMI, De Bilt, The Netherlands.



4.1.1.3 Aerosol optical thickness and single scattering albedo

The OMI aerosol retrieval algorithm will determine the aerosol optical thickness and single scattering albedo over the ocean and most land surfaces. The algorithm will be based on experience with GOME and TOMS data. For the OMI algorithm, approximately 18 narrow wavelength bands will be selected in the spectral range between 340 and 500 nm. The selection criteria for these wavelength bands are a minimum of gaseous absorption and minimal disturbance by the Ring effect.

The algorithm only applies to cloud-free regions. For these regions, the measured reflectance for the selected wavelength bands are fitted using radiative transfer computations for different aerosol types and concentrations (Veefkind et al. 2000, Torres et al. 1998, Torricella et al., 1999). For the best-fit aerosol mixture the aerosol optical thickness and single scattering albedo for the wavelength bands are determined.

To account for surface contributions, a climatology for the surface reflectivity is used in these computations. For most land surfaces the albedo is low in the wavelength range between 340 and 400 nm (Herman and Celarier, 1997). Generally the albedo of the ocean is low in the visible and in general increases towards the UV. Therefore, for aerosol retrieval over land, wavelengths below 400 nm should be used, whereas for retrieval over the ocean the longer wavelengths are favorable.

4.1.1.4 Cloud fraction

The cloud fraction c of a ground pixel is derived from the contrast between the surface and a cloud (see Figure 4.3):

$$c = \frac{R_{\text{meas}} - R_{\text{clear}}}{R_{\text{cloud}} - R_{\text{clear}}}$$

Here R_{meas} is the measured reflectivity, R_{clear} is the calculated reflectivity for clear sky, and R_{cloud} is the calculated reflectivity of a completely cloud covered pixel, where an optically thick cloud is assumed as in the TOMS data processing (see e.g. Koelemeijer and Stammes, 1999; Herman et al., 1996). This algorithm yields an effective cloud fraction by assuming an optically thick cloud. R_{clear} will be determined from time series of minimum reflectivity. A possible wavelength for determining c is 380 nm, as is used for TOMS (Herman et al., 1996).

Besides the cloud cover it is also important to get information about the pixel homogeneity. This can be obtained from one or two wavelengths that have a higher spatial sampling than the nominal pixels. By using this sub-pixel information to evaluate the pixel homogeneity, partly cloudy pixels can be discriminated from pixels with a uniform cloud deck.

4.1.1.5 Cloud scattering pressure

The cloud scattering pressure (see Figure 4.4) will be determined from the Ring effect in the Fraunhofer Ca II lines around 394 nm, as has been done for SBUV (Joiner and Bhartia, 1995; Joiner et al., 1995). The Ring effect is the filling-in of Fraunhofer lines in scattered light from the Earth, due to rotational Raman scattering mainly by N₂ and O₂ in the atmosphere. For cloud covered pixels, the stronger the filling-in, the larger the pressure at the top of the clouds. Alternatively, the DOAS method will be applied to the absorption features of the O₂-O₂ collision complex near 477 nm. Experiments with GOME data suggest that both methods are complementary, therefore combining these two methods may result in a more accurately determined cloud scattering pressure (Koelemeijer, R. private communication).

4.1.1.6 Surface UV-B flux and spectra

Surface UV-B fluxes are calculated using a radiative transfer model from total ozone, cloud cover, solar zenith angle, and possibly aerosols (Krotkov et al., 1998 & 2000; Herman et al., 1999).

Surface UV-B flux (VFD): The algorithm to be used for the VFD processing of the surface UV-B flux is the same as described above. In this case, the ozone vertical column density could come from the TOMS ozone or an another fast algorithm.

UV spectra (both VFD & the off-line but global product): This product is a mapping of UV spectra. As it is under development at the current time, a detailed description of the algorithms involved is premature.

4.1.1.7 Surface reflectance

The spectral surface reflectance is determined for cloud-free scenes with a small aerosol load. For a given geographical area and time frame, these correspond to the darkest scenes. The surface reflectance is computed by performing an atmospheric correction on the scene. The atmospheric correction is for Rayleigh scattering, but can also be extended to correct for aerosols and absorption by gases as well. The cloud and aerosol optical thickness algorithms will use the derived surface reflectivity database.

4.1.1.8 TOMS products

Several geophysical products have been derived from NASA's TOMS instrument series starting in November 1978. TOMS measures at 6 discrete wavelengths in the 300-380 nm spectral range. The combination of these wavelengths is used to derive surface reflectivity and total ozone on an operational basis. The algorithm for deriving these products is described in TOMS User's Guide (McPeters et al., 1996). In addition, several

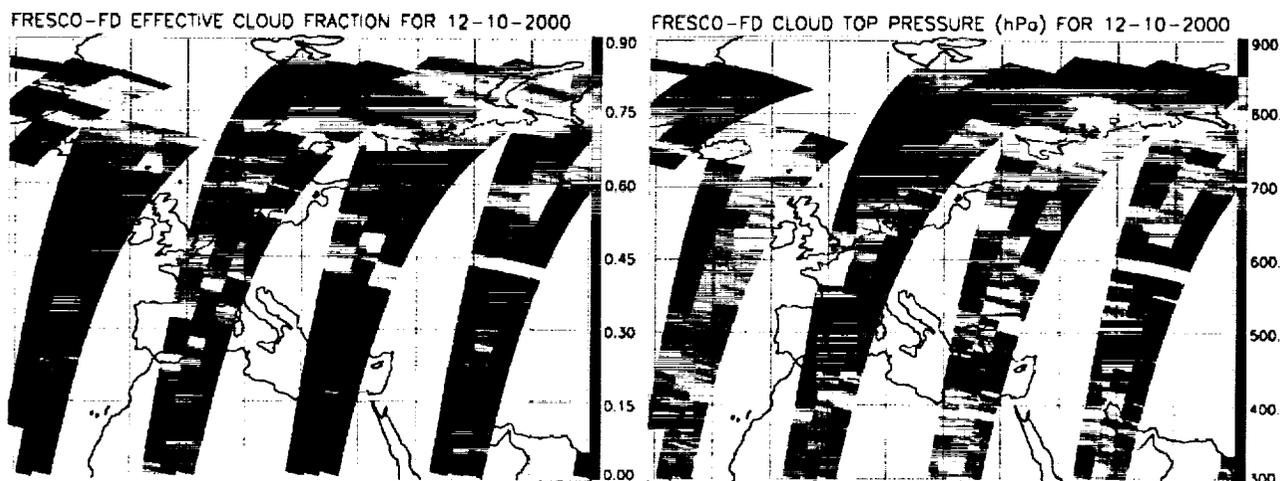


Fig. 4.3 & 4.4 Cloud fraction and cloud top pressure (in hPa), retrieved in NRT from GOME measurements on 12 October 2000. (Courtesy R. Koelemeijer, KNMI, Koelemeijer et al., 2000)

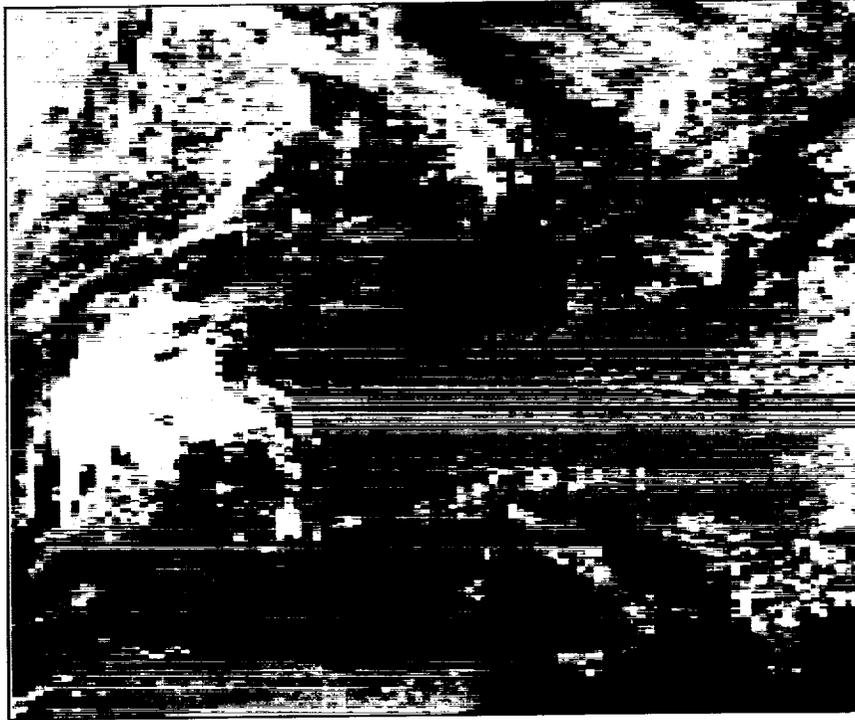


Fig. 4.5 AVHRR channel 2 image over Europe resampled to a grid of approximately $13 \times 40 \text{ km}^2$, to give an impression of the required spatial resolution for OMI.

special products are also produced. These include surface UV-B flux (Krotkov et al., 1998 & 2000; Herman et al., 1999), aerosol optical depth and single scattering albedo (Torres et al., 1998), and tropospheric ozone column (Ziemke et al., 1998).

4.2 Level 1b data products requirements

All Level 2 products will be retrieved from the level 1b products. Therefore, the Level 2 algorithms put requirements on the Level 1b data products. These requirements are identified in this section and are listed in Table 4.1.

4.2.1 Geographical Coverage and Resolution

The Level 1b radiance data shall have daily global coverage (SR 4.2.1.1). The ground pixel size of the Level 1b data shall be $20 \times 20 \text{ km}^2$ at nadir, or smaller (SR 4.2.1.2). For the wavelengths below 310 nm the ground pixel size of the Level 1b data shall be $40 \times 40 \text{ km}^2$ at nadir, or smaller (SR 4.2.1.3). In the Level 1b product, the geolocation of the pixels shall be given, with an accuracy of $1/10^{\text{th}}$ of the ground pixel size (SR 4.2.1.4).

For at least one wavelength per channel, the Level 1b data shall be obtained with a higher spatial sampling than for the nominal pixels (SR 4.2.1.5).

4.2.2 Spectral Range

The spectral ranges that are used by the algorithms described in section 4.1, are listed in Table 4.1. The total spectral range shall at least cover the range between 270 and 500 nm (SR 4.2.2.1). More details can be found in Annex III.

4.2.3 Spectral Resolution and Sampling

For the Level 2 retrieval algorithms the spectral resolution and sampling as listed in Table 5.1 (SR 5.1.1.9 – 5.1.1.15) are sufficient (SR 4.2.3.1), as was tested in several studies (see several of the Annexes).

4.2.4 Spectral Knowledge

Spectral knowledge is defined as the error in the wavelengths assigned to the radiance and irradiance spectra (**Definition 4.2.4.1**). Requirements for the spectral knowledge for specific products were performed. Some of the DOAS products are especially sensitive for shifts in the wavelength scale (Annex IV). The ozone profile is somewhat less sensitive for wavelength shifts. The required spectral knowledge of the radiance and irradiance spectra shall be better than $1/100^{\text{th}}$ of a CCD-pixel above 300 nm and better than $1/50^{\text{th}}$ of a CCD-pixel below 300 nm for ozone profile retrieval. (**SR 4.2.4.1**).

4.2.5 Spectral Stability

Spectral stability is the difference in the wavelength registration of a CCD-pixel between the radiance and irradiance spectra (**Definition 4.2.5.1**). In the retrieval algorithms, the radiance and irradiance data have to be brought onto the same wavelength grid, which involves interpolation. The interpolation to the common wavelength grid introduces errors. This interpolation error increases when differences between the differences between the radiance and irradiance wavelength registration increases. Especially the ozone profile retrieval is very sensitive for such errors. The required spectral stability for Earth and solar measurements is at least $1/20^{\text{th}}$ of a CCD-pixel (see Annex V) (**SR 4.2.5.1**).

4.2.6 Radiometric Precision

The radiometric precision needed for the DOAS product depends on the column density and the amount of structure of the absorption cross section of the specific gas. The required S/N ratios for the DOAS products are described in Annex VI.

S/N ratios are extremely important for O₃ profile retrieval (UV-1 channel). The signal-to-noise ratio below 310 nm affects mainly the retrieval precision in the stratosphere. With a ratio of about 100, the precision is between 5 and 15% in the altitude range from 20 to 50 km.

The required S/N ratios for all products are listed in Table 4.1 (**SR 4.3.1a – SR 4.3.21a**).

4.2.7 Radiometric Accuracy

The physical quantity used by the retrieval algorithms is the ratio of the Earth radiance and the solar irradiance (called the reflectivity (**Definition 4.2.7.1**)) as input. Hence, the radiometric accuracy defined here refers to this ratio. Products that fit the absolute reflectivity, for example for the ozone profile and the aerosol optical thickness, have the most stringent requirements on radiometric accuracy of the absolute reflectivity. When systematic errors in the reflectivity are only weakly dependent on the wavelength, the effects on the DOAS products are limited. The overall requirement for the radiometric accuracy of the reflectivity is 1% (**SR 4.2.7.1**).

4.2.8 Level 1b Product Content

The Level 1b data shall contain radiance and irradiance data, calibration data, geolocation data and metadata. Details of the Level 1b radiance product content and format are given in Annex VII (Veefkind et al, 2000) (**SR 4.2.8.1**).

SR 4.2.8.2 *All Level 1b product content requirements, specified in the latest version of the “OMI Level 1b data format”, shall be applicable.*

4.2.9 Level 1b Product Availability

The level 1b data shall be accessible within 24 hours after arrival of the OMI level 0 at the processing site (**SR 4.2.9.1**). The near-real-time products have a requirement that they shall be available within three hours after observation (**SR 3.2.7.1**). The NRT products are derived from a preliminary version of the Level 1b data. This preliminary version of the Level 1b data has to be available within 2½ hours after observation (**SR 4.2.9.2**). The very fast delivery products shall be available within 30 minutes after the data downlink to

the ground station (SR 3.2.8.2). See “*The Netherlands and Finnish data requirements in the operational phase of OMI*” (Carpay and Mälkki, 2000) (Annex VIII) for more details.

SR 4.2.9.3 *All other Level 1b product availability requirements, specified in the latest version of RS-OMIE-0000-NIVR-007 “The Netherlands and Finnish data requirements in the operational phase of OMI”, shall be applicable.*

4.2.10 Viewing angles: knowledge & precision

The Level 1b-2 algorithms require accurate knowledge of the viewing zenith angle, the solar zenith angle and the relative azimuth angle between the solar and the viewing direction. A requirement on their accuracy can be derived by demanding the computed radiance to be accurate at the 0.1 % level. This derivation can be performed, to a good approximation, by evaluating the sensitivity of the Rayleigh phase function to these three angles for a range of conditions. Therefore, the required accuracy for the solar zenith angle is 0.08° (SR 4.2.10.1), for the viewing zenith angle 0.08° (SR 4.2.10.2) and for the relative azimuth angle 0.05° (SR 4.2.10.3).

4.3 Summary of Level 1b Requirements

In this chapter, the scientific requirements as identified in chapter 3 are translated into requirements on the Level 1b radiance and irradiance products and the reflectivity. In Table 4.1 (SR 4.3.0), these requirements are summarised:

The Level 1b data shall have a pixel size of at most $20 \times 20 \text{ km}^2$. For wavelengths below 310 nm the Level 1b data shall have a pixel size of at most $40 \times 40 \text{ km}^2$. Level 1b data shall be obtained for at least one wavelength with a higher spatial sampling than for the nominal pixels. To be able to derive all the data products listed in table 3.1, a spectral range of at least 270 to 500 nm is required. The spectral resolution and sampling given in Table 5.1 are sufficient. The maximum difference between the wavelength registration for the Earth and solar measurements (spectral stability) shall be $1/20^{\text{th}}$ of a pixel. The error in wavelength registration (spectral knowledge) shall be better than $1/50^{\text{th}}$ of a pixel below 300 nm and better than $1/100^{\text{th}}$ of a pixel above 300 nm. The radiometric accuracy of the ratio of Earthshine radiance and solar irradiance (the reflectivity) shall be better than 1%. The requirements on the radiometric precision (signal-to-noise) depend strongly on the product considered, see Table 4.1. The required accuracy for the solar zenith angle is 0.08° , for the viewing zenith angle 0.08° and for the relative azimuth angle 0.05° . A preliminary version of the Level 1b data shall be available within $2\frac{1}{2}$ hours after observation to derive the Near Real Time products. The Very Fast Delivery products shall be available within 30 minutes after the data downlink to the ground station.

SR 4.3.0 *The general requirements on the Level 1b product are given in SR 4.2.1.1 – SR 4.2.10.3. (i.e. the geographical coverage and resolution requirements are given in SR 4.2.1.1 – SR 4.2.1.5; the spectral (range, resolution, sampling, knowledge and stability) requirements are given in SR 4.2.2.1 – SR 4.2.5.1; the requirement on the overall radiometric accuracy of the reflectivity is given in SR 4.2.7.1; the Level 1b product contents and availability requirements are given in SR 4.2.8.1, SR 4.2.8.2 and SR 4.2.9.1 – SR 4.2.9.3; the knowledge and precision requirements on the viewing angles are specified in SR 4.2.10.1 – SR 4.2.10.3).*

The product depended requirements on the Level 1b product are given in SR 4.3.1 – SR 4.3.21 (i.e. the spectral range, (spectral knowledge), (radiometric accuracy of the reflectivity) and radiometric precision requirements).

4.4 Auxiliary and Ancillary Data Requirements

The Level 2 products are derived from the Level 1b data and other data. Auxiliary data do not originate in the instrument or the satellite platform. The following is a list of auxiliary data needed for the Level 2 algorithms. Detailed information on auxiliary data requirements are given in the “*Auxiliary and Ancillary data requirements document for OMI-EOS*” (Veeffkind [1] et al., 2001).

SR 4.4.1 *All requirements, specified in the latest version of “Auxiliary and Ancillary data requirements document for OMI-EOS”, shall be applicable.*

Auxiliary data for Level 2 algorithms described in section 4.1:

- 1. Atmospheric data**
 - ✓ Meteorological data
 - ✓ Profile data of the species to be retrieved
 - ✓ Cloud coverage and scattering pressure
 - ✓ Spectral Aerosol Optical Thickness
- 2. Surface data**
 - ✓ Spectral surface albedo
 - ✓ Snow and Ice coverage
 - ✓ Terrain height
 - ✓ Chlorophyll concentration
- 3. Spectroscopy data**
 - ✓ Absorption and scattering cross sections of relevant gases and particles
 - ✓ Ring effect source spectrum
 - ✓ OMI instrument transfer function (slit function and CCD pixel response function)

4.5 Level 0-1b processing requirements

The Level 0-1b processing requirements are described in the “*User Requirements Document for the OMI Level 0 to 1b Data Processor (URD)*” (Nugteren, 2000).

SR 4.5.1 *All requirements as specified in the latest version of RS-OMIE-7000-FS-186 “User Requirements Document for the OMI Level 0 to 1b Data Processor”; shall be applicable.*

Table 4.1 Overview of the Level 1b product requirements for the priority 'A' and 'B' OMI data products.

Data product	Spectral Range [nm]	Ground pixel size [km × km]	Spectral knowledge [CCD pixel]	Radiometric accuracy ¹⁾ [%]	Radiometric precision ²⁾ [S/N]
Ozone column	320 – 340	20 × 20	0.01	≤ 3	≥ 250
• DOAS	310 – 380	20 × 20	0.33	≤ 1	≥ 300
• TOMS	270 – 340	40 × 40	0.02	≤ 1	λ < 310 ≥ 100
Ozone profile	340 – 500	20 × 20	not critical	≤ 1	≥ 500
Aerosol optical thickness	340 – 500	20 × 20	not critical	≤ 1	≥ 500
Aerosol single scattering albedo	425 – 450	40 × 40	0.02	≤ 3	≥ 5800
NO ₂ column	390 – 400	20 × 20	0.01	≤ 3	not critical
Cloud scattering pressure	470 – 485	20 × 20	0.01	≤ 3	≥ 1600 ³⁾
Cloud fraction	320 – 500	20 × 20	not critical	≤ 1	not critical
Surface UV-B	280 – 400	20 × 20	not critical	not critical	not critical
SO ₂ column	300 – 330	40 × 40	0.01	≤ 3	≥ 400
BrO column	344 – 360	40 × 40	0.02	≤ 3	≥ 2500
OCIO column	355 – 385	40 × 40	0.01	≤ 3	≥ 1500
HCHO column	335 – 360	40 × 40	0.01	≤ 3	≥ 3200
Surface reflectance	320 – 500	20 × 20	not critical	≤ 1	≥ 100
UV spectra	280 – 400	20 × 20	not critical	not critical	not critical
Near Real Time Products					
Ozone column	320 – 340	20 × 20	0.02	≤ 3	≥ 100
Ozone profile	270 – 340	40 × 40	0.02	≤ 1	λ < 310 ≥ 100
Very Fast Delivery Products					
Ozone column	320 – 340	20 × 20	0.02	≤ 3	≥ 100
Surface UV-B flux	280 – 400	20 × 20	not critical	not critical	not critical
Ozone profile	270 – 340	40 × 40	0.02	≤ 1	λ < 310 ≥ 100
UV spectra	280 – 400	20 × 20	not critical	not critical	not critical
HCHO column	335 – 360	40 × 40	0.01	≤ 3	≥ 3200

Note 1) The radiometric accuracy defined here refers to the reflectivity (i.e. ratio of the Earth radiance and the solar irradiance)

Note 2) S/N requirements are valid for the given ground pixels size in column 3 (i.e. the same ground pixel sizes as in Table 3.1)

Note 3) The most stringent requirement on radiometric precision is given by the method using the 477 nm O₂-O₂ collision complex.

Note 4) A requirement noted as not critical means that other products demand stronger requirements for the Level 1b product.

4.6 References

- Bhartia, P.K., R.D. McPeters, C.L. Mateer, L.E. Flynn, C. Wellemeyer, *Algorithm for the estimation of vertical ozone profiles from the backscattered ultraviolet technique*, J. Geophys. Res. 101, 18,793-18,806, 1996.
- Burrows, J. P., et al., *The Global Ozone Monitoring Experiment (GOME): Mission Concept and First Scientific Results*, J. Atm. Sci., 56, 151-175, 1999.
- Chance, K.V., J.P. Burrows, D. Perner, W. Schneider, *Satellite measurements of tropospheric ozone profiles, including tropospheric ozone, from ultraviolet/visible measurements in the nadir geometry: a potential method to retrieve tropospheric ozone*, J. Quant. Spectrosc. Radiat. Transfer 57, 467-476, 1997.
- Carpay, J. and A. Mälkki, *The Netherlands and Finnish data requirements in the operational phase of OMI*, RS-OMIE-0000-NIVR-007 (version 2.2 of 10 March 2000).
- Diebel, D., J. P. Burrows, R. de Beek, B. Kerridge, L. Marquard, K. Muirhead, R. Munro, and U. Platt, *Detailed Analysis of the Retrieval Algorithms Selected for the Level 1-2 Processing of GOME Data, Final Report*, ESA Contract 10728/94/NL/CN, ESA/ESTEC, Noordwijk, 1995.
- Eisinger, M., J.P. Burrows, and A. Richter, *Studies on the Precision of GOME Irradiance and Radiance Products and GOME Measurements of OCIO and BrO over Antarctica*, in Proc., GOME Geophysical Validation Campaign, ESA WPP-108, pp. 93 - 105, 1996
- Herman, J.R., et al., *Meteor-3 TOMS Data Products User's Guide*, NASA Ref. Publ. 1393, Oct. 1996.
- Herman, J. R. and E. A. Celarier, *Earth surface reflectivity climatology at 340-380 nm from toms data*. J. Geophys. Res., 102: 28003-28011, 1997.
- Herman J.R., N.Krotkov, E.Celarier, D.Larko, and G.Labow, *The distribution of UV radiation at the Earth's surface from TOMS measured UV-Backscattered radiances*, Journ. Geophys. Res., 104, 12059-12076, 1999
- Hoogen, R., V.V. Rozanov, J.P. Burrows, *Ozone profiles from GOME satellite data: Algorithm description and first validation*, J. Geophys. Res. 104, 8263-8280, 1999.
- Joiner, J and P.K. Bhartia, *The determination of cloud pressures from rotational Raman scattering in SBUV measurements*, J. Geophys. Res. D, 100, 23019-23026, 1995.
- Joiner, J., et al., *Rotational Raman scattering (Ring effect) in SBUV measurements*, Appl. Opt. 34, 4513-4525, 1995.
- Koelemeijer, R.B.A., and P. Stammes, *Effects of clouds on the ozone column retrieval from GOME UV measurements*, J. Geophys. Res. D, 104, 8281-8294, 1999.
- Koelemeijer, R.B.A., P. Stammes, J.W. Hovenier and J.F. de Haan, *A fast method for retrieval of cloud parameters using oxygen A-band measurements from the Global Ozone Monitoring Instrument*, J. Geophys. Res. D, in press, 2000.
- Krotkov, N.A., P.K.Bhartia, J.R.Herman, V.Fioletov, J.Kerr, *Satellite estimation of spectral surface UV irradiance in the presence of tropospheric aerosols 1. Cloud-free case*, Journ. Geophys. Res., 103, 8779-8793, 1998.
- Krotkov, N.A., P.K.Bhartia, J.Herman, Z.Ahmad, V. Fioletov, *Satellite estimation of spectral surface UV irradiance 2: Effect of horizontally homogeneous clouds*, Submitted to Journ. Geophys. Res., 2000.
- Noxon, J. F., *Nitrogen Dioxide in the Stratosphere and Troposphere Measured by Ground-Based Absorption Spectroscopy*, Science, 189, 547-549, 1975.
- Noxon, J. F., E. C. Whipple, Jr., and R. S. Hyde, *Stratospheric NO₂. 1. Observational Method and Behaviour at Mid-Latitude*, J. Geophys. Res. 84, 5047-5065, 1979.
- Nugteren, P.R., *User Requirements Document for the OMI Level 0 to 1b Data Processor*, RS-OMIE-7000-FS-186, issue 2 of 20 March 2000.
- McPeters, R.D. et al, *Nimbus-7 Totale Ozone Mapping Spectrometer (TOMS) Data Products User's Guide* (NASA Reference Publication 1384, April 1996).
- OMI Level 1b data format* (see Veeffkind [2] et al., 2001)
- Platt, U., *Differential Optical Absorption Spectroscopy (DOAS)*, in *Air Monitoring by Spectroscopic Techniques*, edited by M. W. Sigrist, pp. 27-84, John Wiley & Sons, New York, 1994.

- Rodgers, C.D., *Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation*, Rev. Geophys. Space Phys. 14609-14624, 1976.
- Singer, S.F., R.C. Wentworth, *A method for the determination of the vertical ozone distribution from a satellite*, J. Geophys. Res. 62, 299-2308, 1957.
- Toricella et al., *Retrieval of aerosol properties over the ocean using Global Ozone Monitoring Experiment measurements: method and application to test cases*, JGR, Vol 104, 12085-12098, 1999.
- Torres, O, P.K. Bhartia, J.R. Herman, Z. Ahmad, and J. Gleason, *Derivation of aerosol properties from satellite measurements of backscattered ultraviolet radiation : Theoretical Basis*, J. Geophys. Res., 103, 17099-17110, 1998.
- Twomey, S., *On the deduction of the vertical distribution of ozone by ultraviolet spectral measurements from a satellite*, J. Geophys. Res. 66, 2153-2162, 1961.
- Van der A, R., R.F. van Oss, H. Kelder, *Ozone profile retrieval from GOME data*, in *Satellite Remote Sensing of Clouds and the Atmosphere III*, Jaqueline E. Russel, Editor, Proceedings of SPIE Vol. 3495, 221-229, 1998.
- Veefkind et al., *Regional distribution of aerosol over land from ATSR-2 and GOME*, Rem. Sensing of the Env., in press, 2000.
- Veefkind [1], J.P., G.W. Leppelmeier, et al, *Auxiliary and Ancillary data requirements document for OMI-EOS* (in preparation), 2001.
- Veefkind [2], J.P., et al, *OMI Level 1b data format*, (in preparation), 2001
- Ziemke, J. R., S. Chandra, and P. K. Bhartia, *Two new methods for deriving tropospheric column ozone from TOMS measurements: The assimilated UARS MLS/HALOE and convective-cloud differential techniques*, J. Geophys. Res., 22,115-22,127, 1998.

Chapter 5 Instrument Requirements

The scientific and algorithm requirements for OMI discussed in the Chapters 3 & 4 lead to instrument requirements, which contain the scientific needs for instrument design. These instrument requirements are listed in this section.

The instrument requirements of this chapter have been formulated in interaction with industry regarding technical capabilities for OMI (see “*OMI-EOS Instrument Specification Document*”, RS-OMIE-0000-FS-021, De Vries (1999)). In this document from Fokker Space, a description of the OMI instrument is given. The rationale for the most important instrument requirements is briefly repeated here, but has more extensively been given in the previous chapters. This leads to the following requirement:

SR 5.0.1 *The OMI instrument shall be built such that it is possible to retrieve the products as listed in Table 3.1 (SR 3.4.0) with the noted accuracies, spatial resolutions etc., using the algorithms as summarised in Chapter 4 (SR 4.3.0).*

Therefore OMI shall measure the Earth radiance and the solar irradiance.

SR 5.0.2 *OMI shall measure the Earth radiance and the solar irradiance spectra*

It is stressed that the design of OMI shall be based on the “lessons learned” of GOME and SCIAMACHY. Advantages of OMI shall include: no scan mirror (to avoid moving parts and spatial aliasing), no polarisation-sensitivity, no etalon effect, no spatial aliasing, smaller ground pixels in order to have better horizontal spatial resolution, and a wider swath in order to have daily global coverage.

SR 5.0.3 *OMI shall not have a scan mirror.*

SR 5.0.4 *OMI shall not be sensitive to polarisation.*

Note: this is quantified with the requirement on rest-polarisation and similar structures in the signal, SR 5.0.10 and with SR 5.2.2.8.

SR 5.0.5 *OMI shall be designed and operated in a way that prevents the etalon effect.*

SR 5.0.6 *OMI ground pixels shall be smaller than $20 \times 20 \text{ km}^2$.*

SR 5.0.7 *OMI shall have a field-of-view that provides cross-track global coverage at all latitudes of the atmosphere in one day from the EOS-Aura spacecraft orbit.*

SR 5.0.8 *OMI shall not suffer from spatial aliasing.*

SR 5.0.9 *The OMI Duty Cycle shall be 100% (continuous operation) in flight.*

SR 5.0.10 *In general, the instrument sensitivity to polarisation shall not be more than 0.5% for fully polarised incident light, for all polarisation directions, over the Full Performance Range.*

This means that fully polarised and unpolarised light should give the same instrumental response within 0.5% over the entire spectral range.

It is expected that the optics, CCD and electronics are to be the best available in order to achieve the mentioned goal (SR 5.0.1). It is expected that optics, CCD and electronics have sufficient reliability (including radiation hardness) for the expected 5-year lifetime of the EOS-Aura mission.

SR 5.0.11 *Optics, detectors and electronics of OMI shall have sufficient reliability (including radiation hardness) for the expected 5-year lifetime of EOS-Aura.*

SR 5.0.12 *OMI shall provide images of atmospheric radiance and the solar irradiance of visible wavelengths.*

SR 5.0.13 *OMI shall provide images of atmospheric radiance and the solar irradiance of ultra-violet wavelengths.*

- SR 5.0.14** *OMI shall view in nadir direction, with a field-of-view in swath direction, which is perpendicular to the spacecraft's flight direction, and a field-of-view in flight direction.*
- SR 5.0.15** *OMI shall use a polarisation scrambler to scramble the polarisation of the incoming atmospheric radiance.*
- SR 5.0.16** *OMI shall convert radiance to spectrum.*
- SR 5.0.17** *OMI shall convert photons to ADC counts.*
- SR 5.0.17-note** *The spacecraft will send the ADC counts to ground.*
- SR 5.0.18** *The OMI Ground Data Processor shall process the data (i.e. ADC counts) to level 1b products.*

5.1 Optical Design

5.1.1 Spectral properties

The following definitions are of specific use for this section:

- Definition 5.1.1.1** The Total Spectral Range is defined as the wavelength range imaged onto the detector, including the overlap regions. In the Global- and Spatial Zoom-in Measurement, this equals to the wavelength range actually present in the instrument data.
- Definition 5.1.1.2** The Full Performance Range is the Total Spectral Range up to the wavelengths where the useful signal from two overlapping channels is equal. This is the wavelength where (about) half of the energy is deposited in each of two overlapping channels.
- Definition 5.1.1.3** The Spectral Sampling Distance is the wavelength range [in nm/pixel] over which a signal is sampled over a pixel.

Avoiding mixing of spectral sampling distance and spectral resolution, the Spectral Resolution is defined as the full width at half maximum (FWHM) for the instrument response for a monochromatic input. The spectral resolution can be expressed in [nm] or pixels, since the sampling distance is known.

- Definition 5.1.1.4** The Spectral Resolution is the full width at half maximum (FWHM) (in [nm] or [pixels]) for the instrument response for a monochromatic input.

OMI shall be an UV-visible imaging spectrometer covering the spectral range 270 - 500 nm, in order to cover the UV and visible absorption bands of O₃, NO₂, BrO, OCIO, HCHO and SO₂, and to observe aerosols, cloud cover and cloud scattering pressure. To achieve best possible performance, the spectral range may be split in sub-channels. However, these sub-channels shall have sufficient overlap so that in the final data, continuous spectra are obtained. In addition, it is preferable that for the most important scientific products, only data from one spectral channel is needed in the retrieval. This ensures that cross-calibration between channels does not affect quality of a single data product. This can be achieved with two channels, denoted by UV and VIS, having the full performance ranges 270 - 365 nm for the UV channel and 365 - 500 nm for the VIS channel. Here 365 nm is the 50 % sensitivity point of both channels. The total overlap of the UV and VIS channels shall be the range 350 - 380 nm.

- SR 5.1.1.1** *OMI shall be a nadir viewing imaging spectrometer with full performance range 270-500 nm.*
- SR 5.1.1.2** *OMI shall have an ultraviolet (UV) channel with full performance range 270-365 nm.*
- SR 5.1.1.3** *OMI shall have a visible (VIS) channel with full performance range 365-500 nm.*
- SR 5.1.1.4** *The 50 % sensitivity point of both channels shall be 365 nm.*
- SR 5.1.1.5** *The total overlap of the UV and VIS channels shall be the range 350-380 nm.*

The dynamic range of the Earth's radiance in the UV from 270 to 330 nm is about three orders of magnitude. Consequently, straylight scattered from the longer UV wavelengths into the shorter UV wavelengths could easily exceed the radiances at the latter wavelengths, thereby endangering measurements of the ozone profile. Therefore, straylight shall be suppressed as much as possible.

This shall be achieved by splitting the UV channel into two parts: a UV-1 part from 270 to 310 nm, and a UV-2 part from 310 to 365 nm. Here 310 nm is the 50% sensitivity point of both channels. The total overlap of the UV-1 and UV-2 channels shall be the range 306 - 314 nm, so all EP-TOMS wavelength bands will be in the same (UV-2) channel.

SR 5.1.1.6 *The UV channel shall be split into two parts, UV-1 and UV-2, with full performance ranges 270-310 nm and 310-365 nm, respectively.*

SR 5.1.1.7 *The 50 % sensitivity point of both UV channels shall be 310 nm.*

SR 5.1.1.8 *The total overlap of the UV-1 and UV-2 channels shall be the range 306-314 nm.*

The spectral resolution of the instrument shall be sufficient to perform DOAS retrieval of trace gases (i.e. O₃, NO₂, BrO, OClO, HCHO and SO₂). Therefore, the spectral resolution (FWHM) expressed in nm shall be equal or better than the values specified in Table 5.1.

SR 5.1.1.9 *The spectral resolution of the UV-1 channel shall equal or better than 0.64 nm*

SR 5.1.1.10 *The spectral resolution of the UV-2 channel shall equal or better than 0.45 nm*

SR 5.1.1.11 *The spectral resolution of the VIS channel shall equal or better than 0.63 nm*

Furthermore, the spectral sampling expressed in detector pixels per FWHM shall be better than 2.7 detector pixels, in order to avoid undersampling. A safe ratio is 3. The spectral sampling distance is the total spectral range divided by the number of CCD pixels covering this range. Given the resolution, the sampling distance follows. In the shortest wavelengths (below 310 nm) a sampling of 2 detector pixels per FWHM is acceptable. This is due to the fact that the ozone Hartley absorption structures in this spectral range are relatively smooth.

SR 5.1.1.12 *The spectral sampling of the UV-1 channel shall equal or better than 0.32 nm while keeping a sampling ratio equal or larger than 2*

SR 5.1.1.13 *The spectral sampling of the UV-2 channel shall equal or better than 0.15 nm while keeping a sampling ratio equal or larger than 3*

SR 5.1.1.15 *The spectral sampling of the VIS channel shall equal or better than 0.21 nm while keeping a sampling ratio equal or larger than 3*

SR 5.1.1.16 *The total range, full performance range, spectral resolution, and spectral sampling distance of OMI shall be as specified in Table 5.1. (Summarise of SR 5.1.1.1 up to SR 5.1.1.15)*

Table 5.1: Required spectral range and resolution of OMI.

“Resolution” means the FWHM of the slit function.

Channel	Total range	Full performance range	Resolution in nm	Resolution in pixels	Sampling distance
UV-1	270 - 314 nm	270 - 310 nm	≤ 0.64 nm	≥ 2	≤ 0.32 nm
UV-2	306 - 380 nm	310 - 365 nm	≤ 0.45 nm	≥ 3	≤ 0.15 nm
VIS	350 - 500 nm	365 - 500 nm	≤ 0.63 nm	≥ 3	≤ 0.21 nm

5.1.2 Spatial properties and observation modes

For global coverage of the Earth in one day, a wide swath of 2600 km is needed. The coverage shall also be contiguous both along and across satellite ground track. This can be achieved by using a large field-of-view

which is imaged onto a CCD detector. Assuming a satellite altitude of 705 km, a 114 degrees wide field of view provides a 2600 km swath.

SR 5.1.2.1 *The UV and VIS channels of OMI shall have a CCD as detector, where the spectrum is imaged in the flight direction and the swath is imaged in the other direction.*

SR 5.1.2.2 *OMI shall have a swath of 2600 km wide or larger to achieve daily global coverage.*

SR 5.1.2.3 *OMI shall have continuous coverage of the Earth both along and across satellite ground track.*

SR 5.1.2.4 *The swath of OMI shall be symmetric around the sub-satellite track (nadir-point).*

The ground pixel size shall be smaller than $20 \times 20 \text{ km}^2$ for ozone column and smaller than or of the order of $40 \times 40 \text{ km}^2$ for ozone profile and other trace gases (see Table 3.1 for specific values). A smaller pixel size of the order of $10 \times 10 \text{ km}^2$ shall be aimed at, in order to obtain cloud-free pixels and to detect and monitor pollution processes in the troposphere.

The Instantaneous Field-Of-View (IFOV) of a sub-satellite OMI pixel shall be $10 \times 10 \text{ km}^2$ or smaller, in order to resolve cloud fields and tropospheric pollution events. The IFOV is defined as the FWHM of the pixel response curve obtained when moving a point source in swath and/or flight direction. OMI shall be able to separate two point sources which are at maximum 10 km separated.

Definition 5.1.2.1 *The Instantaneous Field-Of-View (IFOV) is the FWHM of the pixel response curve obtained when moving a point source in swath and/or flight direction.*

SR 5.1.2.5 *The instantaneous spatial resolution of OMI shall be $10 \times 10 \text{ km}^2$ or smaller at the sub-satellite point.*

Using state-of-the art CCDs it is possible to achieve a pixel size of $13 \times 24 \text{ km}^2$ at nadir for channels UV-2 and VIS, and $13 \times 48 \text{ km}^2$ for channel UV-1 (along \times across track) for a swath of 2600 km (i.e. daily global coverage).

At the extremes of the field of view, the ground pixel size increases, if the instrument sampling (expressed in angle) in the swath direction is constant.

SR 5.1.2.6 *The spatial angles seen by the OMI pixel shall be constant over the swath.*

The observation mode with the 2600 km swath and $13 \times 24 \text{ km}^2$ ground pixels is called the *global observation mode* (**Definition 5.1.2.2**). Next to this mode, there shall be two zoom-in modes, called spatial zoom-in and spectral zoom-in. These zoom-in modes are possible because of the flexibility in programming the CCD read-out and shall be aimed at in order to obtain cloud-free pixels, which is essential for tracing tropospheric pollution.

The *spatial zoom-in mode* shall have a ground pixel size of $13 \times 12 \text{ km}^2$ and full spectral coverage, but is allowed to have a limited swath width of at least 725 km. This swath shall be the central swath, i.e. symmetric with respect to the sub-satellite track (**Definition 5.1.2.3**).

The *spectral zoom-in mode* shall have a ground pixel size of $13 \times 12 \text{ km}^2$ and a full swath of 2600 km. A limited spectral coverage is allowed, but shall be at least 306 - 432 nm to cover the most important scientific products. (**Definition 5.1.2.4**)

In the spectral range of 270 – 310 nm, the pixel size in the across-track direction may be larger, but at most doubled (i.e. $13 \times 48 \text{ km}^2$ in global mode, $13 \times 24 \text{ km}^2$ in zoom-in mode).

SR 5.1.2.7 *The swath width and sub-satellite ground pixel size of OMI shall be as specified in Table 5.2, for the global mode, the spectral zoom-in mode, and the spatial zoom-in mode.*

Table 5.2 Required swath width and sub-satellite ground pixel of OMI for the three different observation modes.

Observation mode	Spectral range	Swath width*	Ground pixel size (along x across track)	Application
Global mode UV-1 UV-2 & VIS	270 - 310 nm 310 - 500 nm	2600 km 2600 km	13 × 48 km ² 13 × 24 km ²	global observation of all products
Spatial zoom-in mode UV-1 UV-2 & VIS	270 - 310 nm 310 - 500 nm	2600 km ≥ 725 km	13 × 24 km ² 13 × 12 km ²	regional studies of all products
Spectral zoom-in mode UV VIS	At least 306 - 364 nm At least 350 - 432 nm	2600 km 2600 km	13 × 12 km ² 13 × 12 km ²	global observation of some products

* and symmetric around sub-satellite track

A *sub-pixel read-out* capability of the CCD shall be implemented for sub-pixel cloud detection. Sub-pixel read-out means that at one selected wavelength per CCD no co-addition of CCD images (see section 5.1.3) in the flight direction is performed (**Definition 5.1.2.5**). This results in a spatial resolution of 10 km (optical resolution) and a sampling distance of 2.7 km in the flight direction (which is nominal exposure time times the spacecraft orbital velocity). Across-track pixel size and swath width shall be the same as for the UV-2 and VIS channels in the chosen observation mode. So, in the global mode, the spatial resolution is 10 × 24 km² for the sub-pixel data. Selection of the wavelength shall be flexible, e.g. in a region without significant gaseous absorption (around 380 nm for the UV, and 480 nm for the VIS), so that sub-pixel cloud detection is possible.

SR 5.1.2.8 *A sub-pixel read-out capability shall exist for one wavelength in the UV channel and one wavelength in the VIS channel of OMI, which is achieved by not co-adding the CCD-images for all three observation modes.*

SR 5.1.2.9 *It shall be possible to choose the wavelengths for sub-pixel data flexible.*

In order to geolocate the OMI Level 1 and 2 data products correctly, the latitude and longitude co-ordinates of each ground pixel shall be known to within 1/10th of the ground pixel size. This geolocation requirement holds after correction for errors in e.g. satellite pointing and instrument pointing.

SR 5.1.2.10 *The latitude and longitude of the centre of each ground pixel shall be known with an accuracy better than 1/10th of the size of the ground pixel of the global, spatial and spectral zoom-in modes (either in an angular unit or in a distance unit on the Earth's surface).*

5.1.3 Detector requirements

The CCD detectors have 2 directions, one of which is the spectral dimension and the other is the swath (see Figure 5.1). The following terminology will be used:

- Row: A CCD row corresponds to the spectral dimension (780 CCD pixels - 750 used).
- Column: A CCD column corresponds to the swath direction (580 CCD pixels - 480 used).

One row contains one spectrum for one viewing direction. One column contains the entire swath for one wavelength. There are 580 rows and 780 columns on the CCD. The CCD technique allows one to measure

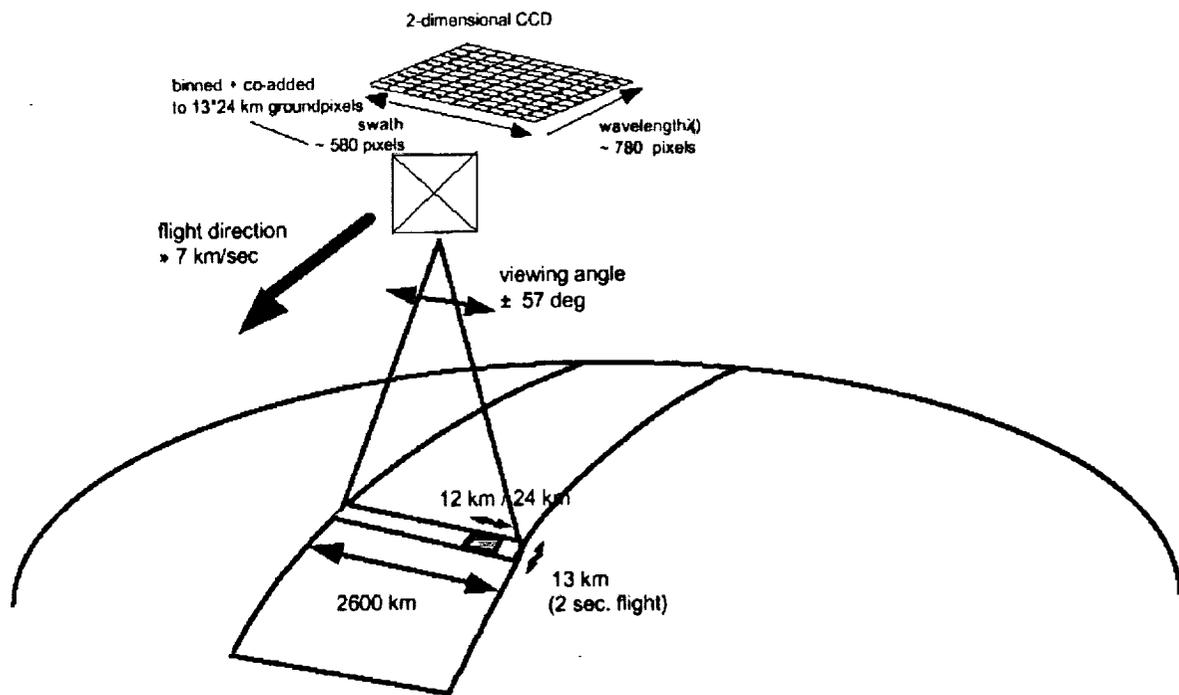


Fig 5.1 OMI CCD measurement principle (Figure with courtesy of Fokker Space)

the entire swath and the entire spectrum simultaneously. In addition, the CCD allows for simultaneous calibration measurements of e.g. dark current and straylight from the rows and columns that are not used for imaging spectra. This gives rise to the following requirements.

SR 5.1.3.1 *At the edges of the CCD, dark current and straylight shall be measured on every exposure.*

SR 5.1.3.2 *Frame transfer smear shall be measured for every exposure.*

It is realised that co-addition of several exposures, to create an image, will result in a summation of the smear measurements.

SR 5.1.3.3 *The spectrum of each viewing direction (i.e. one CCD row) shall be spectrally calibrated separately.*

SR 5.1.3.4 *Gain switching in the preamplifier shall be used to improve S/N in the UV channel.*

SR 5.1.3.5 *There shall be 4 different gains per CCD detector.*

SR 5.1.3.6 *The order of gains shall be programmable in flight.*

SR 5.1.3.7 *The wavelength at which the gain is switched shall be programmable in flight.*

SR 5.1.3.8 *Gain switching shall be such that the range between minimum and maximal radiance permits an optimal use of the full dynamical range of the 12 bits ADC converter.*

The image shall be aligned along the spectral direction, such that every row contains the spectrum of one viewing direction. This leads to the following alignment requirements.

SR 5.1.3.9 *The alignment of the slit of OMI with the CCD shall be accurate within 0.4 CCD pixel. This means that in each spectral channel (UV 1, UV 2 and VIS) each CCD row shall contain the spectrum belonging to one viewing direction, within an accuracy of 0.4 CCD pixel in the swath direction.*

- SR 5.1.3.10** *The co-alignment of the UV-2 and VIS channels shall be within 1 CCD pixel in the swath direction.*
- SR 5.1.3.11** *The co-alignment of the UV-1 and UV-2 channels shall be within 1 CCD pixel in the swath direction.*
- SR 5.1.3.12** *Optical distortion leading to different spectral definition as a function of the viewing angle, like the curved swath image, shall not influence the required spectral range over the entire CCD, according to Table 5.1 (SR 5.1.1.16).*
- SR 5.1.3.13** *The curved swath image shall not influence the required spectral resolution and sampling distance over the entire CCD, according to Table 5.1 (SR 5.1.1.16), to within a margin of 10 % around these values.*
- SR 5.1.3.14** *Spectral lines imaged onto the columns of the CCD for both channels shall be aligned with an accuracy of 0.1 CCD pixel.*

The following definitions are used to describe the measurement and read-out strategy of the CCD:

The *exposure time* is the time the image-part of the CCD is illuminated (nominal exposure time is 0.4 s). After illumination, frame transfer takes place, and the image is transferred to the read-out part of the CCD (**Definition 5.1.3.1**).

The *read-out time* is the time it takes to read this part of the CCD (nominal read-out time is 0.4 s) (**Definition 5.1.3.2**).

In the flight direction, several images are co-added.

The nominal *co-addition time* is 2 s (i.e. 5 images are added) (**Definition 5.1.3.3**).

In the swath-direction (along a column in the CCD) several CCD-pixels are *binned* (in the global mode 8 pixels are binned nominally) (**Definition 5.1.3.4**).

The exposure times of the CCD shall be chosen such that the S/N is optimal and saturation does not occur for the nominal exposure time, not even above bright scenes, such as clouds and snow (see section 5.2). The nominal exposure time shall be 0.4 s. Possible exposure times shall be between 0.1 s and 6 s. The shortest possible integration time of 0.1 s may be needed over very bright targets (clouds, snow, high sun). Exposure times shall be programmable during flight.

SR 5.1.3.15 *CCD exposure times shall be possible between 0.1 s and 6 s.*

SR 5.1.3.16 *OMI shall be able to do long exposures between 6 and 768 s.*

SR 5.1.3.17 *The nominal exposure time shall be 0.4 s.*

SR 5.1.3.18 *The exposure time shall be programmable during flight.*

SR 5.1.3.19 *Read-out time shall not influence data acquisition in the image area of the CCD.*

Co-adding of images (in the flight direction) will be done to improve S/N and reduce data rate. The co-addition period is between 2 s and 6 s and shall be programmable during flight.

In the swath direction, binning of pixels shall be possible to improve S/N and reduce data rate. In the global mode, 8 pixels shall be binned in the swath direction.

SR 5.1.3.20 *Co-adding of images shall be possible, with co-addition period between 2 s and 6 s.*

SR 5.1.3.21 *The co-addition period shall be programmable during flight.*

SR 5.1.3.22 *Binning of pixels (in the swath direction) shall be possible.*

SR 5.1.3.23 *Binning factors between 1 and 15 shall be possible.*

SR 5.1.3.24 *The binning factor shall be programmable during flight.*

SR 5.1.3.25 *It shall be possible to operate the UV and VIS channels independently (so that different exposure time, co-addition period, read-out time and binning factors are possible).*

Definition 5.1.3.5 Bad pixels are: pixels with anomalous dark current, reduced charge transfer efficiency (CTE), reduced quantum efficiency, or anomalous pixel response function and all pixels in columns on the CCD whose signal is transferred through a pixel with one of the aforementioned effects.

Bad pixels shall not influence the retrieval accuracy of the OMI data products (see Annex III for the relevant wavelength ranges). There shall be no bad pixels in the readout register.

SR 5.1.3.26 *The CCD detectors shall not have more than 100 bad or dead pixels.*

SR 5.1.3.27 *Bad/dead pixels shall not influence the retrieval accuracy of any of the OMI data products listed in Table 3.1.*

SR 5.1.3.28 *There shall be no bad or dead pixels in the read-out register.*

There shall be no ice forming on the CCD or on any other optical component in the OMI instrument.

SR 5.1.3.29 *The instrument shall be operated in such a way that no ice forms on the CCD or on any other optical component in the OMI-instrument.*

SR 5.1.3.30 *All channels (UV and VIS) shall start their exposures simultaneously when equal read-out disciplines are used.*

5.2 Radiometric Accuracy

5.2.1 Random errors (required signal-to-noise)

Table 4.1 in Chapter 4 lists the required S/N ratios for the Earth radiances for the different OMI products. Note that the S/N ratios given in Table 4.1 are required for the ground pixel sizes ($20 \times 20 \text{ km}^2$ and $40 \times 40 \text{ km}^2$) as given in Table 3.1.

In this section the S/N ratios are *scaled* to $13 \times 24 \text{ km}^2$ ground pixel in the UV-2 and VIS wavelength range and to a $13 \times 48 \text{ km}^2$ ground pixel in the UV-1 wavelength range, as obtained in the global mode to allow for direct comparison of values with instrument performance (see table 5.3 or Annex VI). These S/N ratios are therefore called “scaled S/N ratio” as opposed to the “required S/N ratios” in Table 4.1. For actual retrieval, a number of ground pixels may have to be combined to achieve the required signal to noise as shown in Table 4.1. The last column of table 5.3 also shows the *scaled* S/N ratio’s for a $13 \times 12 \text{ km}^2$ ground pixel in the UV-2 and VIS and a $13 \times 24 \text{ km}^2$ ground pixel in the UV-1, as obtained in both zoom-in modes.

Table 5.3 Required *scaled* signal-to-noise levels for different wavelength ranges.

The values in this table are derived from the values in Table 4.1, by re-scaling for the ground pixel sizes given in this table.

Wavelength range	Critical trace gas	Scaled S/N (global mode)	Scaled S/N (spatial zoom-in mode)
270 – 310 nm	O ₃ profile	60 ($13 \times 48 \text{ km}^2$)	45 ($13 \times 24 \text{ km}^2$)
310 – 335 nm	O ₃ column	265 ($13 \times 24 \text{ km}^2$)	190 ($13 \times 12 \text{ km}^2$)
335 – 365 nm	HCHO	1450 ($13 \times 24 \text{ km}^2$)	1050 ($13 \times 12 \text{ km}^2$)
365 – 420 nm	OCIO	700 ($13 \times 24 \text{ km}^2$)	470 ($13 \times 12 \text{ km}^2$)
420 – 450 nm	NO ₂	2600 ($13 \times 24 \text{ km}^2$)	1850 ($13 \times 12 \text{ km}^2$)
450 – 500 nm	O ₂ – O ₂	1400 ($13 \times 24 \text{ km}^2$)	1000 ($13 \times 12 \text{ km}^2$)

The selected wavelength ranges are based on the most critical gas, which is defined as being the one that requires the highest S/N ratio in that wavelength range (= **Definition 5.2.1.1**). The determining trace gas in the several wavelength ranges can also be found in Table 5.3. These S/N ratios shall be reached for Earth radiances, which are minimally expected for the OMI instrument (see Figure 5.2 and Annex IX). On the other hand, for the maximal expected Earth radiances OMI will detect, the instrument shall not saturate (see Figure 5.2 and Annex IX).

SR 5.2.1.1 *The S/N ratio's for the Earth radiance measurements as tabulated in Table 5.3 shall be reached for the minimum radiance levels as shown in Figure 5.2.*

SR 5.2.1.2 *The OMI instrument shall not saturate for the maximum Earth radiance levels as defined in Figure 5.2.*

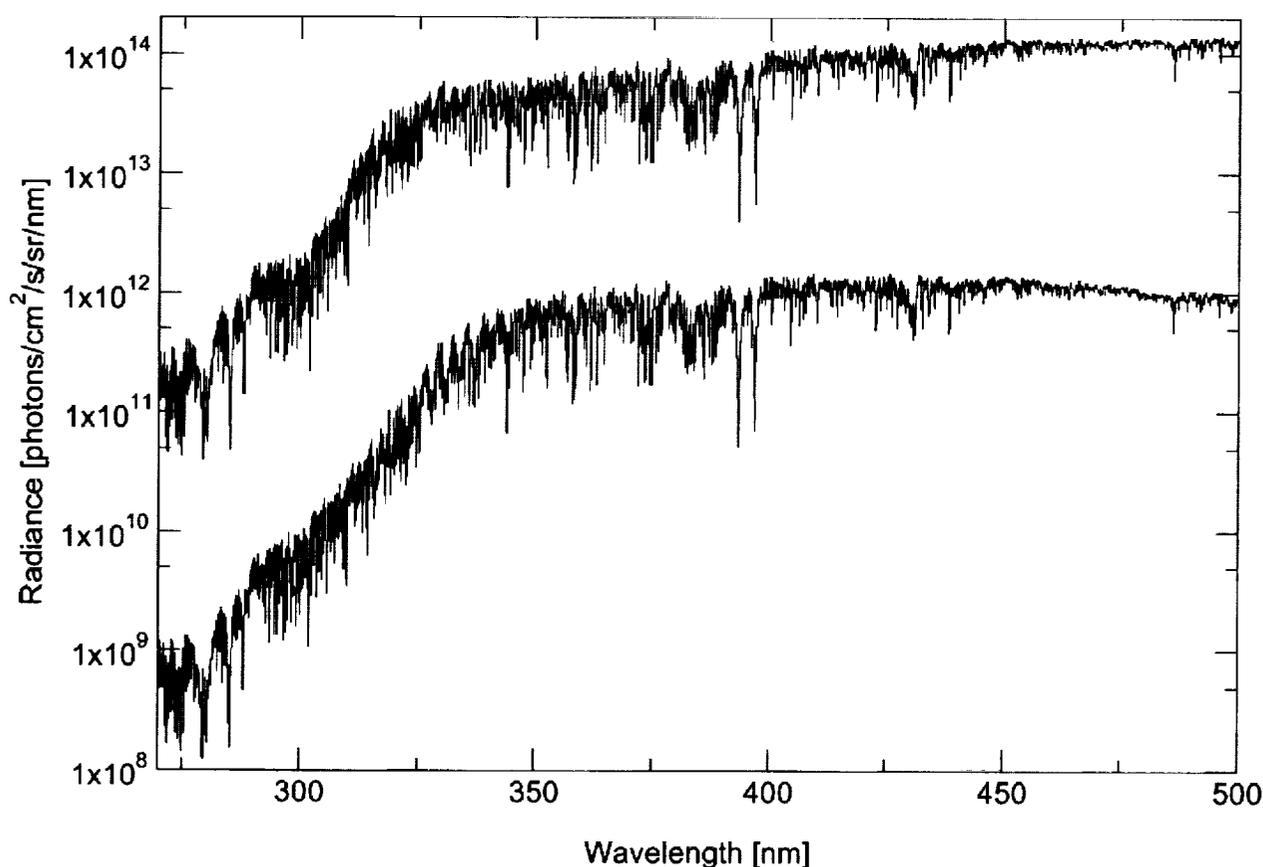


Fig. 5.2 *Overall minimum and maximum radiances to be observed by OMI, as derived from simulations for different scenario's as described in Annex XI.*

The solar irradiance measurements also require a minimal S/N ratio. The requirement on the S/N ratio for the solar irradiance measurements are mainly caused by the wavelength calibration using the Fraunhofer lines of the sun. Moreover, also the solar irradiance levels shall not saturate or damage the instrument.

SR 5.2.1.3 *Solar irradiance measurements, through the calibration port of OMI, shall have S/N ratios of at least 1000, independent of season.*

SR 5.2.1.4 *During solar irradiance measurements OMI shall not saturate, independent of season.*

SR 5.2.1.5 *The OMI Instrument shall not be damaged by high Earth radiances (red line in Figure 5.2) or solar irradiances entering the telescope and/or caused by:*

- *the sun glint effect*
- *lasers used for the alignment (less than 20 mW)*
- *the sun*

5.2.2 Systematic errors

In order to ensure the overall accuracy and long-term stability of the OMI, requirements on the absolute radiometric accuracy are needed. Although not normally needed for the derivation of the OMI-products as listed in Table 3.1 from measurements (which rely on the reflectance, which is the ratio of the Earth radiance over the solar irradiance), it is necessary for the calibration and characterisation of the instrument (in particular the overall throughput) to have in addition an absolute radiometric calibration of both the measured atmospheric radiance and the solar irradiance. It will also confirm that the instrument is working as it should under operational conditions. In order to obtain the accuracies for the different OMI products as defined in Table 3.1, it is necessary to have a radiometric calibration accuracy of $\leq 2\%$, excluding the calibration lamp error. The calibration lamp used shall be a NIST calibrated 1000 W FEL lamp, which shall be calibrated within 2 % (2σ error) over the total spectral range of OMI (270 nm – 500 nm). Moreover, since the intensity of the Earth radiance and solar irradiance measurements will depend on swath angle, wavelength, position in orbit and season, all requirements in section 5.2.2. and section 5.3 shall apply for all these situations.

SR 5.2.2.1 *Requirements SR 5.2.2.4 – SR 5.3.3 shall be met for all swath angles, wavelengths, positions in orbit and seasons.*

SR 5.2.2.2 *The calibration lamp used for the absolute radiometric calibration (see SR 5.2.2.4) shall be a NIST calibrated 1000 W FEL lamp and shall be NIST traceable.*

SR 5.2.2.3 *The NIST calibrated 1000 W FEL lamp shall be calibrated within a 2 % (2σ error) accuracy over the total spectral range of OMI (270 nm – 500 nm).*

SR 5.2.2.4 *The absolute radiometric accuracy of the atmospheric radiance and the solar irradiance spectra shall be known to within $\leq 2\%$, excluding the calibration lamp error.*

Most science products are obtained from the reflectivity, which is the Earth radiance divided by the solar irradiance. In order to ensure the accuracy on the products, as stated in Table 3.1, the absolute reflectivity shall be accurate to $\leq 1.0\%$. This means that the BSDF (Bi-directional Scatter Distribution Function) of the Earth shall be measured within 1 %, which means that the BSDF of the OMI-instrument shall be known within 1 %. In the on-ground calibration the BSDF of the OMI-instrument is measured using an external diffuser (see *Calibration Plan*, PL-OMIE-0000-TPD-127, Zoutman et al., 1999). The error in the BSDF of this external diffuser determines the error in the BSDF of the OMI-instrument and therefore of the absolute reflectivity and shall be not be larger than 1 %.

SR 5.2.2.5 *The error in the absolute reflectivity (defined as the radiance divided by the irradiance) shall be*
 1.0 % for any (collimated to 0.5 degree circular, i.e. Solar like) position in the irradiance Field-Of-View.

The accuracy of the reflectivity can be discussed using the following expression:

$$I_{measured}(\lambda) = m(\lambda, I(\lambda), \varphi, \mathbf{p}) \times I_{true}(\lambda) + a(\lambda, I(\lambda''), \varphi, \mathbf{p})$$

with m the multiplicative factors, a the additive factors, λ and λ'' for wavelength, I for intensity, φ for swath angle and \mathbf{p} for polarisation. I_{true} is the signal at a specific wavelength of interest to the scientists (the ideal reflectivity without biases) and $I_{measured}$ is the signal at the same wavelength as obtained by the OMI. The

multiplicative and additive factors m and a depend on wavelength, intensity, swath angle and polarisation. In an ideal case the multiplicative factors equal unity and the additive factors equal zero.

Definition 5.2.2.1: The effects contributing to *multiplicative factors* are:

1. absolute radiometric calibration taking into account that common optical paths cancel in the calculation of the reflectance.
2. linearity charge transfer efficiencies
3. polarisation effects between the primary mirror and the first scrambler surface
4. spectral structures similar to absorption structures
5. gain settings

Definition 5.2.2.2: The effects contributing to *additive factors* are:

1. stray light
2. dark current
3. exposure smear
4. charge transfer inefficiencies
5. memory effects in CCD, DEM and ELU
6. electronic offset

The relevant science requirements are:

SR 5.2.2.6 *The effect of multiplicative factors on the absolute reflectivity shall be less than 1% of the true signal after correction at all wavelengths and swath angles.*

SR 5.2.2.7 *The effect of additive factors on the absolute reflectivity shall be less than 1% of the true signal after correction at all wavelengths and swath angles.*

Due to the fact that DOAS retrieval is extremely sensitive to spectral structures that resemble absorption structures of the trace gas of interest, a separate requirement is needed for the error caused by “spectral structures similar to absorption structures”. Not only optical instrument effects caused by e.g. the scrambler or an etalon, but e.g. also memory effects in the CCD may cause spectral structures that resemble absorption structures. See Annex X & Annex XI for details. Absorption structures relevant for the OMI-instrument can be found in Annex XII.

SR 5.2.2.8 *The effect of spectral structures similar to absorption structures caused by the instrument and/or its calibration in the reflectivity spectra shall be less than 10^{-4} at all wavelengths and swath angles.*

A separate requirement is also needed for non-linearity, due to the fact that the ozone profile retrieval is extremely sensitive to this. The linearity requirement applies for all illuminations between expected minimum radiance and irradiance and pixel full well. The allowed non-linearity is the maximum excursion relative to linear behaviour, so $|I_{\text{measured}} - I_{\text{true}}| < 0.002 I_{\text{true}}$ (for details, see Annex XIII).

SR 5.2.2.9 *The non-linearity on the reflectivity after correction shall be less than 0.2%.*

Note: Here non-linearity is defined as is the maximum excursion relative to linear behaviour (Definition 5.2.2.3), so $|I_{\text{measured}} - I_{\text{true}}| < 0.002 I_{\text{true}}$. Moreover the linearity requirement applies for all illuminations between expected minimum radiance (and irradiance) and pixel full well.

In case the noise-floor in the measured S/N for the relevant ground pixel size is larger than the non-linearity itself, this requirement can be relaxed and applies to the dynamic range above twice the noise floor.

5.3 Spectral stability and spectral knowledge

Wavelength calibration will be achieved by using the Fraunhofer lines in the solar irradiance and Earth radiance spectra. These lines have well-known positions. Molecular lines in the earth radiance spectrum can possibly contribute to the spectral calibration. The wavelength scale shall be in vacuum wavelengths.

SR 5.3.1 The wavelength scale of the Earth radiance and solar irradiance spectra shall be in vacuum wavelengths.

Spectral knowledge is defined as the error in the wavelengths assigned to the radiance and irradiance spectra (**Definition 5.3.1**). Several studies at KNMI were performed and resulted in requirements for the spectral knowledge for specific products. The required spectral knowledge is $\leq 1/100^{\text{th}}$ of a CCD-pixel above 300 nm and $\leq 1/50^{\text{th}}$ of a CCD-pixel below 300 nm (see Annex IV).

For DOAS retrieval the mechanical and thermal spectral stability of the instrument is, however, also very important. Several studies performed at KNMI showed that the interpolation error made by spectrally co-aligning the Earth radiance and solar irradiance spectra in wavelength scale before calculating the solar irradiance spectra, introduces an error in the retrieved DOAS products. In order to be able to obtain the accuracy on the OMI products as stated in table 3.1, the thermal and mechanical spectral stability of the instrument shall be better than $1/20^{\text{th}}$ of a CCD-pixel. For ozone profile retrieval a minimum of $1/20^{\text{th}}$ of a pixel is also needed (see Annex V).

SR 5.3.2 The spectral knowledge of the radiance and irradiance spectra shall be better than $1/100^{\text{th}}$ of a CCD-pixel above 300 nm and better than $1/50^{\text{th}}$ of a CCD-pixel below 300 nm.

SR 5.3.3 The thermal and mechanical spectral stability of the instrument shall be better than $1/20^{\text{th}}$ of a CCD-pixel.

5.4 OMI On-Ground and Pre-flight Calibration Requirements

The entire instrument shall be calibrated and characterised before flight. Important aspects are: spectral performance and spectral stability, straylight, dark signal, radiometric sensitivity, characterisation of the slit function in the spectral and spatial directions, bad/dead pixels, characterisation of diffuser plates. In the “*OMI On-Ground Calibration and Characterisation Requirement Document*” (Snel, 2000) the requirements for the calibration and characterisation of the instrument can be found. Here only those requirements that have a large financial and schedule impact are mentioned.

For an end-to-end test of the instrument a calibration PI period is essential.

SR 5.4.1 A PI period is needed to measure atmospheric spectra with the Flight Model, and to measure trace gas absorption spectra of, for example, ozone and NO₂.

For a proper spectral calibration using the Fraunhofer lines and for product retrieval using the spectral dependent absorption cross-sections, it is essential to have a very well determined slitfunction. The effective spectral slitfunction is defined as the optical slitfunction convoluted with the Pixel Response Function (PRF) (= **Definition 5.4.1**).

SR 5.4.2 The accuracy of the effective spectral slitfunction of the instrument shall be 1 % of the peak value of the effective spectral slitfunction over the whole spectral range and for all swath-angles and for all relevant measurements modes (nadir and sun diffuser).

There shall be a breadboard/engineering model, called the Development Model (DM), preferably of the complete instrument, but consisting of at least a complete UV-channel placed in the mechanically complete housing (so that for the VIS channel only the optics are missing). This Development Model and the DM measurements shall be ready in time so that the results can be used for the Proto-Flight Model (PFM) design, (especially reduction of straylight), the PFM calibration and characterisation measurements and its preparation, EGSE (Electrical Ground Support Equipment) testing, level 0 → 1b algorithm testing, atmospheric spectra, etc.

- SR 5.4.3 There shall be a Development Model with at least a complete UV-channel. This DM and its measurements shall be available for us in PFM design and the PFM calibration and characterisation measurements.*
- SR 5.4.4 Straylight shall be characterised for all spatial and spectral dimensions.*
- SR 5.4.5 In all measurement modes (measurement and calibration) the instrument response for all sources outside 2 times the IFOV (centred to the IFOV) shall not exceed 1 % of the response for the radiance from inside the IFOV.*
- SR 5.4.6 Straylight determined for the minimum radiance spectrum as shown in Figure 5.2 (blue line) shall be less than 10 % before correction and 0.5 % after correction at all wavelengths and swath angles.*
- SR 5.4.7 The signal from dark current shall not exceed 20% of the useful minimal signal as shown in Figure 5.2 (blue line) before correction and 0.5 % after correction at all wavelengths and swath angles.*
- SR 5.4.8 All other requirements, specified in the latest version "OMI On-Ground Calibration and Characterisation Requirement Document", shall be applicable.*

5.5 In-flight calibration facilities

The accuracy of the OMI Level 1b and 2 data products will strongly depend on the instrument's calibration. The most important calibration steps in the Level 0-1b processing are dark signal correction, straylight correction, and spectral and absolute radiometric calibration.

To perform these calibrations, the following on-board calibration modes shall be possible:

Solar calibration

- SR 5.5.1 The solar calibration shall be used for the absolute radiometric calibration of OMI during flight. Therefore the sun shall be observed at least once each day via a solar port and a diffuser plate.*
- SR 5.5.2 The long-term degradation of the nominally used reflection diffuser shall be monitored by using an identical reflection diffuser that is typically used once per month.*
- SR 5.5.3 In addition, it shall be possible to use the transmission diffuser (which is used for the white light source (WLS)) as a reflection diffuser.*
- SR 5.5.4 In order to correct for spectral effects of the reflection diffuser plate a third reflection diffuser of a different material shall be used.*
- SR 5.5.5 The solar calibration port shall be large enough to observe the total sun in the field-of-view and the useful calibration time shall be about 1 minute.*
- SR 5.5.6 When closed, the solar calibration port shall be light tight.*

White light source calibration

The spectrum of the WLS shall be well known and stable. The WLS observations shall be used for relative radiometric calibration of the instrument optics plus detectors.

SR 5.5.7 There shall be a calibration white light source (WLS) in the instrument. This WLS is used for relative radiometric calibration of the instrument optical path after the primary mirror, plus detectors and for pixel-to-pixel characterisation purposes.

SR 5.5.8 The spectrum of the WLS shall be continuous, well characterised and stable.

Smooth field light source

In front of each CCD there shall be a smooth field light source, required for characterising the pixel-to-pixel sensitivity of the detectors and the efficiency of the CCD pixels.

SR 5.5.9 There shall be a smooth field light source in front of each detector CCD in the wavelength range that can be measured with the CCD, preferably in the wavelength range measured by the channel in question. This means that the UV1, UV2 and VIS channel all preferably shall have a different smooth field light source.

Dark current signal measurements

The dark current signal shall be measured and characterised during the dark side of the orbit and during the illuminated side of the orbit (both are needed because of temperature effects). Comparison of short and long exposure time dark current measurements are needed for separation of electronics offset and dark current in order to correct for both.

SR 5.5.10 The dark current of all CCD pixels shall be measured and characterised during the dark side and the illuminated side of the orbit, in order to characterise temperature variation of the dark current.

SR 5.5.11 Dark current measurements with multiple exposure times of all CCD pixels shall be performed to separate the electronics offset, dark current and noise in order to correct for dark current and electronic off-set in the on-ground software (and characterise the S/N in the measured signal).

Straylight measurements

Straylight should be measured for each image using dedicated CCD rows and should be corrected for.

SR 5.5.12 The straylight shall be measured for each image using dedicated CCD rows and shall be corrected for in on-ground software. This correction shall be based on the dedicated CCD row straylight measurements and the on-ground straylight calibration.

Detector Smear

SR 5.5.13 Detector smear shall be measured using dedicated CCD rows and shall be corrected for in on-ground software.

SR 5.5.14 The OMI in-flight telemetry shall include data which enables on-ground software correction for multiplicative and additive factors as defined in definitions 5.2.2.1 and 5.2.2.2 above.

As mentioned in Chapter 2, the long-term stability of the OMI-instrument is one of the essential requirements from EOS-Aura. This can be achieved by developing special in-flight calibration techniques:

The detailed in-flight calibration requirements can be found in the “*OMI In-flight Calibration Requirements Document*”.

SR 5.5.15 *All other requirements, specified in the latest version “OMI In-flight Calibration Requirements Document”, shall be applicable.*

5.6 References

“*OMI In-flight Calibration Requirements Document*” (in preparation)

Snel, R., “*OMI On-Ground Calibration and Characterisation Requirement Document*” draft version 3,
20 March 2000

Vries, J. de, *OMI-EOS Instrument Specification Document*, RS-OMIE-0000-FS-021 issue 2, 14 September
1999

Zoutman, E., D. de Winter and B. Kruizinga, *Calibration Plan*, PL-OMIE-0000-TPD-127 issue 2,
14 September 1999

Chapter 6 Validation Requirements

6.1 Data validation objectives and strategy

6.1.1 Validation objectives

Validation has been defined by the EOS validation program as the process of assessing by independent means the uncertainties of the data products derived from OMI measurements. The objective of OMI validation is to establish the validity and accuracy of the measurements. It is essential to validate all products of OMI, including level 1b products, in order to determine the quality of the level 2 data products. Validation of level 1b products (radiance and irradiances) is important because all other data products depend on their accuracies.

Validation is an iterative process: Validation results are used to improve existing algorithms (when significant improvements are expected) until the specified accuracy requirements are obtained, or the theoretical accuracy limit is reached.

The validation procedures are described in detail in the OMI Validation Requirements Document, OMI Validation Handbook, and the EOS-Aura Validation Plan.

6.1.2 Validation strategy

The validation shall continue throughout the OMI lifetime (SR 6.1.2.1). Validation is envisaged to consist of three phases, each having a distinct goal. Firstly, the commissioning phase, which aims to provide a quick-look first validation; secondly, the core phase, to ensure a thorough validation of all data products; and finally, a long-term validation, establishing the stability of the instrument which is important for its ability to measure trends (SR 6.1.2.2).

The validation strategy is to rely on measurements based on validated techniques. Preferably, several independent measurement techniques shall be used, at a large number of representative locations and conditions (SR 6.1.2.3). Validation campaigns shall be co-ordinated with other instruments on EOS-Aura (SR 6.1.2.4). New instrumentation shall be considered to provide an intercomparison rather than a validation (SR 6.1.2.5).

To validate OMI data, participation in scientific validation projects, e.g., the NASA-NRA for Aura-validation, shall be encouraged (SR 6.1.2.6).

Experience gained during the validation of GOME and SCIAMACHY shall be exploited (SR 6.1.2.7).

Validation tools which shall be needed are: software for data processing, coincidence predictor, correlative and Aura data database, cataloguing tools, data assimilation tools, auxiliary data (SR 6.1.2.8).

Validation workshops shall be held regularly throughout the OMI lifetime (SR 6.1.2.9).

6.2 Validation phases

6.2.1 Commissioning phase

The first validation phase is the commissioning phase. In this phase absolute irradiance and absolute radiance shall be validated, because all higher level products depend on their accuracies. Furthermore, a preliminary validation of the main level 2 data products shall be provided (SR 6.2.1.1, Definition 6.2.1.1). In this phase, one satellite instrument (with global coverage) and one or two groundbased instruments shall be used as

correlative instruments (SR 6.2.1.2). Typically, this validation phase shall take place after instrument functional tests, and lasts about three months (SR 6.2.1.3).

6.2.2 Core phase

The second validation phase is the core phase, in which all products shall be validated thoroughly in order to determine their accuracy (SR 6.2.2.1, Definition 6.2.2.1). For this purpose, the use of data from existing instruments (ground-based and satellite instruments) as well as from dedicated campaigns shall be needed (SR 6.2.2.2). Campaigns shall be incorporated within the EOS-Aura framework (SR 6.2.2.3). Existing campaigns, outside the scope of EOS-Aura validation, shall also to be exploited (SR 6.2.2.4). During the core phase, data measured by different independent instruments shall be used (SR 6.2.2.5). Data measured within existing networks of instruments shall be exploited, since these are well-validated and often very stable (SR 6.2.2.6). Data from satellite instruments and data-assimilation techniques shall also be included and are essential for obtaining global coverage (SR 6.2.2.7).

Campaigns are an essential part of the core phase. They shall provide data at locations where representative existing measurements are sparse, or where retrieval weaknesses yield results with limited accuracies.

The core phase starts after the commissioning phase and ends when all data products have been validated. It shall span at least one year, to achieve seasonal coverage (SR 6.2.2.8). Campaigns shall not start earlier than 1 year after launch (SR 6.2.2.9). During the core phase, EOS-Aura as well as correlative data shall be available for all validation participants, through (an) easily available database(s) (SR 6.2.2.10).

If data are reprocessed (e.g., based on the validation results), they shall be validated again, using the already available correlative data (SR 6.2.2.11).

6.2.3 Long-term phase

The long-term phase starts after the core phase and lasts during the complete lifetime of the instrument. In the long-term phase, all available data shall be used (SR 6.2.3.1). The main goals for this phase are detection of long-term changes in the accuracies of the products, e.g., due to instrument degradation, and for the validation of newly developed or advanced OMI data products (SR 6.2.3.2, Definition 6.2.3.1). This necessitates a regular, optimised repetition of the essential elements of the core validation phase (SR 6.2.3.3). Validation shall be continued throughout the lifetime of the OMI instrument (SR 6.1.2.1).

6.2.4 Validation rehearsal

Before launch, a validation rehearsal shall be planned (SR 6.2.4.1). Main goals are to provide a check on the data flow and accessibility of the database(s), and to test the validation tools (SR 6.2.4.2). A more extensive set of validation requirements can be found in the “*OMI Validation Requirements Document*” (Valks, 1999), the “*OMI Validation Handbook*” (Brinksma and Boersma, 2001) and the “*EOS-Aura Validation Plan*” (Froidevaux and Douglas, 2000)

SR 6.2.4.3 *All other requirements, specified in the latest versions of the “OMI Validation Requirements Document”, the “OMI Validation Handbook” and the “EOS-Aura Validation Plan” shall be applicable.*

6.3 Availability of validation data sources/campaigns

Based on the availability of correlative data through existing sources, and because it is yet uncertain where and when validation campaigns will be held, and what is to be measured, the following requirements are envisaged:

Correlative measurements of (tropospheric) columns of NO₂ are imperative for validation of this OMI product, however these are sparsely available through existing sources. Thus, it must be guaranteed that

these shall be supplied, either through the NASA-NRA for Aura-validation or through other sources of funding (SR 6.3.1).

For O₃ (column, profile and tropospheric column), in general, sufficient amounts of correlative data are available, but some areas of the world (tropics, polar regions) are not sufficiently covered.

Correlative measurements of HCHO are available from GOME and in situ measurements campaigns for HCHO are ongoing.

Validation sources for BrO and OCIO are SCIAMACHY, GOME-2 and groundbased DOAS instruments.

For aerosols, the AERONET system should be exploited.

Correlative measurements of clouds will be provided by other cloud satellite measurements.

6.4 References

Brinksma, E. and Boersma, F., "*OMI Validation Handbook*", 2001, in preparation

Froidevaux, L. and Douglas, A. (eds), "*EOS-Aura Validation Plan*", Version 1, to be released December 2000

Valks, P., "*OMI Validation Requirements Document*", draft 30 July 1999

List of Acronyms

AATSR	Advanced ATSR
ACE	Atmospheric Chemistry Explorer
ADC	Analog to Digital Converter
AERONET	AERosol ROBotic NETwork
ATSR	Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
BSDF	Bi-directional Scatter Distribution Function
BUV	Backscatter UltraViolet
CCD	Charged Coupled Device
CFC	ChloroFluoroCarbon
CTE	Charge Transfer Efficiency
DEM	Detector Module
DM	Development Model
DOAS	Differential Optical Absorption Spectroscopy
DU	Dobson Unit ($1 \text{ DU} \equiv 2.687 \cdot 10^{16} \text{ molecules/cm}^2$)
ECMWF	European Centre for Medium-range Weather Forecasts
EGSE	Electrical Ground Supply Equipment
ELU	Electronics Unit
Envisat	Environmental satellite
EOS	Earth Observing System
EOS-Aura	Earth Observing Satellites Aura Mission
EP-TOMS	Earth Probe TOMS
ERS	European Remote Sensing satellite
ESA	European Space Agency
FMI	Finnish Meteorological Institute
FOV	Field of View
FS	Fokker Space
FTIR	Fourier Transform InfraRed
FWHM	Full Width at Half Maximum
GCOM	Global Change Observation Mission
GOME	Global Ozone Monitoring Experiment
GOMOS	Global Ozone Monitoring by Occultation of Stars
GSFC	Goddard Space Flight Center
HIRDLS	HIgh-Resolution Dynamics Limb Sounder
IASI	Infrared Atmospheric Sounding Interferometer
IFOV	Instantaneous Field of View
INDOEX	Indian Ocean Experiment
IPCC	Intergovernmental Panel on Climate Change
KNMI	Royal Netherlands Meteorological Institute (Koninklijk Nederlands Meteorologisch Instituut)
MCF	Methylchloroform
MERIS	MEDium Resolution Imaging Specrometer Instrument
METOP	Meteorological OPERational satellite
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology

NIVR	Netherlands Agency for Aerospace Programmes (Nederlands Instituut voor de Vliegtuigontwikkeling en Ruimtevaart)
NOAA	National Oceanic and Atmospheric Administration
NPOESS	National Polar-orbiting Operational Environmental Satellite System
NRT	Near Real Time
NWP	Numerical Weather Prediction
ODUS	Ozone Dynamics Ultraviolet Spectrometer
OMI	Ozone Monitoring Instrument
OMPS	Ozone Mapping and Profiler Suite
OSIRIS	Optical Spectrograph and InfraRed Imaging System
PFM	Proto-Flight Model
PI	Principal Investigator
PMD	Polarisation Measurement Device
PRF	Pixel Response Function
PSC	Polar Stratospheric Cloud
S/N	Signal to Noise
SAO	Smithsonian Astrophysical Observatory
SBUV	Solar Backscatter UltraViolet instrument
SCIAMACHY	Scanning imaging absorption spectrometer for atmospheric cartography
SciSAT	Small Scientific Satellite
SMR	Sub-Millimeter Radiometer
SRON	Space Research Organisation Netherlands
SSBUV	Shuttle Solar Backscatter UltraViolet instrument
SZA	Solar Zenith Angle
TES	Tropospheric Emission Spectrometer
TNO	Netherlands Organisation for Applied Scientific Research (Instituut voor Toegepast Natuurwetenschappelijk Onderzoek)
TOMS	Total Ozone Mapping Spectrometer
TOVS	TIROS Operational Vertical Sounder
TPD	Institute for Applied Physics (Technisch Physische Dienst)
UARS	Upper Atmosphere Research Satellite
UiO	University of Oslo
URD	User Requirements Document
UV	Ultraviolet
VFD	Very Fast Delivery
WLS	White Light Source
WMO	World Meteorological Organisation

List of Annexes

- ANNEX I** “List of Science Requirements”
- ANNEX II** “List of Definitions”
- ANNEX III** KNMI-OMI-2000-008 (version 1.1 of 7 December 2000)
“OMI Level 2 wavelength bands” by J.P. Veefkind
- ANNEX IV** RS-OMIE-KNMI-216 (version 1 of 28 September 2000)
“Spectral knowledge requirements for DOAS products” by R.F. van Oss
- ANNEX V** SN-OMIE-KNMI-203 (version 3 of 7 December 2000)
“Errors in reflectivity due to relative wavelength-shift and width of the slitfunction”
by R.F. van Oss
- ANNEX VI** RS-OMIE-KNMI-210 (version 1 of 28 November)
“Required S/N levels for OMI for DOAS products” by J.P. Veefkind
- ANNEX VII** RS-OMIE-KNMI-206 (version 1 of 31 July 2000)
“Definition of Level 1b Radiance product for OMI” by J.P. Veefkind, A. Mälkki
and R.D. McPeters
- ANNEX VIII** RS-OMIE-0000-NIVR-007 (version 2.2 of 10 March 2000)
“The Netherlands and Finnish data requirements in the operational phase of OMI”,
by J. Carpay & A. Mälkki
- ANNEX IX** KNMI-OMI-2000-004 (version 1 of 11 February 2000)
“Simulated radiances of OMI” by J.P. Veefkind
- ANNEX X** SN-OMIE-KNMI-236 (version 1 of 7 December 2000)
“Effects of spectral structures on DOAS retrieval” by J.P. Veefkind
- ANNEX XI** KNMI-OMI-2000-005 (version 1 of 18 February 2000)
“Effects of scrambler on NO₂ and BrO DOAS retrieval” by J.P. Veefkind
- ANNEX XII** “Reference cross-sections for the OMI data products”
- ANNEX XIII** KNMI-OMIE-2000-009 (version 1 of 8 December 1999)
“The effect of a non-linearity in the radiometric response of the OMI instrument”
by R. van der A

List of all Science Requirements

Introduction

All science and instrument requirements put on OMI-EOS are listed according to the following rule: **SR w.x.y.z**, in which **SR** stands for Science Requirement and **wxyz** stand for respectively chapter (**w**), section (**x**), subsection (**y**) and number of the requirement (**z**) in the SRD.

Science requirements (SRD Chapter 3)

List of priority 'A' products

- SR 3.1.1 OMI shall retrieve the Earth radiance spectrum.*
- SR 3.1.2 OMI shall retrieve the solar irradiance spectrum.*
- SR 3.1.3 OMI shall retrieve the total ozone column (off-line).*
- SR 3.1.4 OMI shall retrieve the ozone profile (off-line).*
- SR 3.1.5 OMI shall retrieve the aerosol optical thickness.*
- SR 3.1.6 OMI shall retrieve the aerosol single scattering albedo.*
- SR 3.1.7 OMI shall retrieve the total NO₂ column.*
- SR 3.1.8 OMI shall retrieve the cloud-scattering pressure.*
- SR 3.1.9 OMI shall retrieve the cloud fraction.*
- SR 3.1.10 OMI shall retrieve the surface UV-B flux.*
- SR 3.1.11 OMI shall retrieve the total ozone column Near Real Time (NRT) product.*
- SR 3.1.12 OMI shall retrieve the ozone profile (NRT) product.*
- SR 3.1.13 OMI shall retrieve the total ozone column Very Fast Delivery (VFD) product.*
- SR 3.1.14 OMI shall retrieve surface UV-B flux (VFD) product.*

List of priority 'B' products

- SR 3.1.15 OMI shall be able to retrieve the total SO₂ column.*
- SR 3.1.16 OMI shall be able to retrieve the total BrO column.*
- SR 3.1.17 OMI shall be able to retrieve the total OCIO column.*
- SR 3.1.18 OMI shall be able to retrieve the total HCHO column.*
- SR 3.1.19 OMI shall be able to retrieve the surface reflectance.*
- SR 3.1.20 OMI shall be able to retrieve UV spectra.*
- SR 3.1.21 OMI shall be able to retrieve the ozone profile Very Fast Delivery (VFD) product.*
- SR 3.1.22 OMI shall be able to retrieve the total HCHO column (VFD) product.*
- SR 3.1.23 OMI shall be able to retrieve UV spectra (VFD) product.*

List of synergetic products

- SR 3.1.24 OMI should be able to retrieve tropospheric O₃ columns by (among others) synergetic use of HIRDLS, TES, MLS and OMI data.*
- SR 3.1.25 OMI should be able to retrieve tropospheric NO₂ columns by (among others) synergetic use of HIRDLS, TES, MLS and OMI data.*

Cloud ground pixel size requirement

- SR 3.2.4.1 Cloud information shall be retrieved on at least the same scale as the smallest ground pixel of any of the OMI data products (a spatial resolution of 20 × 20 km² will be sufficient).*

General Near Real Time (NRT) requirements

- SR 3.2.7.1** *Near Real Time (NRT) products shall be available within 3 hours after observation.*
- SR 3.2.7.2** *NRT products shall have the same ground pixel size as the off-line products.*
- SR 3.2.7.3** *NRT products shall have global coverage in one day.*

General Very Fast Delivery (VFD) requirements

- SR 3.2.8.1** *The OMI data (gathered above Europe and Scandinavia) shall be downloaded to the FMI ground station at Sodankylä (Finland) on one pass per day.*
- SR 3.2.8.2** *Very Fast Delivery (VFD) products shall be available within 30 minutes after the reception of the data.*

Global coverage requirements

- SR 3.3.1** *OMI shall be able to achieve global coverage in one day*
- SR 3.3.2** *Global coverage means that OMI shall be able to measure the UV/VIS spectrum reflected from every part on Earth within 24 hours, except for regions which are not illuminated by sunlight in 24 hours.*
- SR 3.3.3** *Global coverage shall be possible with the ground pixel sizes as specified in Table 3.1 (see **SR 3.4.2b - SR 3.4.23b**)*
- SR 3.3.4** *Global coverage shall be possible with a ground pixel sampling equal to the ground pixel sizes*
- SR 3.3.5** *For solar zenith angles between 85 and 90 degrees, the requirements in Table 3.1 for the ground pixel size for ozone, NO₂, SO₂, HCHO, aerosol, cloud products and the surface reflectance can be slightly relaxed to about 100 × 100 km², in order to measure with sufficient S/N while maintaining the same accuracy.*
- SR 3.3.6** *For BrO and OCIO the requirements in Table 3.1 (see **SR 3.4.12** and **SR 3.4.13**) are applicable for all solar zenith angles.*

Scientific Requirements for the OMI data products from table 3.1

- SR 3.4.0** *Summarise of Table 3.1:
The general product requirements are given in **SR 3.1.1 - SR 3.3.6** and **SR 4.0.1** (i.e. the priority requirements are given in **SR 3.1.1 – SR 3.1.25**; the coverage requirements are given in **SR 3.2.7.3, SR 3.2.8.1** and in **SR 3.3.1 – SR 3.3.6**; the product availability requirements are given in **SR 3.2.7.1, SR 3.2.8.2** and in **SR 4.0.1**).
The product depended requirements are given in **SR 3.4.1 – SR 3.4.23** (i.e. the accuracy, ground pixel size at nadir and vertical resolution requirements).*

Scientific Requirements (from table 3.1) for the off-line products

- SR 3.4.1** *The accuracy of the irradiance product shall be less than or equal to 2 %.*
- SR 3.4.2a** *The accuracy of the radiance product shall be less than or equal to 2 %.*
- SR 3.4.2b** *The ground pixel size at nadir of the radiance product shall be less or equal to 20 × 20 km².*
- SR 3.4.3a** *The accuracy of the ozone column product shall be less than or equal to the largest of either 2 % or 4 DU*
- SR 3.4.3b** *The ground pixel size at nadir of the ozone column product shall be less or equal to 20 × 20 km².*
- SR 3.4.4a** *The accuracy of the ozone profile product shall be less than or equal to 10 % in the stratosphere and less than or equal to 30 % in the troposphere.*
- SR 3.4.4b** *The ground pixel size at nadir of the ozone profile product shall be less or equal to 40 × 40 km².*
- SR 3.4.4c** *The vertical resolution of the ozone profile product shall be about 5 km in stratosphere and less than or equal to 10 km in the troposphere over the vertical altitude range from 0 to 50 km.*
- SR 3.4.5a** *The accuracy of the aerosol optical thickness product shall be less than or equal to the largest of either 10 % or 0.08.*

- SR 3.4.5b** *The ground pixel size at nadir of the aerosol optical thickness product shall be less or equal to 20×20 km².*
- SR 3.4.6a** *The accuracy of the aerosol single scattering albedo product shall be less than or equal to 0.1.*
- SR 3.4.6b** *The ground pixel size at nadir of the aerosol single scattering albedo product shall be less or equal to 20×20 km².*
- SR 3.4.7a** *The accuracy of the NO₂ product shall be less than or equal to the largest of either 10 % or 10^{14} cm⁻² in unpolluted areas and less than or equal to 20 % in polluted areas.*
- SR 3.4.7b** *The ground pixel size at nadir of the NO₂ product shall be less or equal to 40×40 km².*
- SR 3.4.8a** *The accuracy of the cloud scattering pressure product shall be less than or equal to 100 hPa.*
- SR 3.4.8b** *The ground pixel size at nadir of the cloud scattering pressure product shall be less or equal to 20×20 km².*
- SR 3.4.9a** *The accuracy of the cloud fraction product shall be less than or equal to 0.1.*
- SR 3.4.9b** *The ground pixel size at nadir of the cloud fraction product shall be less or equal to 20×20 km².*
- SR 3.4.10a** *The accuracy of the surface UV-B flux product shall be less than or equal to 4 %.*
- SR 3.4.10b** *The ground pixel size at nadir of the surface UV-B flux product shall be less or equal to 20×20 km².*
- SR 3.4.11a** *The accuracy of the SO₂ column product shall be less than or equal to the largest of either 20 % or 0.4 DU.*
- SR 3.4.11b** *The ground pixel size at nadir of the SO₂ column product shall be less or equal to 40×40 km².*
- SR 3.4.12a** *The accuracy of the BrO column product shall be less than or equal to the largest of either 10 % or 10^{13} cm⁻².*
- SR 3.4.12b** *The ground pixel size at nadir of the BrO column product shall be less or equal to 40×40 km².*
- SR 3.4.13a** *The accuracy of the OCIO column product shall be less than or equal to the largest of either 20 % or 10^{15} cm⁻².*
- SR 3.4.13b** *The ground pixel size at nadir of the OCIO column product shall be less or equal to 40×40 km².*
- SR 3.4.14a** *The accuracy of the HCHO column product shall be less than or equal to the largest of either 20 % or 10^{15} cm⁻².*
- SR 3.4.14b** *The ground pixel size at nadir of the HCHO column product shall be less or equal to 40×40 km².*
- SR 3.4.15a** *The accuracy of the surface reflectance product shall be less than or equal to the largest of either 5 % or 0.01.*
- SR 3.4.15b** *The ground pixel size at nadir of the surface reflectance product shall be less or equal to 20×20 km².*
- SR 3.4.16a** *The accuracy of the UV spectra product shall be less than or equal to 10-20 % (depending on wavelength).*
- SR 3.4.16b** *The ground pixel size at nadir of the UV spectra product shall be less or equal to 20×20 km².*

Scientific Requirements (from table 3.1) for the Near Real Time (NRT) products

- SR 3.4.17a** *The accuracy of the ozone column NRT product shall be less than or equal to the largest of either 5 % or 10 DU.*
- SR 3.4.17b** *The ground pixel size at nadir of the ozone column NRT product shall be less or equal to 20×20 km².*
- SR 3.4.18a** *The accuracy of the ozone profile product NRT shall be less than or equal to 10 % in the stratosphere.*
- SR 3.4.18b** *The ground pixel size at nadir of the ozone profile NRT product shall be less or equal to 40×40 km².*
- SR 3.4.18c** *The vertical resolution of the ozone profile NRT product shall be about 5 km in stratosphere over the vertical altitude range from 10 to 50 km.*

Scientific Requirements (from table 3.1) for the Very Fast Delivery (VFD) products

- SR 3.4.19a** *The accuracy of the ozone column VFD product shall be less than or equal to the largest of either 5 % or 10 DU.*

- SR 3.4.19b** *The ground pixel size at nadir of the ozone column VFD product shall be less or equal to $20 \times 20 \text{ km}^2$.*
- SR 3.4.20a** *The accuracy of the surface UV-B flux VFD product shall be less than or equal to 10 %.*
- SR 3.4.20b** *The ground pixel size at nadir of the surface UV-B flux VFD product shall be less or equal to $20 \times 20 \text{ km}^2$.*
- SR 3.4.21a** *The accuracy of the ozone profile product VFD shall be less than or equal to 10 % in the stratosphere.*
- SR 3.4.21b** *The ground pixel size at nadir of the ozone profile VFD product shall be less or equal to $40 \times 40 \text{ km}^2$.*
- SR 3.4.21c** *The vertical resolution of the ozone profile VFD product shall be about 5 km in stratosphere and less than or equal to 10 km in the troposphere over the vertical altitude range from 10 to 50 km.*
- SR 3.4.22a** *The accuracy of the HCHO column VFD product shall be less than or equal to the largest of either 20 % or 10^{15} cm^{-2} .*
- SR 3.4.22b** *The ground pixel size at nadir of the HCHO column VFD product shall be less or equal to $40 \times 40 \text{ km}^2$.*
- SR 3.4.23a** *The accuracy of the UV spectra VFD product shall be less than or equal to 10-20 % (depending on wavelength).*
- SR 3.4.23b** *The ground pixel size at nadir of the UV spectra VFD product shall be less or equal to $20 \times 20 \text{ km}^2$.*

Table 3.1 Overview of the scientific requirements for the priority 'A' and 'B' OMI data products.

In column 2, priorities are listed for each product (in the context of the OMI mission objectives): Priority A indicates highest (at launch availability) priority, priority B is assigned to desired (post launch availability) products. All products are level 2 products, except the 4(ir)radiances which are level 1b products. Each product has a global coverage of one day, except for the Very Fast Delivery (VFD) products. Product delivery requirements are for Near Real Time (NRT) products less than 3 hours after observation and less than 30 minutes after the data receipt for the VFD products, for other products less than two days after observation. The accuracy is defined in the introduction of section 3.2. With column is meant the vertical column. (T) stands for "in the troposphere", (S) stands for "in the stratosphere". 1 DU = $2.687 \cdot 10^{16}$ mol./cm².

Data product	Priority status	Accuracy of observations ¹⁾	Ground pixel size at nadir (km x km)	Vertical resolution (km)	Remarks
Irradiances ^{2), 3)}	A	≤ 2 %	N/A	N/A	
Radiances ²⁾	A	≤ 2 %	≤ 20 x 20	N/A	
Ozone column	A	≤ 2 % / 4 DU	≤ 20 x 20	N/A	
Ozone profile	A	≤ 30 % (T) ≤ 10 % (S)	≤ 40 x 40	≤ 10 km (T) ≥ 5 km (S)	Vertical range is 0-50 km
Aerosol optical thickness	A	≤ 10 % / 0.08	≤ 20 x 20	N/A	At 400 nm
Aerosol single scattering albedo	A	0.1	≤ 20 x 20	N/A	
NO ₂ column ⁴⁾	A	≤ 10 % / 10 ¹⁴ mol. cm ⁻²	≤ 40 x 40	N/A	
Cloud scattering pressure	A ⁵⁾	≤ 100 hPa	≤ 20 x 20	N/A	
Cloud fraction	A ⁵⁾	≤ 0.1	≤ 20 x 20	N/A	
Surface UV-B flux	A	≤ 4%	≤ 20 x 20	N/A	
SO ₂ column	B	≤ 20 % / 0.4 DU	≤ 40 x 40	N/A	Pollution, volcanic
BrO column	B	≤ 10 % / 10 ¹³ mol. cm ⁻²	≤ 40 x 40	N/A	
OCIO column	B	≤ 20 % / 10 ¹³ mol. cm ⁻²	≤ 40 x 40	N/A	Polar vortex
HCHO column	B	≤ 20 % / 10 ¹⁵ mol cm ⁻²	≤ 40 x 40	N/A	Pollution
Surface reflectance	B	≤ 5 % / 0.01	≤ 20 x 20	N/A	
UV spectra	B	≤ 10-20 %	≤ 20 x 20	N/A	Accuracy is wavelength dependent
Near Real Time Products					
Ozone column	A	≤ 5 % / 10 DU	≤ 20 x 20	N/A	
Ozone profile	A	≤ 10 % (S)	≤ 40 x 40	≥ 5 km (S)	Vertical range is 10-50 km
Very Fast Delivery Products					
Ozone column	A	≤ 5 % / 10 DU	≤ 20 x 20	N/A	Over Northern Europe
Surface UV-B flux	A	≤ 10 %	≤ 20 x 20	N/A	Over Northern Europe
Ozone profile	B	≈ 10 % (S)	≤ 40 x 40	≥ 5 km (S)	Vertical range is 10-50 km Over Northern Europe
HCHO column	B	≤ 20 % / 10 ¹⁵ mol. cm ⁻²	≤ 40 x 40	N/A	Over Northern Europe
UV spectra	B	≤ 10-20 %	≤ 20 x 20	N/A	Over Northern Europe Accuracy is wavelength dependent

Note 1) The valid requirement on accuracy will be the largest of the given percentile or absolute number.

Note 2) The requirements for radiance and irradiance follow from Chapter 4.

Note 3) Irradiance is not a separate data product.

Note 4) The required accuracy for the NO₂ column is about 10% in unpolluted areas, but about 20% in polluted areas.

Note 5) Cloud scattering pressure and cloud fraction are also needed for the retrieval of other products by OMI and other instruments.

Algorithm requirements (SRD Chapter 4)

General algorithm requirements

Product availability requirements

SR 4.0.1 *The off-line level 2 products shall be available less than two days after observation.*

Geographical Coverage and Resolution

SR 4.2.1.1 *The Level 1b radiance data shall have daily global coverage.*

SR 4.2.1.2 *The ground pixel size of the Level 1b data shall be $20 \times 20 \text{ km}^2$ at nadir, or smaller.*

SR 4.2.1.3 *For the wavelengths below 310 nm, the ground pixel size of the Level 1b data shall be $40 \times 40 \text{ km}^2$ at nadir, or smaller.*

SR 4.2.1.4 *In the Level 1b product, the geolocation of the pixels shall be given, with an accuracy of $1/10^{\text{th}}$ of the ground pixel size.*

SR 4.2.1.5 *For at least one wavelength, the Level 1b data shall be obtained with a higher spatial sampling than for the nominal pixels.*

Spectral Range

SR 4.2.2.1 *The total spectral range shall at least cover the range between 270 and 500 nm.*

Spectral Resolution and Sampling

SR 4.2.3.1 *The spectral resolution and sampling shall be as listed in Table 5.1 (SR 5.1.1.9 – SR 5.1.1.15).*

Spectral Knowledge

SR 4.2.4.1 *The required spectral knowledge of the radiance and irradiance spectra shall be better than $1/100^{\text{th}}$ of a CCD-pixel above 300 nm and better than $1/50^{\text{th}}$ of a CCD-pixel below 300 nm for ozone profile retrieval.*

Spectral Stability

SR 4.2.5.1 *The required spectral stability for Earth and solar measurements is at least $1/20^{\text{th}}$ of a CCD-pixel.*

Radiometric Accuracy

SR 4.2.7.1 *The overall requirement for the radiometric accuracy of the reflectivity is 1%.*

Level 1b Product Content

SR 4.2.8.2 *All Level 1b product content requirements, specified in the latest version of the "OMI Level 1b data format", shall be applicable.*

Level 1b Product Availability

SR 4.2.9.1 *The level 1b data shall be accessible within 24 hours after arrival of the OMI level 0 at the processing site.*

SR 4.2.9.2 *A preliminary version of the Level 1b data has to be available within 2½ hours after observation to derive the NRT products.*

SR 4.2.9.3 *All other Level 1b product availability requirements, specified in the latest version of RS-OMIE-0000-NIVR-007 "The Netherlands and Finnish data requirements in the operational phase of OMI", shall be applicable.*

Viewing angles: knowledge & precision

- SR 4.2.10.1 The required accuracy knowledge for the Solar Zenith angle is 0.08°.*
- SR 4.2.10.2 The required accuracy knowledge for the viewing zenith angle 0.08°.*
- SR 4.2.10.3 The required accuracy knowledge for the relative azimuth angle 0.05°.*

Level 1b Requirements from table 4.1

SR 4.3.0 Summarise of Table 4.1:

The general requirements on the Level 1b product are given in SR 4.2.1.1 – SR 4.2.10.3. (i.e. the geographical coverage and resolution requirements are given in SR 4.2.1.1 – SR 4.2.1.5; the spectral (range, resolution, sampling, knowledge and stability) requirements are given in SR 4.2.2.1 – SR 4.2.5.1; the requirement on the overall radiometric accuracy of the reflectivity is given in SR 4.2.7.1; the Level 1b product contents and availability requirements are given in SR 4.2.8.1, SR 4.2.8.2 and SR 4.2.9.1 – SR 4.2.9.3; the knowledge and precision requirements on the viewing angles are specified in SR 4.2.10.1 – SR 4.2.10.3).

The product depended requirements on the Level 1b product are given in SR 4.3.1 – SR 4.3.21 (i.e. the spectral range, spectral knowledge, radiometric accuracy of the reflectivity and radiometric precision requirements).

Level 1b Requirements (from table 4.1) for the off-line products

- SR 4.3.1a-1 The available spectral range for the ozone column DOAS product shall be at least 320 – 340 nm.*
- SR 4.3.1a-2 The available spectral range for the ozone column TOMS product shall be at least 310 – 380 nm.*
- SR 4.3.1b-1 The spectral knowledge of the ozone column DOAS product shall be at least 1/100th CCD-pixel.*
- SR 4.3.1b-2 The spectral knowledge of the ozone column TOMS product shall be at least 1/3rd CCD-pixel.*
- SR 4.3.1c-1 The radiometric accuracy of the ozone column DOAS product shall be at least 3%.*
- SR 4.3.1c-2 The radiometric accuracy of the ozone column TOMS product shall be at least 1%.*
- SR 4.3.1d-1 The radiometric precision (S/N) of the ozone column DOAS product shall be at least 250 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.1d-2 The radiometric precision (S/N) of the ozone column TOMS product shall be at least 300 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.2a The available spectral range for the ozone profile product shall be at least 270 – 340 nm.*
- SR 4.3.2b The spectral knowledge of the ozone profile product shall be at least 1/50th CCD-pixel.*
- SR 4.3.2c The radiometric accuracy of the ozone profile product shall be at least 1%.*
- SR 4.3.2d The radiometric precision (S/N) of the ozone profile product shall be at least 100 below 310 nm (for ground pixel size of 40 × 40 km²).*
- SR 4.3.3a The available spectral range for the aerosol optical thickness product shall be at least 340 – 500 nm.*
- SR 4.3.3c The radiometric accuracy of the aerosol optical thickness product shall be at least 1%.*
- SR 4.3.3d The radiometric precision (S/N) of the aerosol optical thickness product shall be at least 500 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.4a The available spectral range for the aerosol single scattering albedo product shall be at least 340 – 500 nm.*
- SR 4.3.4c The radiometric accuracy of the aerosol single scattering albedo product shall be at least 1%.*
- SR 4.3.4d The radiometric precision (S/N) of the aerosol single scattering albedo product shall be at least 500 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.5a The available spectral range for the NO₂ column product shall be at least 425 – 450 nm.*
- SR 4.3.5b The spectral knowledge of the NO₂ column product shall be at least 1/50th CCD-pixel.*

- SR 4.3.5c** *The radiometric accuracy of the NO₂ column product shall be at least 3%.*
- SR 4.3.5d** *The radiometric precision (S/N) of the NO₂ column product shall be at least 5800 (for ground pixel size of 40 × 40 km²).*
- SR 4.3.6a-1** *The available spectral range for the cloud top pressure product shall be at least 390 – 400 nm*
- SR 4.3.6a-2** *Also available for the cloud top pressure product shall be the spectral range of at least 470 – 485 nm.*
- SR 4.3.6b** *The spectral knowledge of the cloud top pressure product shall be at least 1/100th CCD-pixel.*
- SR 4.3.6c** *The radiometric accuracy of the cloud scattering pressure product shall be at least 3%.*
- SR 4.3.6d-2** *The radiometric precision (S/N) of the cloud top pressure product shall be at least 1600 in the spectral range of at least 470 – 480 nm (for ground pixel size of 20 × 20 km²).*
- SR 4.3.7a** *The available spectral range for the cloud fraction product shall be at least 320 – 500 nm.*
- SR 4.3.7c** *The radiometric accuracy of the cloud fraction product shall be at least 1%.*
- SR 4.3.8** *The surface UV-B product requires the fulfilment of the requirements on the ozone column (SR 4.3.1), cloud cover (SR 4.3.7) and aerosol (SR 4.3.3 and SR 4.3.4) products.*
- SR 4.3.9a** *The available spectral range for the SO₂ column product shall be at least 300 – 300 nm.*
- SR 4.3.9b** *The spectral knowledge of the SO₂ column product shall be at least 1/100th CCD-pixel.*
- SR 4.3.9c** *The radiometric accuracy of the SO₂ column product shall be at least 3%.*
- SR 4.3.9d** *The radiometric precision (S/N) of the SO₂ column product shall be at least 400 (for ground pixel size of 40 × 40 km²).*
- SR 4.3.10a** *The available spectral range for the BrO column product shall be at least 344 – 360 nm.*
- SR 4.3.10b** *The spectral knowledge of the BrO column product shall be at least 1/50th CCD-pixel.*
- SR 4.3.10c** *The radiometric accuracy of the BrO column product shall be at least 3%.*
- SR 4.3.10d** *The radiometric precision (S/N) of the BrO column product shall be at least 2500 (for ground pixel size of 40 × 40 km²).*
- SR 4.3.11a** *The available spectral range for the OCIO column product shall be at least 355 – 385 nm.*
- SR 4.3.11b** *The spectral knowledge of the OCIO column product shall be at least 1/100th CCD-pixel.*
- SR 4.3.11c** *The radiometric accuracy of the OCIO column product shall be at least 3%.*
- SR 4.3.11d** *The radiometric precision (S/N) of the OCIO column product shall be at least 1500 (for ground pixel size of 40 × 40 km²).*
- SR 4.3.12a** *The available spectral range for the HCHO column product shall be at least 335 – 360 nm.*
- SR 4.3.12b** *The spectral knowledge of the HCHO column product shall be at least 1/100th CCD-pixel.*
- SR 4.3.12c** *The radiometric accuracy of the HCHO column product shall be at least 3%.*
- SR 4.3.12d** *The radiometric precision (S/N) of the HCHO column product shall be at least 3200 (for ground pixel size of 40 × 40 km²).*
- SR 4.3.13a** *The available spectral range for the surface reflectance product shall be at least 320 – 500 nm.*
- SR 4.3.13c** *The radiometric accuracy of the surface reflectance product shall be at least 1%.*
- SR 4.3.13d** *The radiometric precision (S/N) of the surface reflectance product shall be at least 100 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.14** *The UV spectra product requires the fulfilment of the requirements on the ozone column (SR 4.3.1), cloud cover (SR 4.3.7) and aerosol (SR 4.3.3 and SR 4.3.4).*

Level 1b Requirements (from table 4.1) for the Near Real Time (NRT) products

- SR 4.3.15a** *The available spectral range for the ozone column NRT product shall be at least 320 – 340 nm.*
- SR 4.3.15b** *The spectral knowledge of the ozone column NRT product shall be at least 1/50th CCD-pixel.*
- SR 4.3.15c** *The radiometric accuracy of the ozone column NRT product shall be at least 3%.*
- SR 4.3.15d** *The radiometric precision (S/N) of the ozone column NRT product shall be at least 100 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.16a** *The available spectral range for the ozone profile NRT product shall be at least 270 – 340 nm.*

- SR 4.3.16b** *The spectral knowledge of the ozone profile NRT product shall be at least 1/50th CCD-pixel.*
- SR 4.3.16c** *The radiometric accuracy of the ozone profile NRT product shall be at least 1%.*
- SR 4.3.16d** *The radiometric precision (S/N) of the ozone profile NRT product shall be at least 100 below 310 nm (for ground pixel size of 40 × 40 km²).*

Level 1b Requirements (from table 4.1) for the Very Fast Delivery (VFD) products

- SR 4.3.17a** *The available spectral range for the ozone column VFD product shall be at least 320 – 340 nm.*
- SR 4.3.17b** *The spectral knowledge of the ozone column VFD product shall be at least 1/50th CCD-pixel.*
- SR 4.3.17c** *The radiometric accuracy of the ozone column VFD product shall be at least 3%.*
- SR 4.3.17d** *The radiometric precision (S/N) of the ozone column VFD product shall be at least 100 (for ground pixel size of 20 × 20 km²).*
- SR 4.3.18** *The surface UV-B VFD product requires the fulfilment of the requirements on the ozone column VFD product (SR 4.3.17).*
- SR 4.3.19a** *The available spectral range for the ozone profile VFD product shall be at least 270 – 340 nm.*
- SR 4.3.19b** *The spectral knowledge of the ozone profile VFD product shall be at least 1/50th CCD-pixel.*
- SR 4.3.19c** *The radiometric accuracy of the ozone profile VFD product shall be at least 1%.*
- SR 4.3.19d** *The radiometric precision (S/N) of the ozone profile VFD product shall be at least 100 below 310 nm (for ground pixel size of 40 × 40 km²).*
- SR 4.3.20** *The UV spectra product requires the fulfilment of the requirements on the ozone column VFD product (SR 4.3.17).*
- SR 4.3.21a** *The available spectral range for the HCHO VFD column product shall be at least 335 – 360 nm.*
- SR 4.3.21b** *The spectral knowledge of the HCHO VFD column product shall be at least 1/100th CCD-pixel.*
- SR 4.3.21c** *The radiometric accuracy of the HCHO VFD column product shall be at least 3%.*
- SR 4.3.21d** *The radiometric precision (S/N) of the HCHO VFD column product shall be at least 3200 (for ground pixel size of 40 × 40 km²).*

Auxiliary and Ancillary Data Requirements

- SR 4.4.1** *All requirements, specified in the latest version of “Auxiliary and Ancillary data requirements document for OMI-EOS”, shall be applicable.*

Level 0-1b processing requirements

- SR 4.5.1** *All requirements as specified in the latest version of RS-OMIE-7000-FS-186 “User Requirements Document for the OMI Level 0 to 1b Data Processor”, shall be applicable.*

Table 4.1 Overview of the Level 1b product requirements for the priority 'A' and 'B' OMI data products.

Data product	Spectral Range [nm]	Ground pixel size [km x km]	Spectral knowledge [CCD pixel]	Radiometric accuracy ¹⁾ [%]	Radiometric precision ²⁾ [S/N]
Ozone column	320 – 340	20 x 20	0.01	≤ 3	≥ 250
• DOAS	310 – 380	20 x 20	0.33	≤ 1	≥ 300
• TOMS	270 – 340	40 x 40	0.02	≤ 1	λ < 310 ≥ 100
Ozone profile	340 – 500	20 x 20	not critical	≤ 1	≥ 500
Aerosol optical thickness	340 – 500	20 x 20	not critical	≤ 1	≥ 500
Aerosol single scattering albedo	425 – 450	40 x 40	0.02	≤ 3	≥ 5800
NO ₂ column	390 – 400	20 x 20	0.01	≤ 3	not critical
Cloud scattering pressure	470 – 485	20 x 20	0.01	≤ 3	≥ 1600 ³⁾
Cloud fraction	320 – 500	20 x 20	not critical	≤ 1	not critical
Surface UV-B	280 – 400	20 x 20	not critical	not critical	not critical
SO ₂ column	300 – 330	40 x 40	0.01	≤ 3	≥ 400
BrO column	344 – 360	40 x 40	0.02	≤ 3	≥ 2500
OCIO column	355 – 385	40 x 40	0.01	≤ 3	≥ 1500
HCHO column	335 – 360	40 x 40	0.01	≤ 3	≥ 3200
Surface reflectance	320 – 500	20 x 20	not critical	≤ 1	≥ 100
UV spectra	280 – 400	20 x 20	not critical	not critical	not critical
Near Real Time Products					
Ozone column	320 – 340	20 x 20	0.02	≤ 3	≥ 100
Ozone profile	270 – 340	40 x 40	0.02	≤ 1	λ < 310 ≥ 100
Very Fast Delivery Products					
Ozone column	320 – 340	20 x 20	0.02	≤ 3	≥ 100
Surface UV-B flux	280 – 400	20 x 20	not critical	not critical	not critical
Ozone profile	270 – 340	40 x 40	0.02	≤ 1	λ < 310 ≥ 100
UV spectra	280 – 400	20 x 20	not critical	not critical	not critical
HCHO column	335 – 360	40 x 40	0.01	≤ 3	≥ 3200

Note 1) The radiometric accuracy defined here refers to the reflectivity (i.e. ratio of the Earth radiance and the solar irradiance)
 Note 2) S/N requirements are valid for the given ground pixels size in column 3 (i.e. the same ground pixel sizes as in Table 3.1)
 Note 3) The most stringent requirement on radiometric precision is given by the method using the 477 nm O₂-O₂ collision complex.
 Note 4) A requirement noted as not critical means that other products demand stronger requirements for the Level 1b product.

Instrument requirements (SRD Chapter 5)

Overall characteristics

- SR 5.0.1** *The OMI instrument shall be built such that it is possible to retrieve the products as listed in Table 3.1 (SR 3.4.0) with the noted accuracies, spatial resolutions etc., using the algorithms as summarised in Chapter 4 (SR 4.3.0).*
- SR 5.0.2** *OMI shall measure the Earth radiance and the solar irradiance spectra.*
- SR 5.0.3** *OMI shall not have a scan mirror.*
- SR 5.0.4** *OMI shall not be sensitive to polarisation.
Note: this is quantified with the requirement on rest-polarisation and similar structures in the signal, SR 5.0.10 and with SR 5.2.2.8.*
- SR 5.0.5** *OMI shall be designed and operated in a way that prevents etalon effect.*
- SR 5.0.6** *OMI ground pixel shall be smaller than $20 \times 20 \text{ km}^2$.*
- SR 5.0.7** *OMI shall have a field-of-view that provides cross-track global coverage at all latitudes of the atmosphere in one day from the EOS-Aura spacecraft orbit.*
- SR 5.0.8** *OMI shall not suffer from spatial aliasing.*
- SR 5.0.9** *The OMI Duty Cycle shall be 100% (continuous operation) in flight.*
- SR 5.0.10** *In general, the instrument sensitivity to polarisation shall not be more than 0.5% for fully polarised incident light, for all polarisation directions, over the Full Performance Range.
This means that fully polarised and unpolarised light should give the same instrumental response within 0.5% over the entire spectral range.*
- SR 5.0.11** *Optics, detectors and electronics of OMI shall have sufficient reliability (including radiation hardness) for the expected 5-year lifetime of EOS-Aura.*
- SR 5.0.12** *OMI shall provide images of atmospheric radiance and the solar irradiance of visible wavelengths.*
- SR 5.0.13** *OMI shall provide images of atmospheric radiance and the solar irradiance of ultra-violet wavelengths.*
- SR 5.0.14** *OMI shall view in nadir direction, with a field-of-view in swath direction, which is perpendicular to the spacecraft's flight direction, and a field-of-view in flight direction.*
- SR 5.0.15** *OMI shall use a polarisation scrambler to scramble the polarisation of the incoming atmospheric radiance.*
- SR 5.0.16** *OMI shall convert radiance to spectrum.*
- SR 5.0.17** *OMI shall convert photons to ADC counts.*
- SR 5.0.17-note** *The spacecraft will send the ADC counts to ground.*
- SR 5.0.18** *The OMI Ground Data Processor shall process the data (i.e. ADC counts) to level 1b products.*

Spectral properties

- SR 5.1.1.1** *OMI shall be a nadir viewing imaging spectrometer with full performance range 270-500 nm.*
- SR 5.1.1.2** *OMI shall have an ultraviolet (UV) channel with full performance range 270-365 nm.*
- SR 5.1.1.3** *OMI shall have a visible (VIS) channel with full performance range 365-500 nm.*
- SR 5.1.1.4** *The 50 % sensitivity point of both channels shall be 365 nm.*
- SR 5.1.1.5** *The total overlap of the UV and VIS channels shall be the range 350-380 nm.*
- SR 5.1.1.6** *The UV channel shall be split into two parts, UV-1 and UV-2, with full performance ranges 270-310 nm and 310-365 nm, respectively.*
- SR 5.1.1.7** *The 50 % sensitivity point of both UV channels shall be 310 nm.*
- SR 5.1.1.8** *The total overlap of the UV-1 and UV-2 channels shall be the range 306-314 nm.*
- SR 5.1.1.9** *The spectral resolution of the UV-1 channel shall equal or better than 0.64 nm.*
- SR 5.1.1.10** *The spectral resolution of the UV-2 channel shall equal or better than 0.45 nm.*
- SR 5.1.1.11** *The spectral resolution of the VIS channel shall equal or better than 0.63 nm.*

- SR 5.1.1.12** *The spectral sampling of the UV-1 channel shall equal or better than 0.32 nm while keeping a sampling ratio equal or larger than 2.*
- SR 5.1.1.13** *The spectral sampling of the UV-2 channel shall equal or better than 0.15 nm while keeping a sampling ratio equal or larger than 3.*
- SR 5.1.1.15** *The spectral sampling of the VIS channel shall equal or better than 0.21 nm while keeping a sampling ratio equal or larger than 3.*
- SR 5.1.1.16** *The total range, full performance range, spectral resolution, and spectral sampling distance of OMI shall be as specified in Table 5.1. (Summarise of SR 5.1.1.1 up to SR 5.1.1.15).*

Table 5.1: Required spectral range and resolution of OMI.
“Resolution” means the FWHM of the slit function.

Channel	Total range	Full performance range	Resolution in nm	Resolution in pixels	Sampling distance
UV-1	270 - 314 nm	270 - 310 nm	≤ 0.64 nm	≥ 2	≤ 0.32 nm
UV-2	306 - 380 nm	310 - 365 nm	≤ 0.45 nm	≥ 3	≤ 0.15 nm
VIS	350 - 500 nm	365 - 500 nm	≤ 0.63 nm	≥ 3	≤ 0.21 nm

Spatial properties and observation modes

- SR 5.1.2.1** *The UV and VIS channels of OMI shall have a CCD as detector, where the spectrum is imaged in one direction and the swath is imaged in the other direction.*
- SR 5.1.2.2** *OMI shall have a swath of 2600 km wide or larger to achieve daily global coverage.*
- SR 5.1.2.3** *OMI shall have contiguous coverage of the Earth both along and across satellite ground track.*
- SR 5.1.2.4** *The instantaneous spatial resolution of OMI shall be 10 × 10 km² or smaller at the sub-satellite point.*
- SR 5.1.2.5** *The instantaneous spatial resolution of OMI shall be 10 × 10 km² or smaller at the sub-satellite point.*
- SR 5.1.2.6** *The spatial angles seen by the OMI pixel shall be constant over the swath.*
- SR 5.1.2.7** *The swath width and sub-satellite ground pixel size of OMI shall be as specified in Table 5.2, for the global mode, the spectral zoom-in mode, and the spatial zoom-in mode.*

Table 5.2 Required swath width and sub-satellite ground pixel of OMI for the three different observation modes.

Observation mode	Spectral range	Swath width*	Ground pixel size (along x across track)	Application
Global mode				
UV-1	270 - 310 nm	2600 km	13 × 48 km ²	global observation of all products
UV-2 & VIS	310 - 500 nm	2600 km	13 × 24 km ²	
Spatial zoom-in mode				
UV-1	270 - 310 nm	2600 km	13 × 24 km ²	regional studies of all products
UV-2 & VIS	310 - 500 nm	≥ 725 km	13 × 12 km ²	
Spectral zoom-in mode				
UV	At least 306 - 364 nm	2600 km	13 × 12 km ²	global observation of some products
VIS	At least 350 - 432 nm	2600 km	13 × 12 km ²	

* and symmetric around sub-satellite track

- SR 5.1.2.8** *A sub-pixel read-out capability shall exist for one wavelength in the UV channel and one wavelength in the VIS channel of OMI, which is achieved by not co-adding the CCD-images for all three observation modes.*
- SR 5.1.2.9** *It shall be possible to choose the wavelengths for sub-pixel data flexible.*
- SR 5.1.2.10** *The latitude and longitude of the centre of each ground pixel shall be known with an accuracy better than $1/10^{\text{th}}$ of the size of the ground pixel of the global, spatial and spectral zoom in modes (either in an angular unit or in a distance unit on the Earth's surface).*

Detector requirements

- SR 5.1.3.1** *At the edges of the CCD, dark current and straylight shall be measured on every exposure.*
- SR 5.1.3.2** *Frame transfer smear shall be measured for every exposure.*
- SR 5.1.3.3** *The spectrum of each viewing direction (i.e. one CCD row) shall be spectrally calibrated separately.*
- SR 5.1.3.4** *Gain switching in the preamplifier shall be used to improve S/N in the UV channel.*
- SR 5.1.3.5** *There shall be 4 different gains per CCD detector.*
- SR 5.1.3.6** *The order of gains shall be programmable in flight.*
- SR 5.1.3.7** *The wavelength at which the gain is switched shall be programmable in flight.*
- SR 5.1.3.8** *Gain switching shall be such that the range between minimum and maximal radiance permits an optimal use of the full dynamical range of the 12 bits ADC converter.*
- SR 5.1.3.9** *The alignment of the slit of OMI with the CCD shall be accurate within 0.4 CCD pixel. This means that in each spectral channel (UV 1, UV 2 and VIS) each CCD row shall contain the spectrum belonging to one viewing direction, within an accuracy of 0.4 CCD pixel in the swath direction.*
- SR 5.1.3.10** *The co-alignment of the UV-2 and VIS channels shall be within 1 CCD pixel in the swath direction.*
- SR 5.1.3.11** *The co-alignment of the UV-1 and UV-2 channels shall be within 1 CCD pixel in the swath direction.*
- SR 5.1.3.12** *Optical distortion leading to different spectral definition as a function of the viewing angle, like the curved swath image, shall not influence the required spectral range over the entire CCD, according to Table 5.1 (SR 5.1.1.16).*
- SR 5.1.3.13** *The curved swath image shall not influence the required spectral resolution and sampling distance over the entire CCD, according to Table 5.1 (SR 5.1.1.16), to within a margin of 10 % around these values.*
- SR 5.1.3.14** *Spectral lines imaged onto the columns of the CCD for both channels shall be aligned with an accuracy of 0.1 CCD pixel.*
- SR 5.1.3.15** *CCD exposure times shall be possible between 0.1 s and 6 s.*
- SR 5.1.3.16** *OMI shall be able to do long exposures between 6 and 768 s.*
- SR 5.1.3.17** *The nominal exposure time shall be 0.4 s.*
- SR 5.1.3.18** *The exposure time shall be programmable during flight.*
- SR 5.1.3.19** *Read-out time shall not influence data acquisition in the image area of the CCD.*
- SR 5.1.3.20** *Co-adding of images shall be possible, with co-addition period between 2 s and 6 s.*
- SR 5.1.3.21** *The co-addition period shall be programmable during flight.*
- SR 5.1.3.22** *Binning of pixels (in the swath direction) shall be possible.*
- SR 5.1.3.23** *Binning factors between 1 and 15 shall be possible.*
- SR 5.1.3.24** *The binning factor shall be programmable during flight.*
- SR 5.1.3.25** *It shall be possible to operate the UV and VIS channels independently (so that different exposure time, co-addition period, read-out time and binning factors are possible).*
- SR 5.1.3.26** *The CCD detectors shall not have more than 100 bad or dead pixels.*
- SR 5.1.3.27** *Bad/dead pixels shall not influence the retrieval accuracy of any of the OMI data products listed in Table 3.1.*
- SR 5.1.3.28** *There shall be no bad or dead pixels in the read-out register.*

- SR 5.1.3.29** *The instrument shall be operated in such a way that no ice forms on the CCD or on any other optical component in the OMI-instrument.*
- SR 5.1.3.30** *All channels (UV and VIS) shall start their exposures simultaneously when equal read-out disciplines are used.*

Radiometric Accuracy: Random errors (required signal-to-noise)

- SR 5.2.1.1** *The S/N ratio's for the Earth radiance measurements as tabulated in Table 5.3 shall be reached for the minimum radiance levels as shown in Figure 5.2.*
- SR 5.2.1.2** *The OMI instrument shall not saturate for the maximum Earth radiance levels as defined in Figure 5.2*

Table 5.3 **Required scaled signal-to-noise levels for different wavelength ranges.**
The values in this table are derived from the values in Table 4.1. by re-scaling for the ground pixel sizes given in this table.

Wavelength range	Critical trace gas	Scaled S/N (global mode)	Scaled S/N (spatial zoom-in mode)
270 – 310 nm	O ₃ profile	60 (13 × 48 km ²)	45 (13 × 24 km ²)
310 – 335 nm	O ₃ column	265 (13 × 24 km ²)	190 (13 × 12 km ²)
335 – 365 nm	HCHO	1450 (13 × 24 km ²)	1050 (13 × 12 km ²)
365 – 420 nm	OCIO	700 (13 × 24 km ²)	470 (13 × 12 km ²)
420 – 450 nm	NO ₂	2600 (13 × 24 km ²)	1850 (13 × 12 km ²)
450 – 500 nm	O ₂ – O ₂	1400 (13 × 24 km ²)	1000 (13 × 12 km ²)

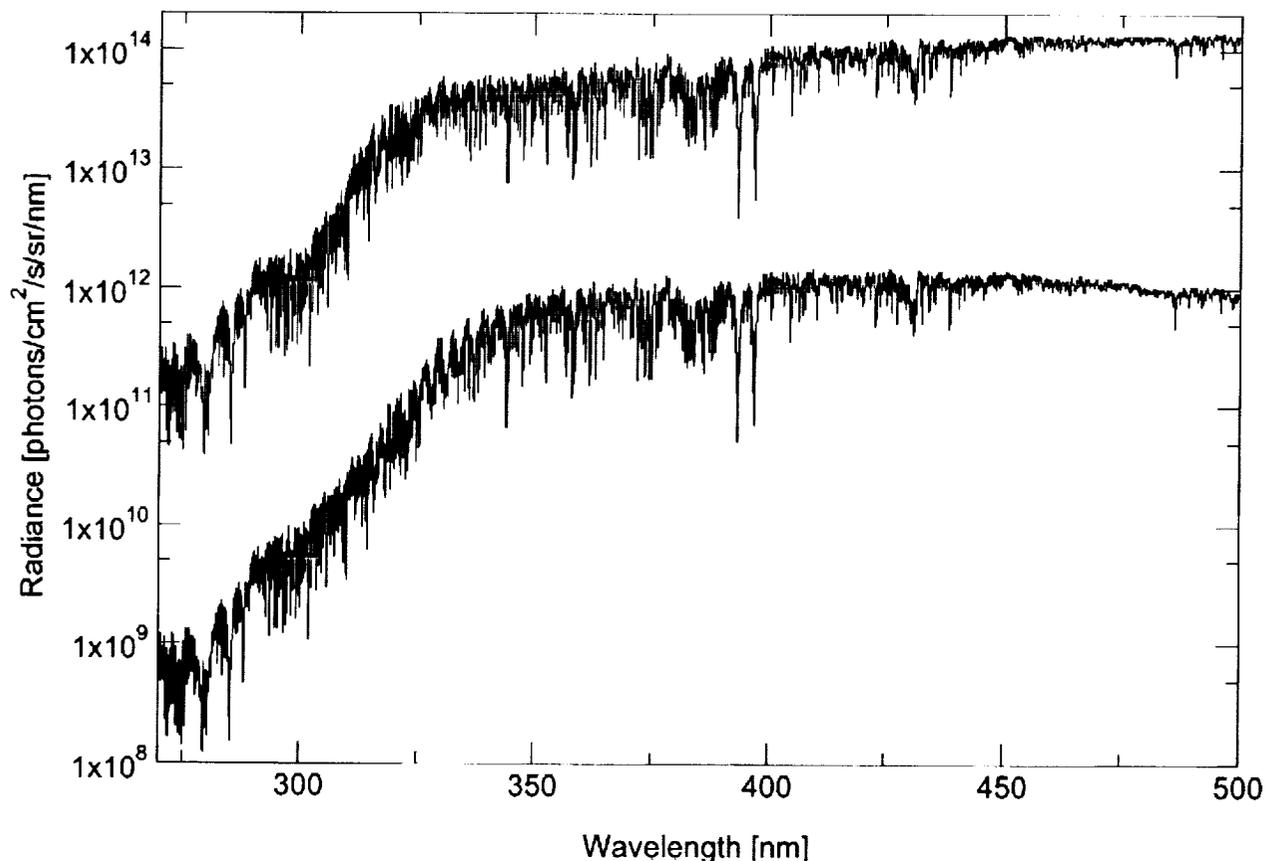


Fig. 5.2 *Overall minimum and maximum radiances to be observed by OMI, as derived from simulations for different scenario's as described in Annex XII.*

- SR 5.2.1.3** *Solar irradiance measurements, through the calibration port of OMI, shall have S/N ratios of at least 1000, independent of season.*
- SR 5.2.1.4** *During solar irradiance measurements OMI shall not saturate, independent of season.*
- SR 5.2.1.5** *The OMI Instrument shall not be damaged by high Earth radiances (red line in Figure 5.2) or solar irradiances entering the telescope and/or caused by:*
- the sun glint effect*
 - lasers used for the alignment (less than 20 mW)*
 - the sun*

Radiometric Accuracy: Systematic errors

- SR 5.2.2.1** *Requirements SR 5.2.2.4 – SR 5.3.3 shall be met for all swath angles, wavelengths, positions in orbit and seasons.*
- SR 5.2.2.2** *The calibration lamp used for the absolute radiometric calibration (see SR 5.2.2.4) shall be a NIST calibrated 1000 W FEL lamp and shall be NIST traceable.*
- SR 5.2.2.3** *The NIST calibrated 1000 W FEL lamp shall be calibrated within a 2 % (2σ error) accuracy over the total spectral range of OMI (270 nm – 500 nm).*
- SR 5.2.2.4** *The absolute radiometric accuracy of the atmospheric radiance and the solar irradiance spectra shall be known to within $\leq 2\%$, excluding the calibration lamp error.*
- SR 5.2.2.5** *The error in the absolute reflectivity (defined as the radiance divided by the irradiance) shall be $= 1.0\%$ for any (collimated to 0.5 degree circular, i.e. Solar like) position in the irradiance Field-Of-View.*
- SR 5.2.2.6** *The effect of multiplicative factors on the absolute reflectivity shall be less than 1% of the true signal after correction at all wavelengths and swath angles.*
- SR 5.2.2.7** *The effect of additive factors on the absolute reflectivity shall be less than 1% of the true signal after correction at all wavelengths and swath angles.*
- SR 5.2.2.8** *The effect of spectral structures similar to absorption structures caused by the instrument and/or its calibration in the reflectivity spectra shall be less than 10^{-4} at all wavelengths and swath angles.*
- SR 5.2.2.9** *The non-linearity on the reflectivity after correction shall be less than 0.2%.*
Note: Here non-linearity is defined as is the maximum excursion relative to linear behaviour (= Definition 5.2.2.3), so $|I_{measured} - I_{true}| < 0.002 I_{true}$. Moreover the linearity requirement applies for all illuminations between expected minimum radiance (and irradiance) and pixel full well.
In case the noise-floor in the measured S/N for the relevant ground pixel size is larger than the non-linearity itself, this requirement can be relaxed and applies to the dynamic range above twice the noise floor.

Spectral stability and spectral knowledge

- SR 5.3.1** *The wavelength scale of the Earth radiance and solar irradiance spectra shall be in vacuum wavelengths.*
- SR 5.3.2** *The spectral knowledge of the radiance and irradiance spectra shall be better than $1/100^{\text{th}}$ of a CCD-pixel above 300 nm and better than $1/50^{\text{th}}$ of a CCD-pixel below 300 nm.*
- SR 5.3.3** *The thermal and mechanical spectral stability of the instrument shall be better than $1/20^{\text{th}}$ of a CCD-pixel.*

OMI On-Ground and Preflight Calibration Requirements

- SR 5.4.1** *A PI period is needed to measure atmospheric spectra with the Flight Model, and to measure trace gas absorption spectra of, for example, ozone and NO_2 .*

- SR 5.4.2** *The accuracy of the effective spectral slitfunction of the instrument shall be 1 % of the peak value of the effective spectral slitfunction over the whole spectral range and for all swath-angles and for all relevant measurements modes (nadir and sun diffuser).*
- SR 5.4.3** *There shall be a Development Model with at least a complete UV-channel. This DM and its measurements shall be available for us in PFM design and the PFM calibration and characterisation measurements.*
- SR 5.4.4** *Straylight shall be characterised for all spatial and spectral dimensions.*
- SR 5.4.5** *In all measurement modes (measurement and calibration) the instrument response for all sources outside 2 times the IFOV (centred to the IFOV) shall not exceed 1 % of the response for the radiance from inside the IFOV.*
- SR 5.4.6** *Straylight determined for the minimum radiance spectrum as shown in Figure 5.2 (blue line) shall be less than 10 % before correction and 0.5 % after correction at all wavelengths and swath angles.*
- SR 5.4.7** *The signal from dark current shall not exceed 20% of the useful minimal signal as shown in Figure 5.2 (blue line) before correction and 0.5 % after correction at all wavelengths and swath angles.*
- SR 5.4.8** *All other requirements, specified in the latest version "OMI On-Ground Calibration and Characterisation Requirement Document", shall be applicable.*

In-flight calibration facilities

Solar calibration

- SR 5.5.1** *The solar calibration shall be used for the absolute radiometric calibration of OMI during flight. Therefore the sun shall be observed at least once each day via a solar port and a diffuser plate.*
- SR 5.5.2** *The long-term degradation of the nominally used reflection diffuser shall be monitored by using an identical reflection diffuser that is typically used once per month.*
- SR 5.5.3** *In addition, it shall be possible to use the transmission diffuser (which is used for the white light source (WLS)) as a reflection diffuser.*
- SR 5.5.4** *In order to correct for spectral effects of the reflection diffuser plate a third reflection diffuser of a different material shall be used.*
- SR 5.5.5** *The solar calibration port shall be large enough to observe the total sun in the field-of-view and the useful calibration time shall be about 1 minute.*
- SR 5.5.6** *When closed, the solar calibration port shall be light tight.*

White light source calibration

- SR 5.5.7** *There shall be a calibration white light source (WLS) in the instrument. This WLS is used for relative radiometric calibration of the instrument optical path after the primary mirror, plus detectors and for pixel-to-pixel characterisation purposes.*
- SR 5.5.8** *The spectrum of the WLS shall be continuous, well characterised and stable.*

Smooth field light source

- SR 5.5.9** *There shall be a smooth field light source in front of each detector CCD in the wavelength range that can be measured with the CCD, preferably in the wavelength range measured by the channel in question. This means that the UV1, UV2 and VIS channel all preferably shall have a different smooth field light source.*

Dark current signal measurements

- SR 5.5.10** *The dark current of all CCD pixels shall be measured and characterised during the dark side and the illuminated side of the orbit, in order to characterise temperature variation of the dark current.*
- SR 5.5.11** *Dark current measurements with multiple exposure times of all CCD pixels shall be performed to separate the electronics offset, dark current and noise in order to correct for dark current and electronic off-set in the on-ground software (and characterise the S/N in the measured signal).*

Straylight measurements

SR 5.5.12 *The straylight shall be measured for each image using dedicated CCD rows and shall be corrected for in on-ground software. This correction shall be based on the dedicated CCD row straylight measurements and the on-ground straylight calibration.*

Detector Smear

SR 5.5.13 *Detector smear shall be measured using dedicated CCD rows and shall be corrected for in on-ground software.*

SR 5.5.14 *The OMI in-flight telemetry shall include data which enables on-ground software correction for multiplicative and additive factors as defined in definitions 5.2.2.1 and 5.2.2.2 above.*

SR 5.5.15 *All other requirements, specified in the latest version "OMI In-flight Calibration Requirements Document", shall be applicable.*

Validation requirements (SRD Chapter 6)

Validation strategy

- SR 6.1.2.1** *The validation shall continue throughout the OMI lifetime.*
- SR 6.1.2.2** *Validation is envisaged to consist of three phases, each having a distinct goal. Firstly, the commissioning phase, which aims to provide a quick-look first validation; secondly, the core phase, to ensure a thorough validation of all data products; and finally, a long-term validation, establishing the stability of the instrument which is important for its ability to measure trends.*
- SR 6.1.2.3** *The validation strategy is to rely on measurements based on validated techniques. Preferably, several independent measurement techniques shall be used, at a large number of representative locations and conditions.*
- SR 6.1.2.4** *Validation campaigns shall be co-ordinated with other instruments on EOS-Aura.*
- SR 6.1.2.5** *New instrumentation shall be considered to provide an intercomparison rather than a validation.*
- SR 6.1.2.6** *To validate OMI data, participation in scientific validation projects, e.g., the NASA-NRA for Aura-validation, shall be encouraged.*
- SR 6.1.2.7** *Experience gained during the validation of GOME and SCIAMACHY shall be exploited.*
- SR 6.1.2.8** *Validation tools which shall be needed are: software for data processing, coincidence predictor, correlative and Aura data database, cataloguing tools, data assimilation tools, auxiliary data.*
- SR 6.1.2.9** *Validation workshops shall be held regularly throughout the OMI lifetime.*

Commissioning phase

- SR 6.2.1.1** *In the commissioning phase absolute irradiance and absolute radiance shall be validate and a preliminary validation of the main level 2 data products shall be provided.*
- SR 6.2.1.2** *In the commissioning phase, one satellite instrument (with global coverage) and one or two groundbased instruments shall be used as correlative instruments.*
- SR 6.2.1.3** *The commissioning phase shall take place after instrument functional tests, and lasts about three months.*

Core phase

- SR 6.2.2.1** *In the core phase, all products shall be validated thoroughly in order to determine their accuracy.*
- SR 6.2.2.2** *Data from existing instruments (ground-based and satellite instruments) as well as from dedicated campaigns shall be needed.*
- SR 6.2.2.3** *Campaigns shall be incorporated within the EOS-Aura framework.*
- SR 6.2.2.4** *Existing campaigns, outside the scope of EOS-Aura validation, shall also to be exploited.*
- SR 6.2.2.5** *During the core phase, data measured by different independent instruments shall be used.*
- SR 6.2.2.6** *Data measured within existing networks of instruments shall be exploited, since these are well-validated and often very stable.*
- SR 6.2.2.7** *Data from satellite instruments and data-assimilation techniques shall also be included and are essential for obtaining global coverage.*
- SR 6.2.2.8** *The core phase starts after the commissioning phase and ends when all data products have been validated. It shall span at least one year, to achieve seasonal coverage.*
- SR 6.2.2.9** *Campaigns shall not start earlier than 1 year after launch.*
- SR 6.2.2.10** *During the core phase, EOS-Aura as well as correlative data shall be available for all validation participants, through (an) easily available database(s).*
- SR 6.2.2.11** *If data are reprocessed (e.g., based on the validation results), they shall be validated again, using the already available correlative data.*

Long-term phase

- SR 6.2.3.1** *The long-term phase starts after the core phase and last during the complete lifetime of the instrument. In the long-term phase, all available data shall be used.*
- SR 6.2.3.2** *In the long-term phase, long-term changes in the accuracies of the products, e.g., due to instrument degradation, shall be detected and newly developed or advanced OMI data products shall be validated.*
- SR 6.2.3.3** *In the long-term phase, a regular, optimised repetition of the essential elements of the core validation phase is necessary.*

Validation rehearsal

- SR 6.2.4.1** *A validation rehearsal shall be planned before launch.*
- SR 6.2.4.2** *The main goals of a validation rehearsal are to provide a check on the data flow and accessibility of the database(s), and to test the validation tools.*
- SR 6.2.4.3** *All other requirements, specified in the latest versions of the “OMI Validation Requirements Document”, the “OMI Validation Handbook” and the “EOS-Aura Validation Plan” shall be applicable.*

Availability of validation data sources/campaigns

- SR 6.3.1** *Correlative measurements of (tropospheric) columns of NO₂ shall be supplied, either through the NASA-NRA for Aura-validation or through other sources of funding.*

List of the relevant Definitions, **associated with the Science Requirements**

Introduction

All definitions mentioned in the OMI-EOS Science Requirements Document (SRD) (RS-OMIE-KNMI-001, Version 2 of 7 December 2000) are listed according to the following rule: **Definition w.x.y.z**, in which **wxyz** stand for respectively chapter (**w**), section (**x**), subsection (**y**) and number of the definition (**z**) in the SRD.

Science requirements (SRD Chapter 3)

- Definition 3.1.1** Priority 'A' products are those products which shall be retrieved by OMI to fulfil the OMI mission objectives and they shall be available directly after launch.
- Definition 3.1.2** Priority 'B' products are those products which shall be possible to retrieve by OMI and which are desirable products that provide an extra contribution to the OMI mission objectives, but which are not necessarily available directly after launch.
- Definition 3.2.1** The pragmatic definition of the accuracy is: the RMS difference between 1) product values retrieved from simulated ("measured" and calibrated) theoretical Earth radiance spectra generated with a state of the art radiative transfer model (including well-defined atmospheres) and 2) the input product values used for the generation of these spectra. The theoretical spectra should be fed into instrument simulation software ("measured"), with all known error sources included; and calibrated with level 0-1b software.
- Definition 3.3.1** Global coverage means that OMI shall be able to measure the UV/VIS spectrum reflected from every part on Earth within 24 hours, except for regions which are not illuminated by sunlight in 24 hours.

Algorithm requirements (SRD Chapter 4)

- Definition 4.0.1** Level 0 data is the raw instrument data at original resolution, time ordered, with duplicate packets removed.
- Definition 4.0.2** Level 1b data is the radiometrically corrected and calibrated data in physical units at full instrument resolution as acquired.
- Definition 4.0.3** Level 2 data is the geolocated geophysical product, e.g. ozone column
- Definition 4.0.4** Ancillary data is data other than instrument measurements, originating in the instrument itself or from the satellite, required to perform processing of the data.. They include orbit data, attitude data, time information, spacecraft engineering data, calibration data, data quality information and data from other instruments.
- Definition 4.05** Auxiliary data is the data required for instrument processing, which does not originate in the instrument itself or from the satellite. Some auxiliary data will be generated in the ground segment, whilst other data will be provided from external sources.
- Definition 4.2.4.1** Spectral knowledge is defined as the error in the wavelengths assigned to the radiance and irradiance spectra.
- Definition 4.2.5.1** Spectral stability is the difference in the wavelength registration of a CCD-pixel between the radiance and irradiance spectra.
- Definition 4.2.7.1** The reflectivity is defined as the ratio of the Earth radiance and the solar irradiance.

Instrument requirements (SRD Chapter 5)

- Definition 5.1.1.1** The Total Spectral Range is defined as the wavelength range imaged onto the detector, including the overlap regions. In the Global- and Spatial Zoom-in Measurement, this equals to the wavelength range actually present in the instrument data.
- Definition 5.1.1.2** The Full Performance Range is the Total Spectral Range up to the wavelengths where the useful signal from two overlapping channels is equal. This is the wavelength where (about) half of the energy is deposited in each of two overlapping channels.
- Definition 5.1.1.3** The Spectral Sampling Distance is the wavelength range [in nm/pixel] over which a signal is sampled over a pixel.
- Definition 5.1.1.4** The Spectral Resolution is the full width at half maximum (FWHM) (in [nm] or [pixels]) for the instrument response for a monochromatic input.
- Definition 5.1.2.1** The Instantaneous Field-Of-View (IFOV) is the FWHM of the pixel response curve obtained when moving a point source in swath and/or flight direction.
- Definition 5.1.2.2** The global observation mode is the observation mode with the 2600 km swath and $13 \times 24 \text{ km}^2$ ground pixels. In the spectral range of 270 – 310 nm, the pixel size in the across-track direction may be larger, but at most doubled (i.e. $13 \times 48 \text{ km}^2$). The swath will be symmetric with respect to the sub-satellite track.
- Definition 5.1.2.3** The spatial zoom-in mode is the observation mode with a ground pixel size of $13 \times 12 \text{ km}^2$ and full spectral coverage, but is allowed to have a limited swath width of at least 725 km. In the spectral range of 270 – 310 nm, the pixel size in the across-track direction may be larger, but at most doubled (i.e. $13 \times 24 \text{ km}^2$). The swath will be symmetric with respect to the sub-satellite track.
- Definition 5.1.2.4** The spectral zoom-in mode is the observation mode with a ground pixel size of $13 \times 12 \text{ km}^2$ and a full swath of 2600 km. A limited spectral coverage is allowed, but shall be at least 306 - 432 nm to cover the most important scientific products. The swath will be symmetric with respect to the sub-satellite track.
- Definition 5.1.2.5** Sub-pixel read-out means that at one selected wavelength per CCD no co-addition of CCD images in the flight direction is performed.
- Definition 5.1.3.1** The exposure time is the time the image-part of the CCD is illuminated (the nominal exposure time is 0.4 s). After illumination, frame transfer takes place, and the image is transferred to the read-out part of the CCD.
- Definition 5.1.3.2** The read-out time is the time it takes to read the read-out part of the CCD (the nominal read-out time is 0.4 s).
- Definition 5.1.3.3** The co-addition time is the time in which several images are co-added. The nominal co-addition time is 2 s (i.e. 5 images are co-added to one: data is summated in the flight direction to improve S/N and reduce data rate).
- Definition 5.1.3.4** Binning is the summation of data of several CCD pixels along a column in the CCD (i.e. in the swath-direction) into one larger ground pixel to improve S/N and reduce data rate. (Nominally, 8 pixels are binned in the global mode).

Definition 5.1.3.5 Bad pixels are: pixels with anomalous dark current, reduced charge transfer efficiency (CTE), reduced quantum efficiency, or anomalous pixel response function and all pixels in columns on the CCD whose signal is transferred through a pixel with one of the aforementioned effects.

Definition 5.2.1.1 The most critical gas, which is defined as being the data product that requires the highest S/N ratio in a specific wavelength range.

Definition 5.2.2.1: The effects contributing to multiplicative factors are:

1. absolute radiometric calibration taking into account that common optical paths cancel in the calculation of the reflectance.
2. linearity charge transfer efficiencies
3. polarisation effects between the primary mirror and the first scrambler surface
4. spectral structures similar to absorption structures
5. gain settings

Definition 5.2.2.2: The effects contributing to additive factors are:

1. stray light
2. dark current
3. exposure smear
4. charge transfer inefficiencies
5. memory effects in CCD, DEM and ELU
6. electronic offset

Definition 5.2.2.3 Non-linearity is defined as is the maximum excursion relative to linear behaviour.

Definition 5.4.1 The effective spectral slitfunction is defined as the optical slitfunction convoluted with the Pixel Response Function (PRF).

Validation requirements (SRD Chapter 6)

- Definition 6.2.1.1** The commissioning phase is the first validation phase, in which absolute irradiance and absolute radiance shall be validate and a preliminary validation of the main level 2 data products shall be provided.
- Definition 6.2.2.1** The core phase is the second validation phase, in which all products shall be validated thoroughly in order to determine their accuracy.
- Definition 6.2.3.1** The long-term phase is the third validation phase, in which long-term changes in the accuracies of the products, e.g., due to instrument degradation, shall be detected and in which newly developed or advanced OMI data products shall be validated.

ID: KNMI-OMI-2000-008
 Title: OMI Level 2 wavelength bands
 Author: J.P. Veefkind
 Version: 1.1 of 7 December 2000
 Checked: J. de Haan
 Approved: P.F. Levelt

OMI Level 2 wavelength bands

History

This document replaces version 1 of 14 February 2000. A few minor changes were made:

- The terminology "priority", "standard products" and "special products" was changed to reflect the terminology used in the OMI Science Requirements Document Version 2 (SRD).
- The BrO retrieval window is 344 – 360 nm instead of 345 – 359 nm.
- The wavelength bands for the surface UV-B flux and UV spectra and for the cloud scattering pressure (via the O₂-O₂ collision complex around 477 nm) data products were added.

OMI level 2 wavelength bands

An overview is given of the wavelength bands that are used for OMI Level 2 data products. For each band a class identification from 1-3 is given, according to the following criteria:

1. Priority 'A' products (which shall be available directly after launch) that use a relatively small wavelength region: i.e DOAS & Cloud products, and TOMS wavelengths.
2. Same as 1, but for priority 'B' products (which provide a valuable contribution to the OMI mission objectives, but which are not necessarily available directly after launch) and CIO (OCI will be difficult to retrieve with OMI).
3. Products (of both the priority 'A' as 'B' type) that use broad wavelength regions: profile retrieval, aerosol optical thickness, surface reflectance, UV-B and spectra.

The class identification is based on the severity of the loss of a single wavelength and if a product is a priority 'A' or 'B' product. Loss of (a) wavelength(s) in a class 1 band has the most severe impact on the fulfillment of the OMI Mission Objects, as defined in the SRD.

The product bands, the number of wavelength pixels, and the wavelength band class identification are given in Table 2, 3 and 4, for the UV-1, UV-2 and VIS channel of OMI, respectively. The wavelength range of the OMI channels is given in Table 1. The TOMS wavelengths are based on EP-TOMS. For products with priority 3, like ozone profile and aerosol optical thickness, there are many alternative wavelength pixels, however not all wavelengths can be used. In this case no number of pixels is included in the tables.

Note that in Table 2, 3 and 4 the spectral windows related to the spectral calibration of the OMI are not included.

Table 1. Spectral range of the OMI UV and VIS channels.

Channel	Total range	Full performance range
UV-1	270 - 314 nm	270 - 310 nm
UV-2	306 - 380 nm	310 - 365 nm
VIS	350 - 500 nm	365 - 500 nm

Table 2. Product bands in UV-1.

Product name	Channel	Band [nm]	# of pixels	Class	Comments
O ₃ Profile	UV-1	270 - 314		3	Continues in UV-2 and VIS
CIO DOAS	UV-1	290 - 314	75	2	Difficult to retrieve with OMI
TOMS#5 312.5	UV-1	311.5-313.5	6	1	Also in UV-2
TOMS#6 308.6	UV-1	307.5-309.5	6	1	Also in UV-2
Surface UV-B & spectra	UV-1	280 - 314		3	Continues in UV-2 and VIS

Table 3. Product bands in UV-2.

Product name	Channel	Band [nm]	# of pixels	Class	Comments
Cloud Top Pressure	UV-2	390 - 400	66	1	
Cloud Cover	UV-2	378 - 383	33	1	
O ₃ column DOAS	UV-2	325 - 335	66	1	
O ₃ Profile	UV-2	306 - 314		3	Continues in UV-1 and VIS
Aerosol	UV-2	340 - 400		3	Continues in VIS
BrO column DOAS	UV-2	344 - 360	114	2	Priority 'B' Product
SO ₂ column DOAS	UV-2	314 - 327	86	2	Priority 'B' Product
OCIO column DOAS	UV-2	357 - 381	160	2	Also in VIS Priority 'B' Product
HCHO column DOAS	UV-2	336 - 357	140	2	Priority 'B' Product
Surface Reflectance	UV-2	320 - 380		3	Continues in VIS
Surface UV-B & spectra	UV-2	306 - 380		3	Continues in UV-1 and VIS
TOMS#1 360.0	UV-2	359 - 361	13	1	Also in VIS
TOMS#2 331.2	UV-2	330.2-332.2	13	1	
TOMS#3 322.3	UV-2	321.3-323.3	13	1	
TOMS#4 317.5	UV-2	316.5- 318.5	13	1	
TOMS#5 312.5	UV-2	311.5- 313.5	13	1	Also in UV-1
TOMS#6 308.6	UV-2	307.5-309.5	6	1	Also in UV-1

Table 4. Product bands in VIS.

Product name	Channel	Band [nm]	# of pixels	Class	Comments
NO ₂ column	VIS	425 - 450	119	1	
Cloud Top Pressure	VIS	470 - 485	72	1	O ₂ -O ₂ collision complex
O ₃ column DOAS VIS	VIS	450 - 500	238	2	
O ₃ Profile	VIS	350 - 500		3	Continues in UV-1 and UV-2
Aerosol	VIS	350 - 400		3	Continues in UV-2
OCIO column DOAS	VIS	357 - 381	114	2	Also in UV-2 Priority 'B' Product
Surface Reflectance	VIS	350 - 500		3	Continues in UV-2
Surface UV-B & spectra	VIS	350 - 400		3	Continues in UV-1 and UV-2
TOMS#1 360 nm	VIS	359 - 361	9	1	Also in UV-2

ID: RS-OMIE-KNMI-216
Title: Spectral Knowledge Requirements for DOAS Products
Author: R.F. van Oss Checked: J. de Haan
Version: 1 of 28 September 2000 Approved: P.F. Levelt

Spectral Knowledge Requirements for DOAS Products

History

This research was the result of an action item towards the OMI science team, raised during the OMI Instrument Preliminary Design Review (I-PDR), held at TNO-TPD, Delft in The Netherlands from 2 to 4 December 1998. The background of the issue was the difference between the Instrument Specification Document (RS-OMIE-0000-FS-021, version 1 of 22 June 1998) and the Science Requirements Document (RS-OMIE-KNMI-001, version 1 of 18 November 1998).

The relevant Review Item Descriptions (RIDs) were I-PDR NIVR-52 (originator J. Callies), I-PDR NIVR-84 (originator P. Levelt) and I-PDR NIVR-140 (originator P. Levelt), resulting in:

AI and/or RID description

The science requirement is that the spectral stability should be better than 1/100th spectral pixel, while the current design has a much lower stability.

Action item

AI on the science team to investigate if the requirement on the spectral stability of 1/100th pixel is really necessary or that this requirement can be relaxed to 1/50th pixel.

In forthcoming meetings between the OMI industry and the OMI science team, it was recognised that action mentioned above applies to the spectral knowledge (after software correction), while spectral stability refers to the mechanical and thermal stability of the instrument (which introduces interpolation errors when co-aligning Earth radiances and solar irradiance spectra).

The I-PDR action item was replaced by several new actions, which can be summarised in the following action:

KNMI to test what are the spectral requirements on the wavelength grid for ozone profile and DOAS retrieval and define it in terms of two separate requirements: a **mechanical and thermal stability** requirement and in a **spectral knowledge** requirement.

This study focuses on the spectral knowledge requirements of the DOAS products and replaces the draft version "Spectral stability - Consequences for DOAS retrieval" of 11 June 1999.

The spectral knowledge requirements for the ozone profile are described in RS-OMIE-KNMI-226 (version 1, in preparation) and the mechanical spectral stability requirements are described in SN-OMIE-KNMI-203 (version 3 of 7 December 2000).

Description of action

The effect of an error in the wavelength registration of 1/50th and of 1/100th CCD- pixel in the level 1b OMI spectra on the DOAS slant column density retrievals of Ozone (UV and VIS), NO₂, SO₂, and BrO has been studied.

The method employed here is an "end-to-end" calculation. This means that OMI level 1b spectra are simulated using a radiation transfer model and an instrument model. Distorted spectra, containing errors in the wavelength registration, as well as undistorted spectra are generated. On these simulated spectra slant column densities are retrieved using the DOAS method. In this way, the errors on the slant column resulting from errors in

wavelength registration are determined. The effect of an erroneous spectrum is established for a number (16) of cases, differing in ground albedo, solar zenith angle, viewing angle and vertical column density of the gas. These cases cover the range of realistic parameter values relevant for the OMI observations.

The spectra are calculated for a mid-latitude summer standard atmosphere. The concentrations of gasses, other than the one under consideration, have been set to zero. The vertical column of the gas is tuned by a multiplication factor that is constant with height. For the radiative transfer calculations, MODTRAN (version 3.7) was used. The spectral resolution of MODTRAN is sufficient in view of the slit function of OMI.

The DOAS fit is employed using only the absorption spectrum of the gas. Since the perturbation only affects the slant column density and not the air mass factor, the effect on the slant column density is calculated.

Table 1 summarises the details of the radiation transfer model.

Table 2 summarises the details of the OMI instrument model.

The instrument simulation involves (i) the convolution of the calculated high-resolution spectrum with a (nearly Gaussian) slit function, (ii) the sampling of the radiances on the instrument wavelength grid and (iii) adding noise using a Gaussian random generator. The noise amplitude is calculated including only shot noise and electronic & detector noise (Ref b). A co-adding factor is used. For the present purposes this factor has been given an unrealistic high value (1e6) to make the noise artificially low to be able to detect small changes in the radiance and the resulting DOAS columns. Simulations with a more realistic noise level will not change the magnitudes of the consequences of the wavelength distortions, only that small consequences can not be detected anymore.

Table 3 presents the 16 cases used for the calculations.

Table 3a gives the vertical column densities.

The SO₂ low column density is based on the reported threshold for GOME (Eisinger & Burrows, ESAMS Scientific Sessions, ESTEC, Jan. 1999) (Ref. (e))

Table 4 presents for each gas the channel and wavelength region used and the details of the errors in wavelength registration ("shift or squeeze") that have been introduced in the simulated spectra.

The wavelength ranges used for the DOAS fit are chosen identical to those used for GOME retrievals. Note that other ranges could be more suitable for OMI.

The shift (in nm) represents a constant wavelength perturbation, $\pm 1/50$ and $\pm 1/100$ pixel are used. The squeeze leaves the central wavelength in the window unchanged but results in a wavelength shift, which is linear in distance from the center. The magnitude of the squeeze is such that at the boundaries the wavelengths change an amount $\pm 1/50$ or $\pm 1/100$ pixel.

*Definition: $wl := wl_center + (wl - wl_center) * squeeze + shift$,*

The shift and squeeze are always employed separately.

The shifts and squeezes are only applied to the earthshine spectrum and not on the solar spectrum. This has more severe consequences for the retrieval compared to an equal shift for the sun and the earth spectrum, but it is nonetheless a realistic error.

A total of eight perturbed spectra are produced resulting from four shifts and four squeezes.

Results

In Figure 1 the perturbations of the slant column density are shown, defined as:

$$\text{Perturbation} = 100\% * (N_{dis} - N_{undis}) / N_{undis}$$

with N_{dis} the slant column derived from the distorted spectrum and N_{undis} the slant column from the undistorted spectrum.

Conclusions and discussion

The effect on the slant column density of a relative wavelength shift between the earthshine and the solar spectrum depends critically on the specie and the wavelength range used in the DOAS fit.

O₃ UV:

The effect on the slant column is less than 0.6 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 0.3%.

O₃ VIS:

The effect on the slant column is less than 5 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 2%.

NO₂:

The effect on the slant column is less than 10 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 5%.

BrO:

The effect on the slant column is less than 8 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 5%.

SO₂:

The simulated spectra of the low vertical column density appeared to be extremely sensitive to wavelength shifts and squeezes. For the low column (GOME threshold), the effect on the slant column reaches up to 520% for a wavelength distortion of 1/50th pixel. For 1/100th the effect is 270%. For the high vertical column density the effect on the slant column reaches up to 75% for a wavelength distortion of 1/50th pixel. For 1/100th the effect is 30%. We note that for a more realistic model which includes O₃ and SO₂ a somewhat higher accuracy may be required.

When we compare the effect of the wavelength distortions on the slant column to the requirements on the accuracy listed in Table 3.1 of Ref (c), the following conclusions can be drawn.

For Ozone UV (Req: 2 %), NO₂ (Req: 10 %) and BrO (Req: 10 %) a stability of 1/50th CCD-pixel is barely enough to satisfy the requirement. If the wavelength grid is stable up to 1/100th of a pixel the requirements can be safely met.

For Ozone VIS even a stability of 1/100th pixel is not enough to meet the required accuracy.

For SO₂ (Req: 20 %) the spectral stability of 1/100th pixel is even for the high column density (10x GOME threshold) not good enough to ensure the required accuracy.

Note that this report only discusses the effect of the spectral knowledge on the slant column. Since the noise level has been turned artificially low, a more realistic noise level will result in an even more reduced accuracy.

References

- (a) Information for the industry needed to close RIDs of the OMI Preliminary Design Review meeting at TNO/TPD in Delft on December 2-4, 1998, KNMI-FAX of 5 March 1999
- (b) Van der A, R., Noise levels of OMI instrument, personal communication, Jan 1999
- (c) Science Requirements Document for OMI-EOS, RS-OMIE-KNMI-001, V. 2-draft of 22 August, 2000.
- (d) Kruizinga, B., Radiometric effects of remnant polarisation in OMI due to the polarisation scrambler, Jan 1999, TNO-TPD
- (e) Eisinger, M. and J.P. Burrows, *GOME observations of tropospheric sulphur dioxide*, in proceedings ESAMS'99 European Symposium on Atmospheric Measurements from Space, ESTEC, Noordwijk, The Netherlands 18-22 January 1999, ESA WPP 161 ISSN 1022-6656, p. 415-419, March 1999.

Table 1: Atmospheric and observational parameters

Radiation transport model	MODTRAN version 3.7
Spectral sampling	5 cm ⁻¹ (= 0.08 nm at 400 nm)
Multiple scattering	DISORT 8 stream
Solar irradiance spectrum	Kurucz, 1 cm ⁻¹ tabulation, 5 cm ⁻¹ resolution
Atmospheric profiles of constituents	Mid Latitude summer, with constant factors to adjust columns of selected gasses (Tbl. 3)
Albedo	0.2 or 0.8, Lambertian (Tbl. 3)
Aerosol model	No aerosols
Solar zenith angle	20° or 80° (Table 3)
Viewing zenith angle	180° or 130° (Table 3)
Wavelength range	Specific for gas (Table 4)

Table 2: Instrument model

Slit function	tabulated slit function (GOME instrument model)															
Resolution	Channel 1: 1.00 nm Channel 2: 0.45 nm Channel 3: 0.63 nm															
Spectral sampling	Channel 1: 0.32 nm Channel 2: 0.15 nm Channel 3: 0.21 nm															
Channel bounds	Channel 1: 270 – 314 nm Channel 2: 306 – 380 nm Channel 3: 350 – 500 nm															
Noise	Noise (rms) = C * sqrt(S/C + N*N)/SQRT(co-adding) (co-adding = 1e6) With: S signal in photon/(s*sr*cm ² *nm) Noise in photon/(s*sr*cm ² *nm) N, C depend on channel: <table border="1" style="margin-left: 40px;"> <thead> <tr> <th></th> <th>N</th> <th>C</th> </tr> </thead> <tbody> <tr> <td>Channel 1A</td> <td>30</td> <td>1.47e7</td> </tr> <tr> <td>Channel 1B</td> <td>260</td> <td>1.47e7</td> </tr> <tr> <td>Channel 2</td> <td>260</td> <td>8.97e7</td> </tr> <tr> <td>Channel 3</td> <td>260</td> <td>3.15e8</td> </tr> </tbody> </table> Channel 1A < 300 nm, Channel 1B > 300nm		N	C	Channel 1A	30	1.47e7	Channel 1B	260	1.47e7	Channel 2	260	8.97e7	Channel 3	260	3.15e8
	N	C														
Channel 1A	30	1.47e7														
Channel 1B	260	1.47e7														
Channel 2	260	8.97e7														
Channel 3	260	3.15e8														

Table 3:

Case	Solar zenith angle	Viewing zenith angle	Albedo	Column density ¹⁾
1	20°	180°	0.05	low
2	80°	180°	0.05	low
3	20°	180°	0.80	low
4	80°	180°	0.80	low
5	20°	130°	0.05	low
6	80°	130°	0.05	low
7	20°	130°	0.80	low
8	80°	130°	0.80	low
9	20°	180°	0.05	high
10	80°	180°	0.05	high
11	20°	180°	0.80	high
12	80°	180°	0.80	high
13	20°	130°	0.05	high
14	80°	130°	0.05	high
15	20°	130°	0.80	high
16	80°	130°	0.80	high

1) See Table 3a

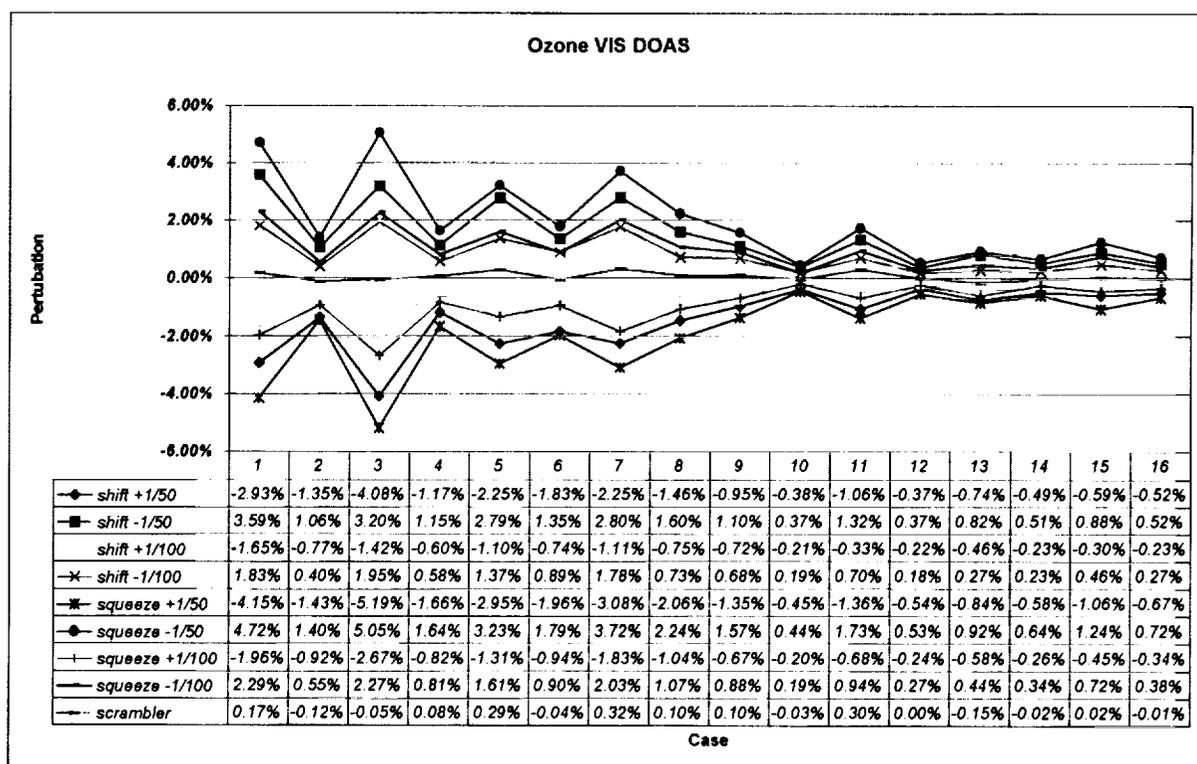
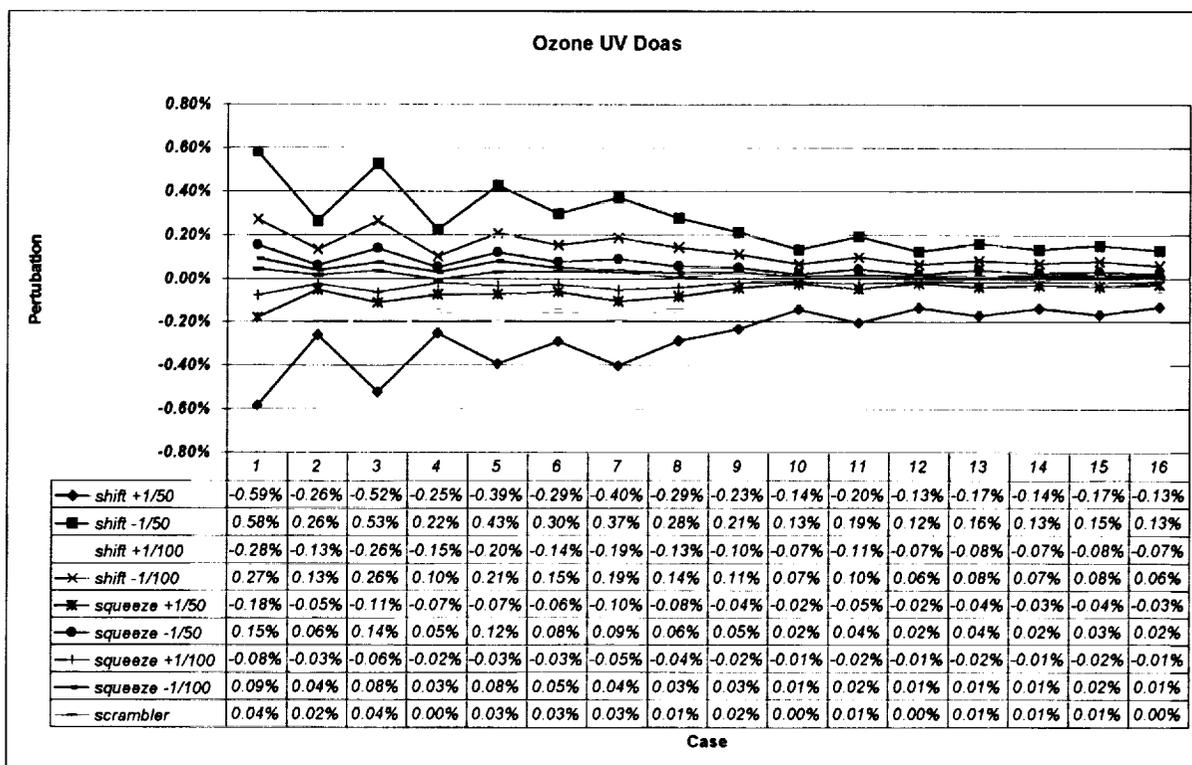
Table 3a

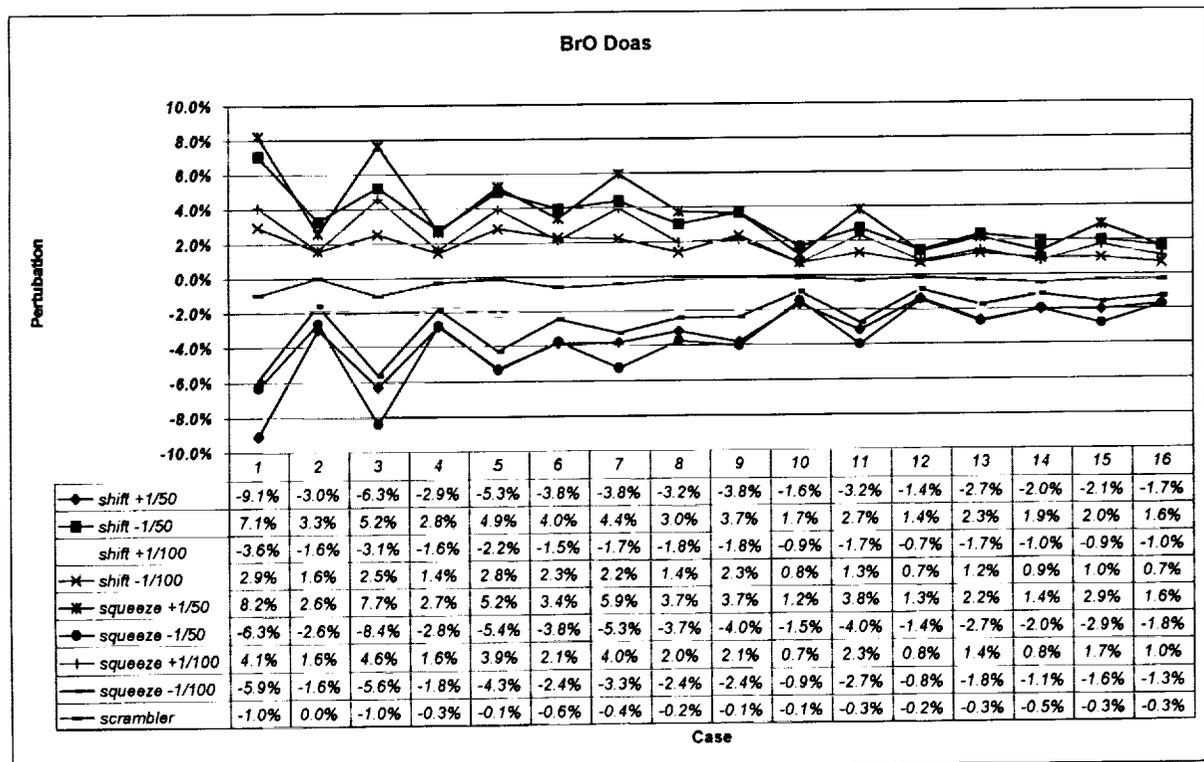
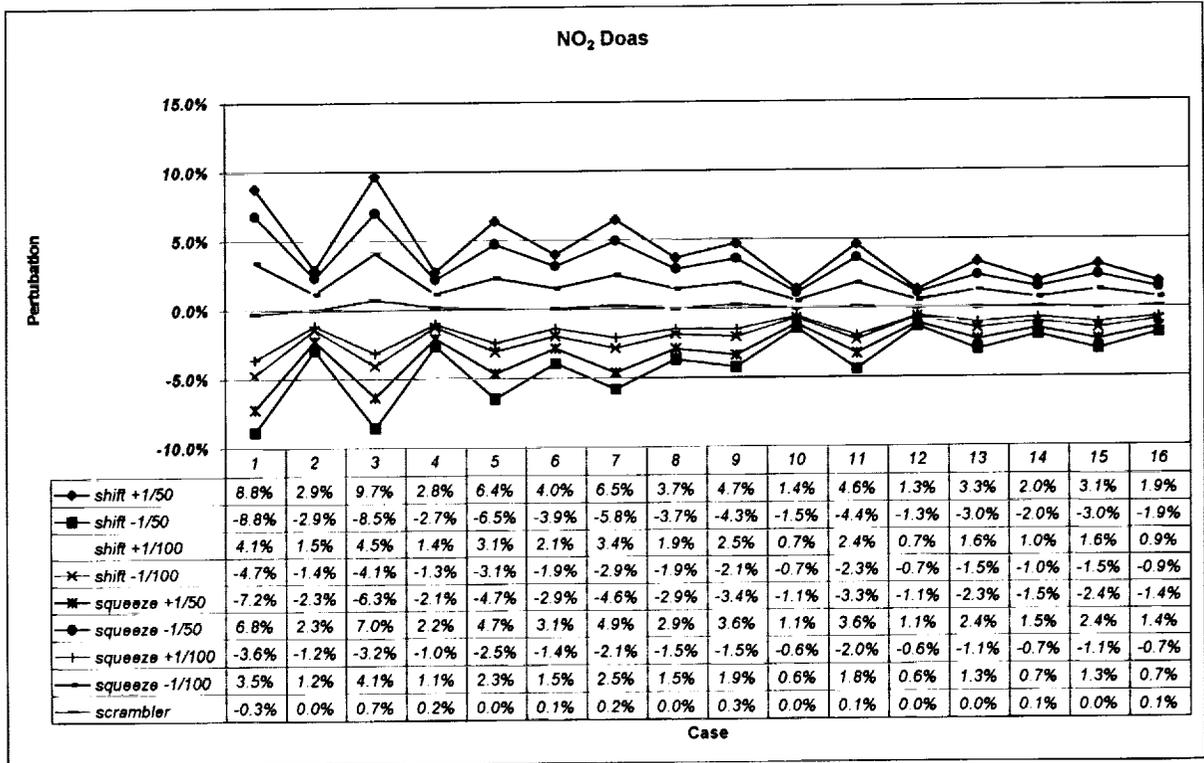
	High column density	Low column density
O3 UV/VIS	501 DU	167 DU
NO ₂	(0.4 DU) $1.2 \times 10^{16} \text{ cm}^{-2}$	(0.2 DU) $5.9 \times 10^{15} \text{ cm}^{-2}$
BrO	$1.3 \times 10^{14} \text{ cm}^{-2}$	$6.3 \times 10^{13} \text{ cm}^{-2}$
SO ₂	(5.6 DU) $1.5 \times 10^{17} \text{ cm}^{-2}$	(0.6 DU) $1.5 \times 10^{16} \text{ cm}^{-2}$

Table 4

	O ₃ -UV	O ₃ -VIS	NO ₂	BrO	SO ₂
Channel	2	3	3	2	2
Wavelength range [nm]	325 – 335	450 - 500	425 – 450	345 - 360	314 – 327
Shift [nm]	±0.003	±0.0042	±0.0042	±0.003	±0.003
	±0.0015	±0.0021	±0.0021	±0.0015	±0.0015
Squeeze [-]	1.0006, 0.9994	1.000168, 0.999832	1.000336, 0.999664	1.0004, 0.9996	1.00046, 0.99954
	1.0003, 0.9997	1.000084, 0.999916	1.000168, 0.999832	1.0002, 0.9998	1.00023, 0.99977

Figure 1: Perturbation in slant column density resulting from 9 perturbations in the simulated OMI level 1 spectra for 16 cases. a: O3UV, b: O3VIS, c: NO2, d: BrO, e: SO2.





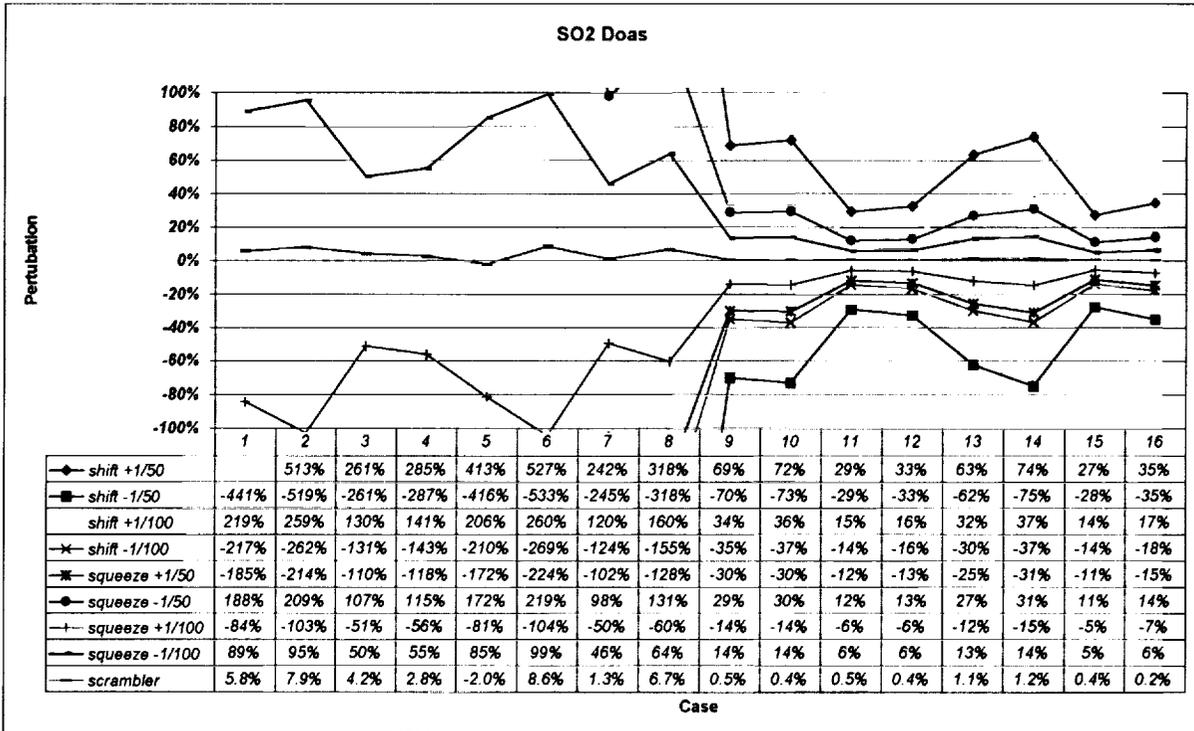


Figure 1(abcde) shows the relative deviation between two reflectance-values for the three OMI channels for the five values of the relative shift. For this figure the channel UV-1 S-FWHM is three pixels. Figure 2 shows the relative deviation for channel UV-1 for the five values of the relative shift and the five values for the S-FWHM. The maximum deviation per channel for each shift is presented in Table 1. Also, for channel UV-1 the results for five values for the S-FWHM are shown.

Table 1: The maximum deviation [in %] between the 'correct' and the 'OMI' reflectance, per channel, for each of the five values for the relative shift between the OMI -sun and -earthshine spectrum and, for channel UV-1, for each of the five values for the S-FWHM.

Shift [pixel]	UV-1					UV-2	VIS
	S-FWHM = 1 pixel	S-FWHM = 2 pixels	S-FWHM = 3 pixels	S-FWHM = 4 pixels	S-FWHM = 5 pixels	S-FWHM = 3 pixels	S-FWHM = 3 pixels
0.10	4.4%	1.6%	2.7%	3.7%	4.2%	1.7%	0.5%
0.05	2.7%	1.7%	2.8%	3.7%	4.2%	1.7%	0.3%
0.00	1.4%	1.8%	2.8%	3.7%	4.2%	1.7%	0.1%
-0.05	1.8%	2.1%	2.8%	3.7%	4.2%	1.7%	0.3%
-0.10	3.4%	2.5%	2.8%	4.2%	4.2%	1.7%	0.5%

From the figures in Table 1 a few observations can be made:

- (i) The error in the reflectance introduced by the degrading of the physical sun and earthshine spectra by OMI is non-negligible for a zero relative shift. This is due to the fact that "the ratio of two averages is generally not equal to the average of the ratio". This is an intrinsic error that cannot be avoided.
- (ii) The errors are largest in channel UV-1, smaller in channel UV-2 and smallest in channel VIS. This is caused by differences in the structure in the atmospheric reflectance spectrum and by the different amount of averaging in the channels. The larger errors in channel UV-1 are mainly due to the larger sampling per pixel (0.32 nm versus 0.15 nm in UV-2 and 0.21 in VIS), while the smaller errors in the VIS channel are due to the small amount of structure in the reflectance spectrum.
- (iii) The three channels show a different sensitivity to the amount of shift between the sun and earthshine spectra. Restricted to the case where for all channels S-FWHM = 3 pixels, the maximum error is relatively insensitive to the amount of shift for channels UV-1 and 2, while for channel VIS there is a clear increase with increasing shift. It is not clear why this is so. Note that the error in the window [340-350 nm] in channel UV-2 does depend on the shift and the error is small for zero shift.
- (iv) Since the error can be large in the vicinity of strong lines in the solar spectrum, the retrieval of cloud-top-height, using the Ring effect at the Calcium lines at 395 nm in the VIS, will be affected by this error. It is therefore advisable not to use the reflectance obtained from the OMI sun and earthshine spectra, but instead make use of a high-resolution sun spectrum.
- (v) The large values of the error (even at zero shift) in channel UV-2 between 310 and 320 nm can affect the DOAS retrieval of SO₂ in this window.
- (vi) The effect of the error in channel UV-2 between 325 and 335 nm on the DOAS retrieval of ozone should be looked into, in view of the strict requirement of 2% on the accuracy of the ozone column. Currently this effect is, partly, accounted for by the Ring spectrum. However, since the error depends on the amount of structure in the reflectance, it depends on the ozone column.

Conclusions

- (i) The magnitude of a relative wavelength shift between the sun and the earthshine OMI-spectra affects the error on the reflectance in the visual channel and the large-wavelength side of channel UV-2. A shift of 1/10th of a pixel gives an error of 0.5%, 1/20th gives an error of 0.3%, and a zero shift gives an error of 0.1%.
- (ii) For channel UV-1 the value of the IRF-FWHM affects the dependence of the error in the reflectance on the shift: undersampling (IRF-FWHM = 1 pixel) results in a large sensitivity of the error on the shift; increasing the sampling suppresses this.
- (iii) The error in the reflectivity for a zero shift has to be dealt with in the level 1b to 2 retrievals.
- (iv) For channel UV-1 larger values of the IRF-FWHM lead to larger errors on the reflectivity at zero shift.

Fig. 1a The relative deviation between two reflectance-values for the three OMI channels for a relative shift of - 0.10

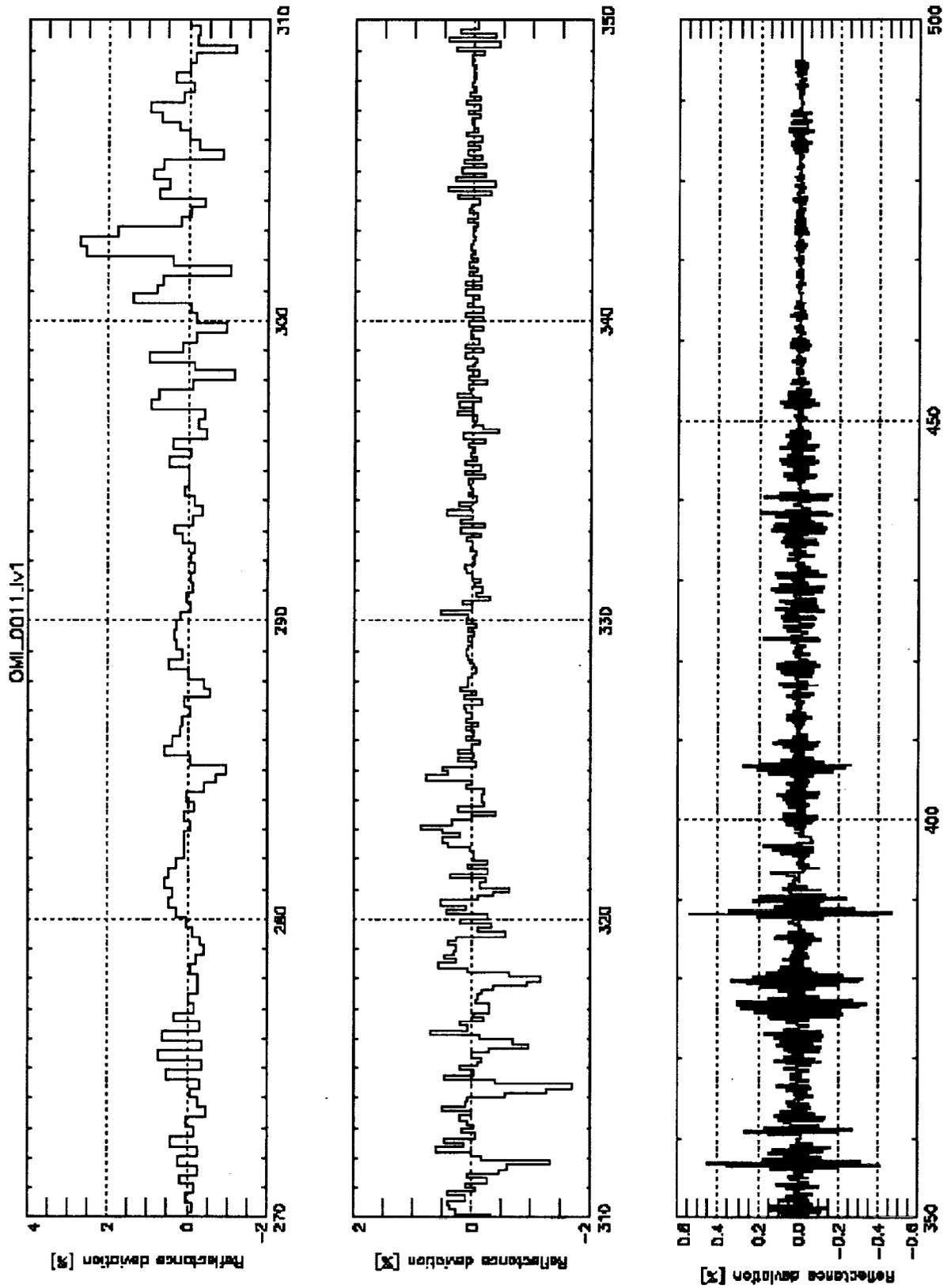


Fig. 1b The relative deviation between two reflectance-values for the three OMI channels for a relative shift of - 0.05

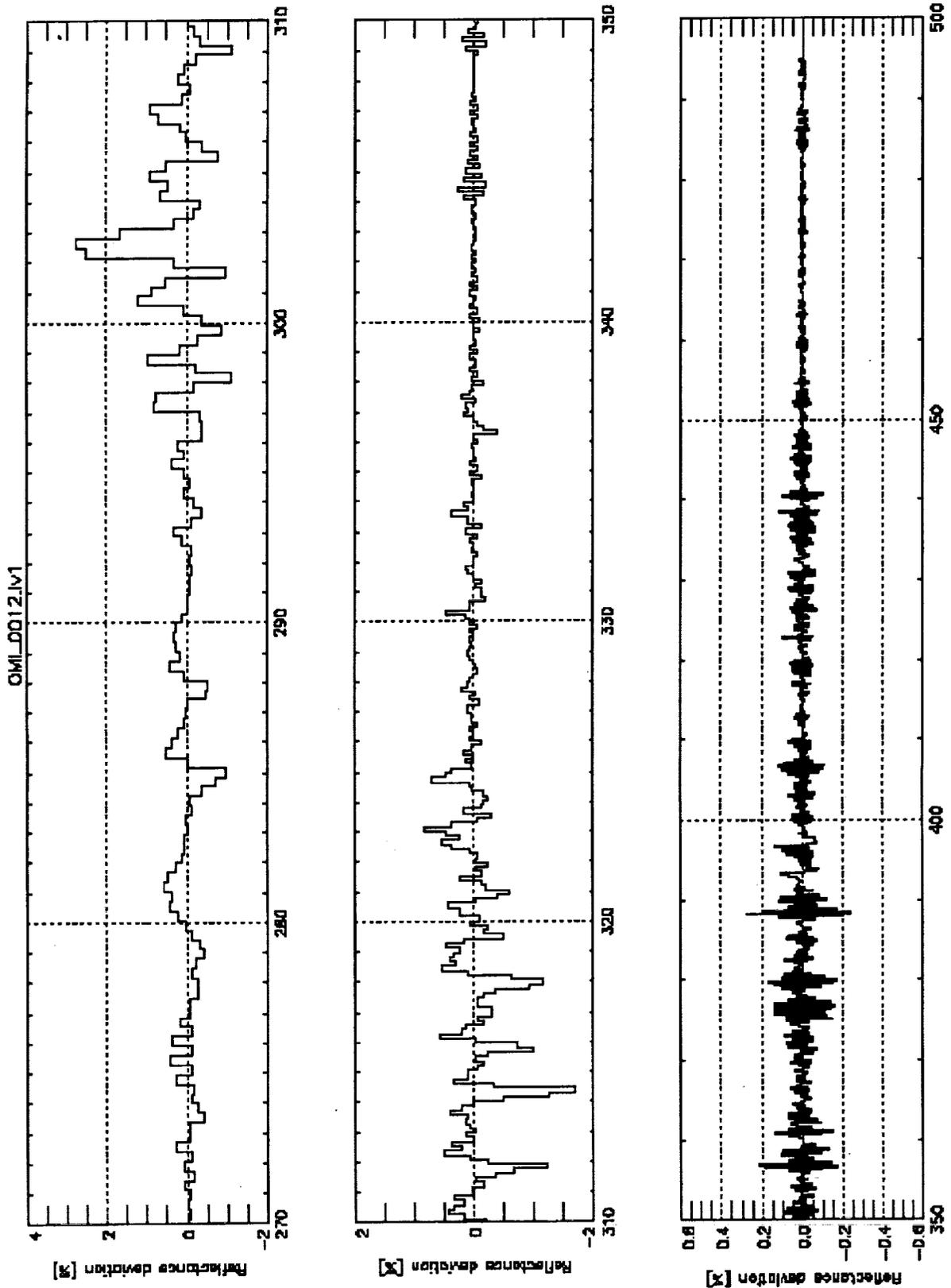


Fig. 1c The relative deviation between two reflectance-values for the three OMI channels for a relative shift of 0.0

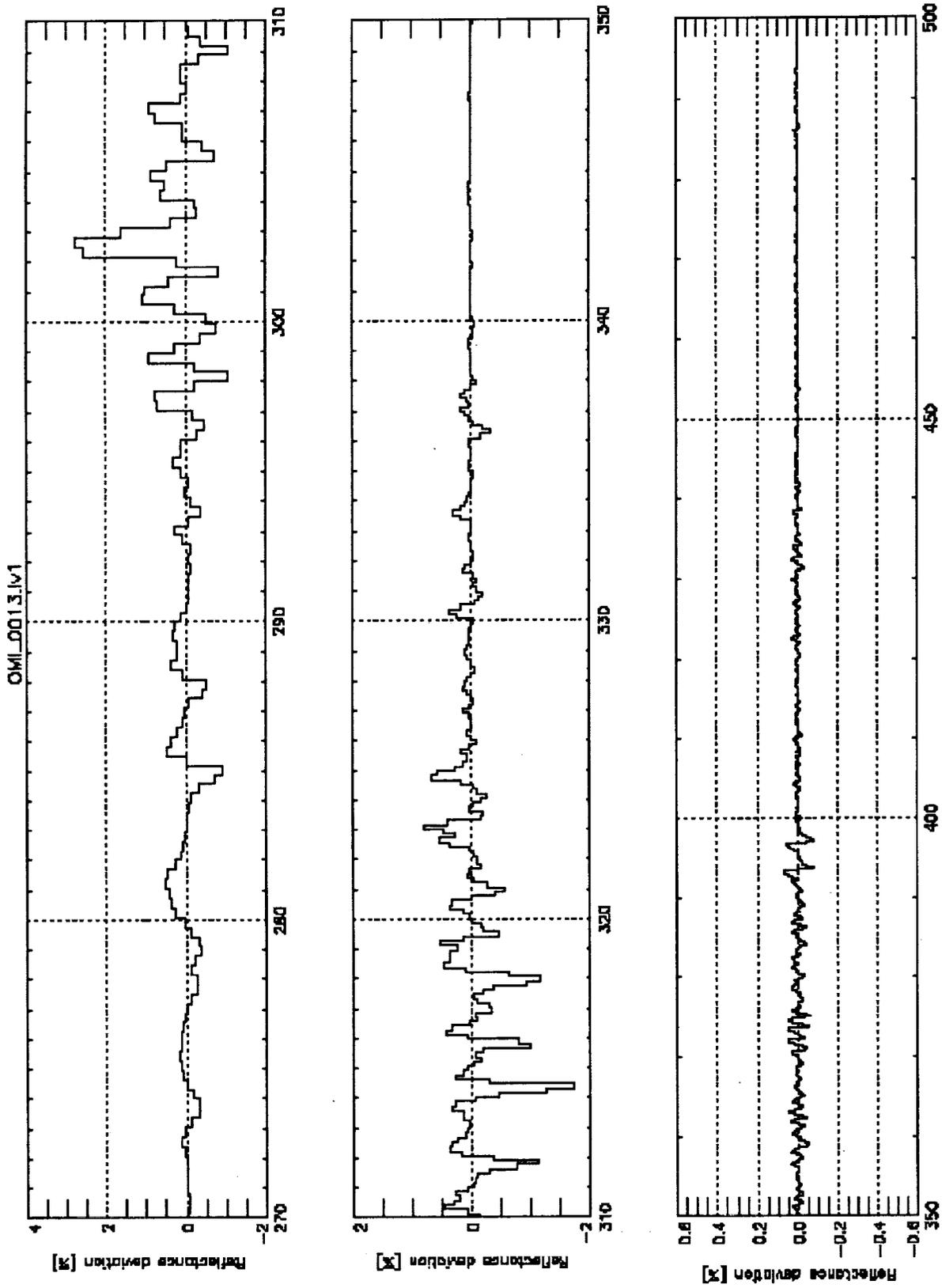


Fig. 1d The relative deviation between two reflectance-values for the three OMI channels for a relative shift of + 0.05

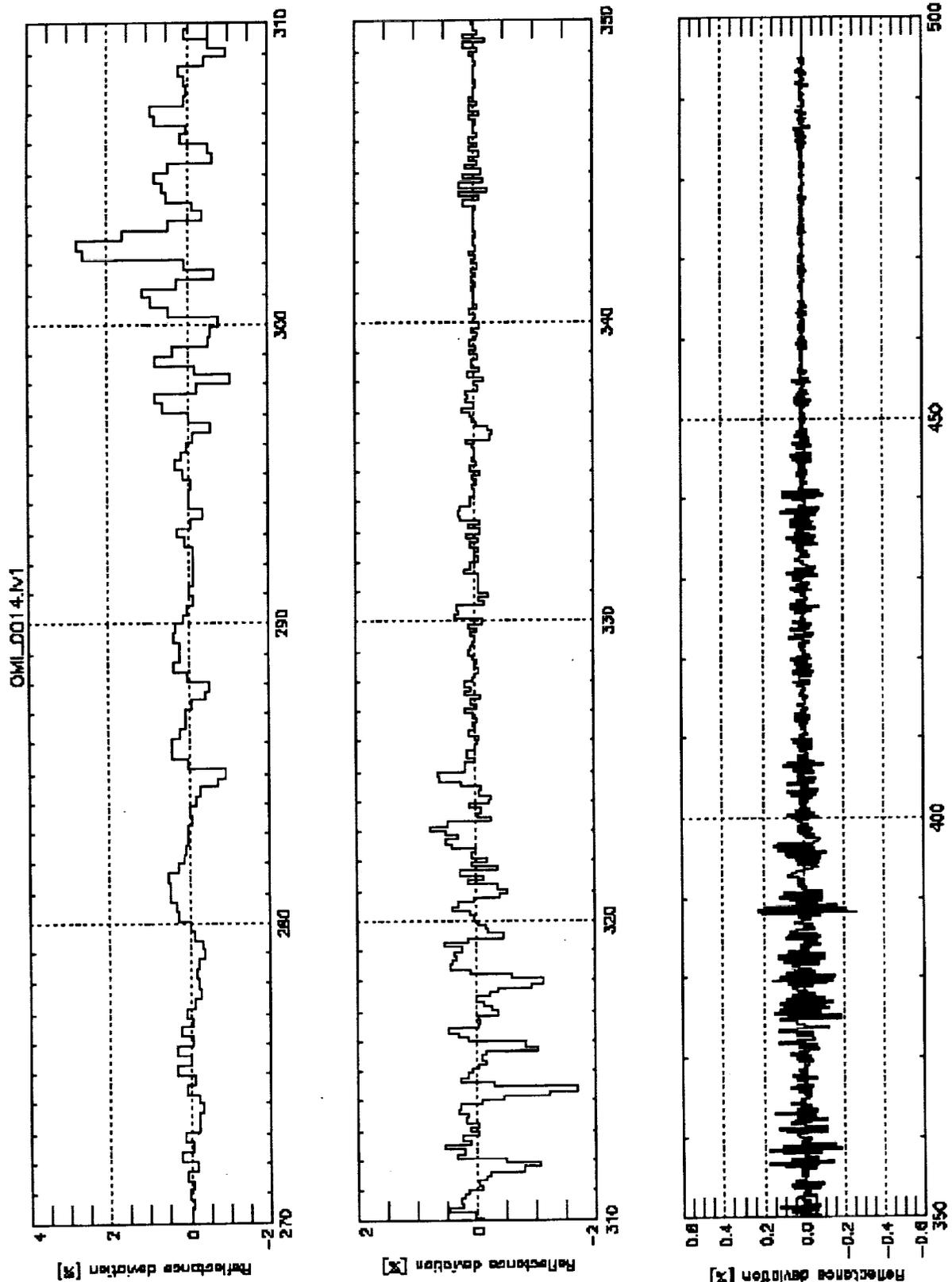


Fig. 1e The relative deviation between two reflectance-values for the three OMI channels for a relative shift of + 0.10

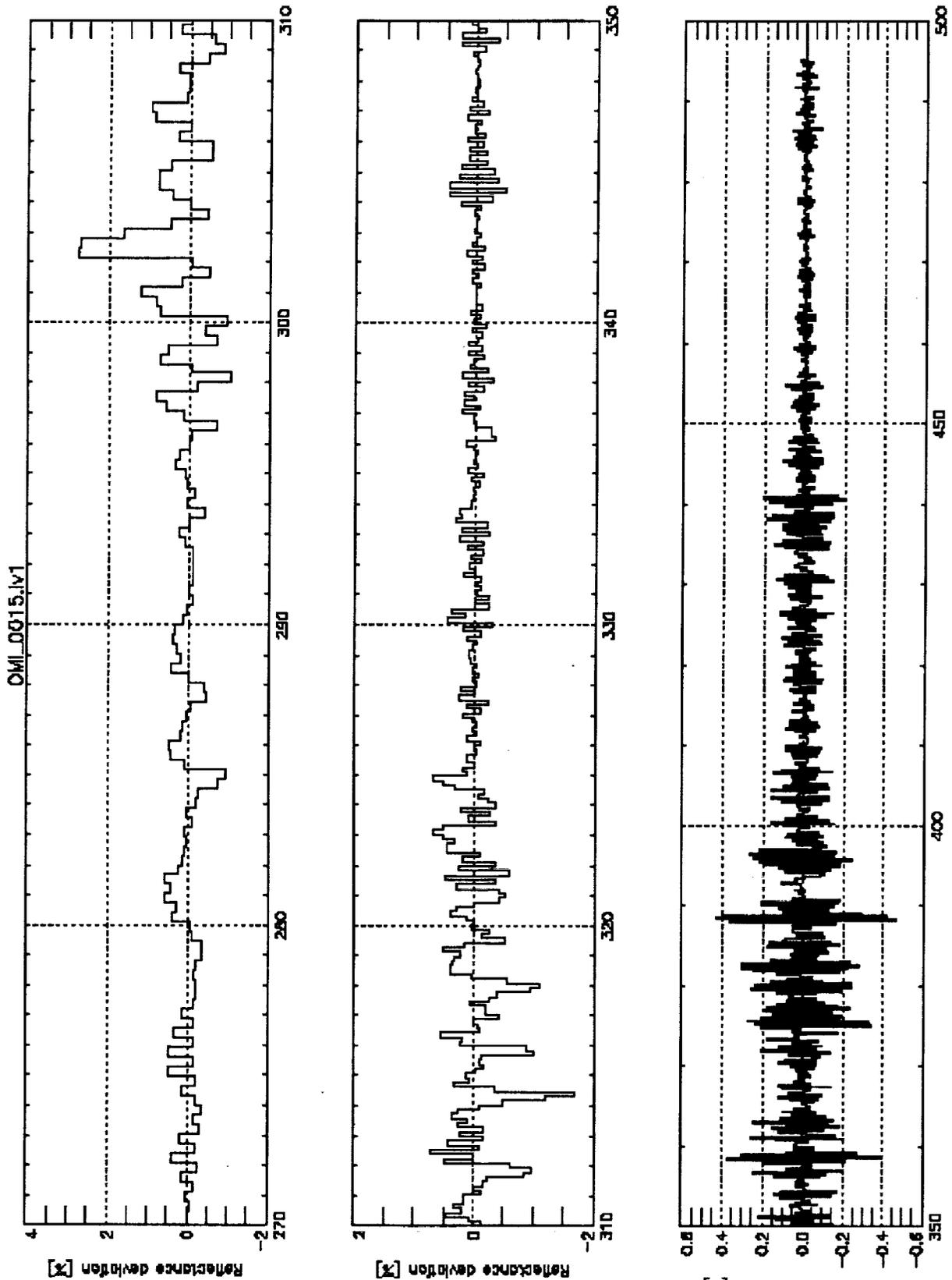
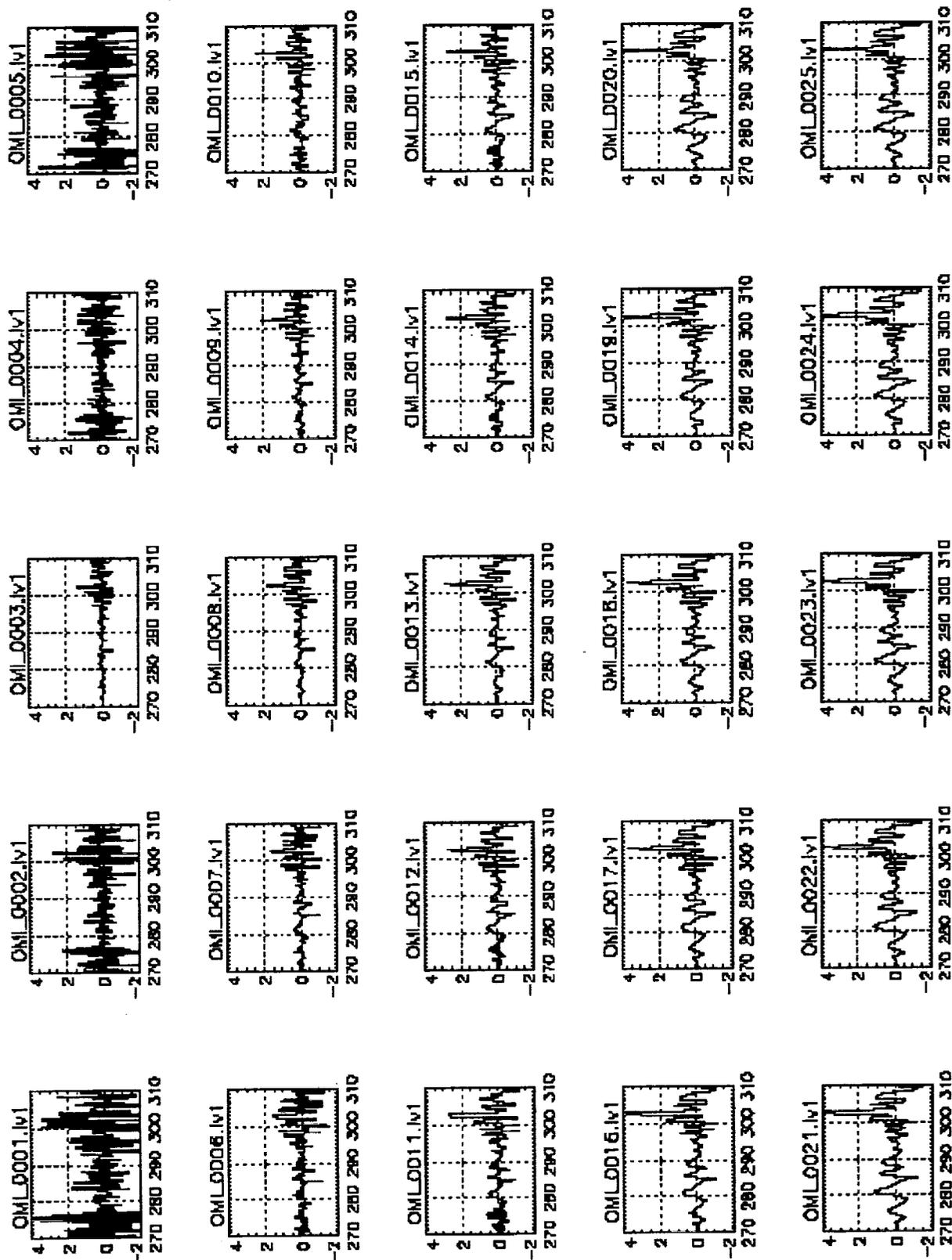


Fig. 2 The relative deviation for channel UV-1 for the five values of the relative shift (from left to right, $+0.1 \rightarrow -0.1$) and the five values for the S-FWHM (from top to bottom, $S=1 \rightarrow 5$).





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 Title: Required Signal-to-noise levels for OMI for DOAS products
 Author: J.P. Veefkind
 Version: 1 of 28 November 2000
 Checked: R.F. van Oss, J. de Haan
 Approved: P.F. Levelt

Required Signal-to-Noise levels for OMI DOAS products

Abstract

The required signal-to-noise (S/N) levels for OMI DOAS products are determined.

1. Method

The method to estimate the required S/N for DOAS products is described in R1. As shown in R1, there is a relation between the S/N ratio and the error in the slant column density:

$$S/N = [\Delta SCD]^{-1} [stdev(\sigma_x)\sqrt{N}]^{-1} \quad (1)$$

where ΔSCD is the error in the slant column density

$[stdev(\sigma_x)\sqrt{N}]$ is a factor that is determined by the differential absorption cross section of the species x and the number of wavelengths used in the DOAS fit. The values for $[stdev(\sigma_x)\sqrt{N}]$ for ozone, NO₂, BrO, SO₂, OCIO and HCHO for OMI are given in Table 1.

Using equation 1 the required S/N are determined by using the errors in the SCD as input.

Table 1. $[stdev(\sigma_x)\sqrt{N}]$ for ozone, NO₂, BrO and SO₂, OCIO and HCHO

	Fit window [nm]	$[stdev(\sigma_x)\sqrt{N}]^{-1}$ [DU]
Ozone	325 - 335	2100 *
NO ₂	425 - 450	43 *
BrO	345 - 360	1.8 *
SO ₂	314 - 327	320 *
OCIO	355 - 385	1.1
HCHO	335 - 360	240

* From R1

2. Results

In R2 requirements are given for the accuracy of OMI data products. These requirements are for the vertical column densities. In Table 2 the minimum error for vertical column densities are given, and the pixel size for which they are valid. To use these numbers, they are translated to errors in the slant column by multiplying them with an airmass factor of 2, representing the case when OMI is looking at nadir and the solar zenith angle is 0 degrees. The resulting error in the slant column is also given in Table 2.

The required S/N is calculated using equation 1 using the information provided in Tables 1 and 2. The resulting S/N values are given in the third column of Table 3. Note that these values are for the pixel size given in Table 2. Also given in Table 3 are the required S/N for a pixel of 13 × 24 km² (OMI global mode) and for 13 × 12 km² (OMI zoom-in mode).

Table 2. Minimum values for the vertical column densities for the given pixel size. Also given are the errors in the slant column densities assuming an air mass factor of 2.

	Pixel Size [km ²]	Δ VCD [molec/cm ²]	Δ VCD [DU]	Δ SCD [DU]
Ozone	20 × 20		4	8
NO ₂	40 × 40	1·10 ¹⁴	3.7·10 ⁻³	7.4·10 ⁻³
BrO	40 × 40	1·10 ¹³	3.7·10 ⁻⁴	7.4·10 ⁻⁴
SO ₂	40 × 40		0.4	0.8
OCIO	40 × 40	1·10 ¹³	3.7·10 ⁻⁴	7.4·10 ⁻⁴
HCHO	40 × 40	1·10 ¹⁵	3.7·10 ⁻²	7.4·10 ⁻²

Table 3. Required S/N for the SCD errors listed in Table 2. The third column is the S/N for the pixel size given in Table 2, the fourth column is for OMI global mode pixel (13 × 24 km²) and the last column for OMI zoom-in pixels (13 × 12 km²).

	Fit window [nm]	S/N	S/N Global	S/N Zoom-in
Ozone	325 - 335	263	232	164
NO ₂	425 - 450	5805	2563	1813
BrO	345 - 360	2430	1073	759
SO ₂	314 - 327	400	177	125
OCIO	355 - 385	1485	656	464
HCHO	335 - 360	3240	1431	1012

3. Conclusions

The required S/N values for DOAS products of ozone, NO₂, BrO, SO₂, OCIO and HCHO for OMI are determined. The S/N for OMI global mode and zoom-in mode pixels is given in Table 3. Note that these required S/N values are only given for the DOAS products. For other products, additional S/N requirements are needed.

4. References

- R1. Van Oss, R.F., Relation between signal-to-noise of Earth radiance measurements on DOAS column error, 20 October 1999.
- R2. Science Requirements Document for OMI-EOS version 2 draft, RS-OMIE-000-KNMI-001, 22 August 2000

Definition of Level 1B Radiance product for OMI

document: RS-OMIE-KNMI-206
version: 1.0
date: 31 July 2000
authors: J.P. Veefkind KNMI veefkind@knmi.nl
A. Mälkki FMI anssi.malkki@fmi.fi
R.D. McPeters NASA mcpeters@wrabbit.gsfc.nasa.gov
approved: B. van den Oord
checked: B. van den Oord

1. Introduction

The data format of the Level 1B radiance product for the Ozone Monitoring Instrument (OMI) on EOS Aura, as defined by the international OMI science team, is described.

1. The drivers for the Level 1B format are:
 - Information Content. No information shall be lost by storing the data
2. User accessibility. Easy access must be provided for all (potential) OMI users.
3. Size. Size reduction to reduce archiving and transport costs.
4. External Interface. HDF-EOS swath structure.

Note that these drivers may have conflicting interests. For example: user the accessibility and information content may drive to a larger data product, which is clearly in opposite direction of the size driver.

2. File Organization

OMI is an UV/VIS spectrometer. It has two CCD detectors, one for the ultra violet (UV) and one for the visible (VIS) wavelength range. The UV CCD is used to image two channels: UV-1 and UV-2. The VIS CCD is used for only one channel. Thus OMI has three channels: UV-1, UV-2, and VIS.

Most of the data products that are derived for the OMI Level 1B radiances use only a part of the spectrum within one of the channels. An exception is the UV-1: most data products that are derived from this channel will also use the UV-2. Therefore the OMI Level 1B radiances are split into two data products, one for the UV-1 and UV-2 (UV CCD), and one for the VIS channel (VIS CCD). The main advantage of having two products is that users that need only part of the spectrum reduces considerably on their storage and transportation costs. The UV OMI data product will use separate HDF-EOS swath structures for the UV-1 and the UV-2.

For each CCD readout discipline (global, spatial and spectral zoom-in) a separate product is created. Users that are interested in the zoom products can thus easily find, transport and store the data that they are interested in. Additionally, the zoom-in data is also re-binned to the binning factor of the global readout discipline and stored in the global readout discipline product. This is done for users that derive global products, so that they find all data of an orbit in one file and in one swath data structure. Note that using spectral or spatial zoom-in results in missing parts of the spectrum or missing parts of the swath. In the global readout discipline files, data from different readout discipline can be present. In this product a flag is used to indicate the used readout discipline.

3. Information Content

The OMI Level 1B radiance product contains three classes of information:

- Metadata
- Radiance data
- Geolocation data.

Definition of Level 1B Radiance Product for OMI

The information that shall be provided in each of the classes is listed below.

Metadata

- ECS core metadata
- GDPS version number
- OPF version number
- Auxiliary and ancillary files
- Temporal coverage
- Spatial Coverage
- CCD Readout Discipline
- CCD Readout Discipline Statistics (Global data products only)
- Binning Factor
- Co-addition factor
- Integration time
- DEM gain (factor and column)
- ELU gain
- ELU mode
- Number of binned dark/smear rows
- Number of skipped rows
- Number of binned rows read
- Number of readout register pixels skipped
- Number of pixels per binned row read
- Folding Mirror position
- Solar port open/closed
- Diffuser Position
- WLS state
- LEDs state
- Day/night flag
- Small pixel data column numbers
- Quality Flag Statistics
- Number of measurements

Radiance Data

- Radiance Data
- Small Pixel Data
- Wavelength information
- Quality Flags
- CCD Readout Discipline

Geolocation Data

- Latitude
- Longitude
- Time
- Terrain Height
- Solar Zenith Angle
- Solar Azimuth Angle
- Line-of-sight Zenith Angle
- Line-of-sight Azimuth Angle
- Spacecraft Latitude
- Spacecraft Longitude
- Spacecraft Altitude
- Land/Sea/Ice flag
- Sunlint flag

4. Packing of Data

The efficient packing of the data considerably reduces the costs for archiving and transportation. The bulk of the OMI data are the radiances and their precisions. If stored as 4 byte reals, the radiances and their precisions use 8 byte per (binned and co-added) pixel. Several options were investigated to store the information in less bytes. The packing method that uses the least bytes, without losing significant information is to store the mantissa of the radiance, the mantissa of the radiance precision and a shared exponent. (For example $469.7 \pm 1.1 \cdot 10^9$ is stored as 4697 (mantissa radiance, 2 byte integer), 11 (mantissa precision, 2 byte integer), 8 (shared exponent, 1 byte integer). In total 5 bytes are used to store the radiance and its precision, which is a reduction of 37.5% compared to the 8 bytes needed if stored as reals.

Each pixel of OMI data has its own wavelength registration. However, the result of the wavelength calibration algorithm of the Level 0→1B GDPS is a fourth order polynomial describing the relation between pixel number and the wavelength. This information is present for each pixel in the swath and for each of the channels. In the Level 1B radiance products, the five coefficients and their variances of the fourth order polynomials are stored.

5. Product Size

Based on the detailed definition given in appendix A, the size of the products for global modes are estimated as 500 MB for the UV product and 620 MB for the VIS products. These estimates are based on 2000 measurements per orbit, assuming 2/3 of the orbit to be sunlit. As the total number of entries is approximately the same, the size of the zoom mode products will only be slightly larger. The increase is caused by more geolocation information and more small pixel data.

6. Summary

The following are the major aspects concerning the OMI Level 1B radiance product:

1. The OMI Level 1B radiance product shall be orbit based
2. There shall be separate products for the UV and the VIS channels
3. Data from special measurement modes is stored as special products
4. Data from special measurement modes are re-binned to, and stored in, the global mode product

APPENDIX A Detailed Product Definition

UV PRODUCTS

Product short name: Name convention OMu<ReadoutID>R1,
 OMu01R1B Global
 OMu02R1B Spectral zoom-in
 OMu03R1B Spatial zoom-in

Product long name: OMI/Aura Level 1B for UV-1 and UV-2 channel

Product description: This product contains the geolocated backscattered radiances for the OMI UV-1 (270-314 nm) and UV-2 (306-380 nm) channels. Also contained in this products are the Solar zenith and azimuth angles and viewing zenith and azimuth angles.

Data format: HDF-EOS

Data structure: Simple swath structures for UV-1 and UV-2. Name UV1radiance, UV2radiance

Dimensions in swath

nTimes	number of measurements
nXtrack	number of OMI swath angles
nWavel	number of wavelengths
nTimesSmallPixel	number of small pixel data
nWavelCoef	number of wavelength coefficients

VIS PRODUCTS

Product short name: Name convention OMv<ReadoutID>R1,
 OMv01R1B Global
 OMv02R1B Spectral zoom-in
 OMv03R1B Spatial zoom-in

Product long name: OMI/Aura Level 1B for VIS channel

Product description: This product contains the geolocated backscattered radiances for the VIS channel (350 – 500 nm). Also contained in this products are the Solar zenith and azimuth angles and viewing zenith and azimuth angles.

Data format: HDF-EOS

Data structure: Simple swath structures for VIS. Name VISradiance

Dimensions in swath

nTimes	number of measurements
nXtrack	number of OMI swath angles
nWavel	number of wavelengths
nTimesSmallPixel	number of small pixel data
nWavelCoef	number of wavelength coefficients

SWATH CONTENTS

Metadata

Core Metadata

Product Specific Metadata

Radiance data

RadianceMantissa	(nTimes,nXtrack,nWavel)	2 byte integer
RadiancePrecisionMantissa	(nTimes,nXtrack,nWavel)	2 byte integer
RadianceExponent	(nTimes,nXtrack,nWavel)	1 byte integer
WavelengthCoefficient	(nTimes,nXtrack,nWavelCoef)	4 byte real
WavelengthCoefficientPrecision	(nTimes,nXtrack,nWavelCoef)	4 byte real
UVsmallPixelRadiance ¹	(nTimesSmallPixel,nXtrack)	4 byte real
VISsmallPixelRadiance ¹	(nTimesSmallPixel,nXtrack)	4 byte real
UVsmallPixelWavelength ¹	(nTimesSmallPixel,nXtrack)	4 byte real
VISsmallPixelWavelength ¹	(nTimesSmallPixel,nXtrack)	4 byte real
AutomatedFlags ²	(nTimes,nXtrack,nWavel)	2 byte integer
ReadOutDiscipline ³	(nTimes,nXtrack)	1 byte integer

Geolocation

Time ⁴	(nTimes)	8 byte double
SecondsInDay ⁴	(nTimes)	4 byte float
Latitude	(nTimes,nXtrack)	4 byte real
Longitude	(nTimes,nXtrack)	4 byte real
Terrain Height	(nTimes,n Xtrack)	2 byte integer
SolarZenithAngle	(nTimes,nXtrack)	4 byte real
SolarAzimuthAngle	(nTimes,nXtrack)	4 byte real
LOSzenithAngle	(nTimes,nXtrack)	4 byte real
LOSazimuthAngle	(nTimes,nXtrack)	4 byte real
SpacecraftLatitude	(nTimes)	4 byte real
SpacecraftLatitude	(nTimes)	4 byte real
SpacecraftLongitude	(nTimes)	4 byte real
SpacecraftAltitude	(nTimes)	4 byte real
GeoFlags ²	(nTimes,nXtrack)	2 byte integer

1) not in UV-I swath

2) used for bitwise flag storage: 2 byte integer contains 16 flags.

3) Global measurement mode only.

4) Time is in TAI format (as required by HDF-EOS), SecondsInDay is in UTC format.



The Netherlands and Finnish data requirements in the operational phase of OMI

	name:	date:	sign.:
Prepared:	J. Carpay	10-3-00	
Approved:	H. Förster		



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1. Reference documents

- a. OMI-EOS Data Volume and Data Rate Budgets LE-OMI-0033-FS/98, 23 July 1998
- b. OMI Science Requirements Document RS-OMIE-000-KNMI-001 issue 1, 18 Nov. 1998
- c. Finnish Ground Station for EOS-Chem, LE-OMIE-0002-FMI/98, 18 Sept. 1998

2. Summary of the requirements

The current requirements for data delivery from the OMI instrument to the Netherlands' and Finnish scientific parties can be summarised as follows:

1. A level 1b dataset of each orbit – possibly a subset in spectral range-, together with the necessary engineering, calibration and ancillary data shall be accessible to NIVR within 70 minutes after delivery to the ground station, for the generation of Near Real Time level 2 products. If this is not possible rate buffered or level 0 data and necessary engineering and ancillary data shall be accessible within 50 minutes after delivery to the ground station.
2.
 - a) The whole set or a spatial (Finland) and spectral range subset of raw data for Very Fast-Delivery (VFD) regional products shall be broadcast to a Finnish ground station at least once a day during overpass of the EOS-Chem satellite over Finland.
 - b) The whole set or a spatial (Netherlands) and spectral range subset of raw data for Very Fast-Delivery regional products shall be broadcast to a Netherlands ground station at least once a day during overpass of the EOS-Chem satellite over The Netherlands (TBC).
3. A subset (i.e. a number of ground pixels) of level 0 data and necessary engineering and ancillary data of TBD amount shall be available on request to NIVR within 1 week after the request is received at the DAAC
4. All level 0 data and necessary engineering and ancillary data shall be available on request to NIVR within 2 weeks after the request is received at the DAAC
5. The level 1b data shall be accessible to NIVR within 24 hours after arrival of the OMI data at the 0-1 processing site (EOSDIS requirement)
6. The necessary housekeeping data shall be available routinely at the OMI Support Terminals in the Netherlands and Finland within 24 hours
7. The level 2 standard products shall be accessible to NIVR within 24 hours after the level 1b data has become available at the level 2 processing site



3. Introduction

The Netherlands, jointly with Finland, will deliver the ozone-monitoring instrument OMI-EOS to NASA for EOS-Chem, an atmospheric chemistry mission due to be launched in December of 2002. This paper has the purpose to describe the current data needs from the Netherlands-Finnish user community *in the operational phase* of the mission. It will mainly focus on the requirements for OMI data, but where applicable also other instruments are mentioned.

During the commissioning phase, when the instrument will be calibrated and the products validated, the data requirements will be different. For that phase, separate facilities for data distribution will have to be planned and set up to ensure fast delivery of calibration and validation data to the research groups carrying out those activities.

OMI Support Terminals from which the instrument operations support and monitoring will be carried out, will be installed in The Netherlands and Finland (TBC). These have a separate need for engineering and housekeeping data. This is mentioned in this document where relevant, but data quantities can at the moment only be estimated.

The requirements listed in this document have been defined independently from the EOS-DIS requirements. Some of the requirements go beyond the routine specs of EOS-DIS and probably will have to be fulfilled via a different road. One example is the use of an additional ground station in Finland, which will receive the data needed for regional (i.e. above Finland) special products. This ground station could also be used in a different way as a backup for the Norwegian ground station in Svalbard. The latter is discussed separately between FMI and NASA. This requirements document has been written taking into account that the requirement for EOS-DIS is to deliver at least 95 % of the data recorded by the instrument. Therefore where "all data" is mentioned, this means all data available at EOS-DIS.

The assumption for this version of the document is that level 0-1 processing will take place at the Goddard DAAC, the level 1-2 processing site is TBD. The fast-delivery products will be generated at a KNMI owned computer installed at GSFC, in a similar way to the NOAA system for MODIS (TBC). The Very Fast Delivery product is processed in and distributed from Finland.

Since the data requirements may change with time, this document remains a living document.

4. Data usage

Three types of data use can be distinguished.

- a. operational use
- b. scientific use
- c. engineering use

a: Operational use:

For operational applications like weather forecasting the delivery of operational data has a time constraint: for instance, ozone columns need to be available for input into the weather models within 3 hours after observation. In general the most critical requirement for operational data is the timely delivery, rather than accuracy. It is also called Near-Real Time data (NRT). With the present processing scenario, the minimal requirement is a subset (roughly 6%, GOME experience at KNMI) of the data for operational NRT purposes (ozone column retrieval).



Very Fast delivery (VFD) is direct broadcast of OMI raw data, which is received by a ground station and subsequently processed into higher level products.

The following NRT, VFD and/or operational special products are foreseen at the moment (note that this is not related to the NASA/EOS-DIS data products or requirements):

- NRT global level 2 O₃ column (Netherlands)
- level 4 assimilated global ozone field (Netherlands)
- regional VFD level 2 O₃ column (Finland, from raw data acquired and processed in Finland, possibly also in The Netherlands (TBC))
- regional VFD level 2 O₃ profile (Finland, processed in Finland, possibly also in The Netherlands (TBC))
- regional VFD UVB index maps (Finland, processed in Finland, possibly also in The Netherlands (TBC))

Recent developments at KNMI show that there are possibilities for more operational NRT products. These are:

- ozone profile (input for weather models)
- NO₂ column (biomass burning)
- aerosol index (biomass burning, volcanoes)

Another optional product is NRT delivery of global or local level 3 or 4 SO₂ map in case of volcanic outbursts. The main goal for this is tracking of volcanic clouds for air traffic safety purposes. It has not yet been determined who will produce this.

NRT availability of level 0 data for these products is a probable future requirement.

b: Scientific use

For scientific use of the data, the requirement is accuracy rather than fast delivery. As a minimum the following (level 2 and higher) products are foreseen:

- O₃ total column (standard product)
- UVB flux (standard product)
- O₃ vertical profile (standard product TBC)
- NO₂ column (standard product TBC)
- aerosol optical thickness (standard product TBC)
- cloud information (effective cover and top pressure, standard product TBC)
- SO₂
- BrO

c: Engineering use

Engineering data is used for health checks of the instrument on a routine basis. In addition to the engineering data also sample spectra (calibration data and earth radiances), dark current et cetera are needed for instrument health monitoring. This data has to be available to the engineers monitoring the instrument at the OMI Support Terminals in The Netherlands and Finland



5. Data requirements

5.1 Data rates

It is estimated that the instrument generates science data at 1 Mbit/s = 750 Mbytes/orbit, including the dark side of the orbit. For this estimate it is assumed that the necessary calibration data is obtained on the dark side of the orbit. The engineering datastream is 9,6 kbit/s = 7.2 Mbytes/orbit.

5.2 Operational data use

The requirements for operational data depend on which algorithms are selected for processing. With the currently foreseen approach (fast DOAS method), a subset of roughly 6% of the level 1 data is needed for the operational products listed above. The fast delivery ozone product (total column) is generated from the wavelength band from 325 to 335 nm.

For cloud information, a narrow spectral window at longer wavelengths (TBD) is needed in addition to the wavelength band of 325-335 nm. Calibration spectra, dark current and straylight data of a **TBD** amount are also needed (the calibration spectra must be in the same wavelength windows (TBC)). The earlier mentioned possible NRT products are not yet included in the mentioned data budget.

5.2.1 KNMI operational data needs

KNMI will need the data operationally for use in an operational level 1b-2 processor, developed at KNMI and running at a TBD site (for instance at GSFC, as to reduce the amount of data to be transferred overseas). The level 2 product will be used as input for generation of the higher-level ozone maps and for operational weather forecasts at ECMWF and NOAA. Although level 1b data is preferred, it is also possible to use level 0 or rate-buffered data for level 0-2 processing at the processing site.

Estimated total amount for ozone column: **60 kbit/s**. Data amounts for the other possible operational products are not yet estimated.

Availability:

If level 0 data is delivered to the processing site it needs to be delivered 20-30 minutes earlier than level 1b data (see below, steps 2 and 3). The time steps in the process are as follows (in reverse order):

1. transport from processing site to the weather model:	5 minutes
2. level 1-2 processing at processing site:	5 minutes
3. rate-buffered/level 0-1 processing at processing site , including transport:	30 minutes (TBC)
4. transport from spacecraft to SIPS or EOS-DIS	40 minutes
5. orbit	100 minutes
Total	180 minutes

Since OMI is the only instrument on board of EOS-CHEM with this Near-real time requirement, it appears that by giving OMI data the highest priority in the time schedule these requirements can be met.

5.2.2 FMI operational data needs

To fulfil the requirement for a very fast delivery of the data, it is required that the spacecraft is in broadcast mode over Finland, i.e. during one overpass per day when Finland is within the swath. During the broadcast, OMI raw data is also recorded on board. With the broadcast mode no uplink is needed.



The use of OMI-EOS with the direct broadcast mode will also serve as a technology demonstrator and pilot project for the Finnish ground station

5.3 Scientific data use

The constraint on the delivery time is less strict for scientific use, but the amount of data is much larger.

Level 0 (science and engineering data):

Subset of groundpixels : available within **1 week** after request (amount TBD): Essential
All : available within **2 weeks** after request: Desirable

The foreseen use of level 0 data includes the further development of processing algorithms.

Level 1b:

All : available within **24 hours** after arrival of OMI data at the level 0-1 processing site: Essential (this is also an EOS-DIS requirement (TBC))

Depending on data amounts and actual delivery times, the delivery might be on-line, via satellite link or on physical media (CD, tape...). This has to be discussed. The planned use for level 1b data is for generation of additional scientific level 2 products and further development of algorithms for the currently foreseen level 2 products.

5.4 Engineering data

Because the instrument operations are supported from The Netherlands, it is necessary that housekeeping data (a subset of engineering data) (i.e. a subset of 7.2 Mbyte/orbit) is delivered routinely to the OMI Instrument Support Terminals (TBC).

Some of this data is also needed for the Very fast delivery and the Near-Realtime ozone products.

6. Other EOS-Chem instruments

General

No NRT delivery of other EOS-Chem instrument data is required (TBC) on Netherlands or Finnish side.

No level 0 and level 1 data from these instruments are required. However, the level 2 and 3 data of HIRDLS, MLS and TES are needed for comparison and validation of OMI products. In addition, these data are needed for processing into synergetic products. An example is tropospheric ozone column, which can be derived from the OMI total ozone column by subtracting integrated stratospheric ozone profiles provided by the other instruments.

The following level 2 and 3 data products are needed

HIRDLS: profiles of O₃, NO₂, SO₂, BrO, H₂O, temperature etc.

TES: columns and profiles of O₃, NO₂, SO₂, BrO, etc.

MLS: profiles of O₃, NO₂, SO₂, BrO, H₂O, temperature etc.



Annex 1: Levels of product processing

The different levels of the OMI data products are defined in EOS-DIS as follows:

Raw	As received from OMI.
Rate-Buffered	Intermediate product between raw and level 0, with limited quality checks and overlaps not removed
Level 0	Raw instrument data at original resolution, time ordered, with duplicate packets removed.
Level 1A	level 0 data that may have been reformatted or transformed reversibly, located to a co-ordinate system, and packaged with needed ancillary and engineering data.
Level 1B	radiometrically corrected and calibrated data in physical units at full instrument resolution as acquired.
Level 2	Geolocated geophysical product, e.g. ozone column
Level 3	Regridded ("interpolated") level 2 data
Level 4	Level 2 products enhanced with other data or model calculations ("value added products").

Annex 2: definitions

Accessible	The data can be picked up electronically, e.g. at an FTP server
Available	The data is sent to NIVR or an NIVR designated site, e.g. on tapes or CD ROM
Request	This means a request from NIVR to EOS-DIS to make the data available. This could also be a standing order (i.e. an order to send the data every week)
Rate buffered data	data from a single instrument (APID) from a single spacecraft contact. It consists of packets extracted from the telemetry stream, augmented with an EDOS service header and placed in a file to be sent to customer. The EDOS service header contains EDOS supplied quality and accounting information, including: <ul style="list-style-type: none">• time stamp (ground receipt)• out-of-sequence flag• playback flag• test data indicator• RS decoding error count• source VCID
Special Data Products.	Generated as part of a research investigation using EOS data and produced for a limited region or time period, or products that are not accepted as standard by the PI, IWG and NASA Headquarters. They will be generated at research users' computer facilities.
Standard Data Products.	Generated as part of a research investigation, of wide research utility, accepted by the PI, the IWG and the EOS Program Office, routinely produced, and, in general, spatially and/or temporally extensive data products. Standard Level 1 data products will be generated for all EOS instruments; standard Level 2 data products will be generated for most EOS instruments. Some EOS interdisciplinary investigations will also generate standard data products.
Ancillary data.	Data other than instrument data required to perform an instrument's data processing. They include orbit data, attitude data, time information, spacecraft engineering data, calibration data, data quality information, and data from other instruments.

Simulated Radiances for OMI

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author: J.P. Veefkind
approved: G.H.J. van den Oord
checked: J. de Haan

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0. Abstract

OMI radiance spectra simulations are presented for ozone hole, tropical summer and midlatitude conditions. Orbit simulations were performed using the Satellite Tool Kit (STK). Radiative transfer calculations were performed using MODTRAN. Expected minimum and maximum radiances for OMI are derived and compared to other radiance data used in the OMI documentation. Variations of the minimum and maximum radiances for selected wavelengths over the orbit are presented. This document replaces the document "Radiance percentile values for small-pixel GOME earthshine measurements" (R2).

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1. Introduction

For tuning the optics and gain settings of OMI realistic radiance spectra are needed. Especially important for signal-to-noise (S/N) and saturation issues are the minimum and maximum radiance levels. Two different sets of radiance levels are used in the OMI documentation for S/N calculations: the minimum/nominal/maximum values (R1, [link to file in ASCII](#)) and the GOME percentile values (R2, [link to file in ASCII](#)).

For the present study three scenario's are used:

1. Antarctic
2. Tropical Summer
3. Midlatitude

The scenario's 1 and 2 are expected to give the lowest and highest radiances.

For the three scenario's the Sun/satellite geometries were calculated using the Satellite Tool Kit (STK). Orbit simulations were performed for the EOS-CHEM orbit: Sun synchronous with an altitude of 705 km and a local equator crossing time of 13:45:00.

The radiances were calculated using MODTRAN 3.7 . MODTRAN was chosen because of its quasi spherical approach, which is important for the ozone hole scenario. Two values for the surface albedo are used: 0.0 and 0.9. The MODTRAN computations do not include the Ring effect and the effects of Sun glint.

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2. Scenario's

2.1 Antarctic

Simulations of OMI measurements were performed for two stations on Antarctica: station S75 (Lat -75, Lon 0) and station S85 (Lat -85, Lon 0). Orbit simulations were performed to predict measurements by OMI of ground pixels at the locations of S75 and S85, in the time period between 1 September and 1 November 2003. This is the time of year that ozone hole situations occur. The orbit simulations were started at 0N, 0E, at 1 September 2003 13:45:00 GMT. They provide the Sun/satellite geometry for the overpasses over S75 and S85, i.e. the Solar zenith angle, the viewing zenith angle, and the relative azimuth angle between the Sun and the line-of-sight (LOS).



Figure 2.1. Locations of stations S75 and S85 and an example of an OMI overpass on 16 September 2003. The green lines are OMI ascending overpasses for a single day. The cyan and magenta lines indicate the art of the orbit when OMI measurements for the two stations are possible.

Due to the wide swath of OMI, multiple overpasses per day are available at high latitudes. For each day, the overpass with the smallest Solar zenith angle was used in the MODTRAN calculations. This criterion selects the highest radiance levels for a given location and day. Thus, the optimum daily measurement of OMI for a given location is selected. Simulations were performed for five days in the period between 1 September and 1 November 2003. The Sun/satellite geometry for the overpasses over S75 and S85 are given in Table 2.1 and Table 2.2, respectively.

Table 2.1. Sun/satellite geometry for station S75 (75S, 0E).

Date	Time	Sun zenith angle	LOS zenith angle	Sun-LOS azimuth angle
1 Sep 2003	15:03:10.75	88.818	24.140	66.638
16 Sep 2003	13:05:52.49	82.753	54.317	64.042
2 Oct 2003	13:32:16.01	77.005	50.555	61.047
15 Oct 2003	15:01:27.11	73.372	25.201	58.878
2 Nov 2003	13:40:02.15	66.647	49.2830	56.358

Table 2.2. Sun/satellite geometry for station S85 (85S, 0E).

Date	Time	Sun zenith angle	LOS zenith angle	Sun-LOS azimuth angle
1 Sep 2003	-	-	-	-
16 Sep 2003	13:03:03	91.903	51.290	63.581
2 Oct 2003	13:29:26	85.954	49.841	61.129
16 Oct 2003	12:25:48	81.136	53.119	59.252
1 Nov 2003	14:31:13	75.603	45.776	57.726

In the MODTRAN calculations two model atmospheres were used: the subarctic winter model to simulate "normal" ozone conditions and a modified subarctic winter model to simulate ozone hole conditions. For the ozone hole conditions, the ozone concentration between 16 and 45 km altitude was set to zero, resulting in an total ozone column of 100 DU. The following are links to the MODTRAN input files:

Normal ozone conditions:

- station S75, albedo 0.0
- station S75, albedo 0.9
- station S85, albedo 0.0
- station S85, albedo 0.9

Ozone hole conditions

- station S75, albedo 0.0
- station S75, albedo 0.9
- station S85, albedo 0.0
- station S85, albedo 0.9

[Jump to Antarctic Results](#)

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2.2 Tropical Summer

For the tropical summer scenario a station on the equator was defined: S0 (0N, 0E). Orbit simulations were performed between 21 and 25 September 2003. At low latitudes only one ascending overpass per day is available for OMI, see Figure 2.2. The Sun/satellite geometries for the overpasses over S0 are listed in Table 2.3.

In addition to the simulations for station S0, also the simulations were performed for the minimum Solar zenith angle observed by OMI. Therefore, orbit simulations were performed for the 1st and 15th of each month. For this period, the smallest solar zenith angle occurred at 28.13N 155.36W for 1 July 2004 23:52:44 GMT, and was 20.221 degrees. The Sun/satellite geometries are listed in Table 2.4.

In finding the extreme radiances that OMI will measure, the Sun-Earth distance should also be taken into account. The minimum Solar zenith angles are observed in early July, when the Sun-Earth distance is at its maximum. In early January the incoming Solar irradiance is about 7 % higher. To account for this effect, orbit simulations were also performed to find the minimum Solar zenith angle observed by OMI during the time of the year when the Sun-Earth distance is at its

minim, i.e. around 4 January. Orbit simulations were performed between 5 and 8 January 2004. The minimum Solar zenith angle for this period is 26.434 degrees, which occurred for 20.83S, 139.1W for 7 January 2004 23:16:18.61 GMT. For the minimum Solar zenith angle cases, MODTRAN calculations for nadir and extreme swath angles were performed. The Sun/satellite geometries are listed in Table 2.4.

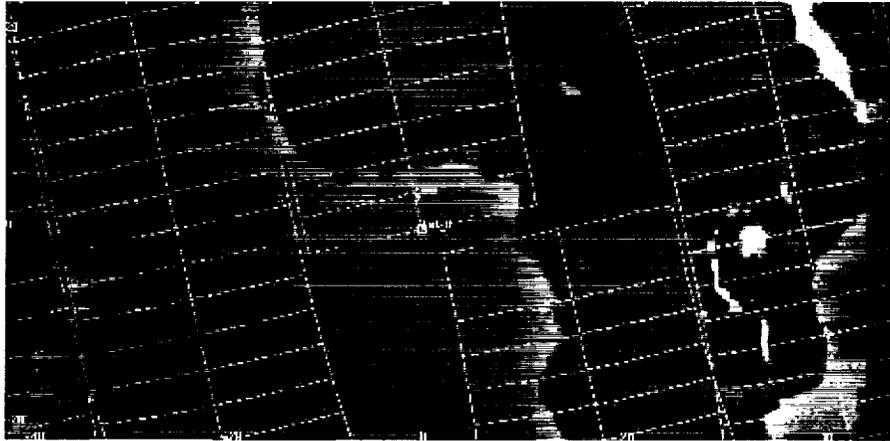


Figure 2.1. OMI coverage from 21 September 2003 13:45 GMT to 22 September 2003 13:45 GMT.

Green lines show swath middles and the swath extremes.

Table 2.3. Sun/satellite geometry for station S0 (0S, 0E).

Date	Time	Sun zenith angle	LOS zenith angle	Sun-LOS azimuth angle
21 Sep 2003	13:53:08	28.032	17.045	190.520
22 Sep 2003	12:59:37	27.852	56.436	5.786
23 Sep 2003	13:44:09	28.143	2.520	17.725
24 Sep 2003	14:28:40	28.486	55.494	189.980
25 Sep 2003	13:35:09	28.307	21.428	6.019

Table 2.4. Sun/satellite geometry for minimal Solar zenith angle (28.133N 155.361W) in July and January..

Date	Time	Sun zenith angle	LOS zenith angle	Sun-LOS azimuth angle
1 Jul 2004	23:52:44	20.221	57.000	180.000
1 Jul 2004	23:52:44	20.221	0.000	180.000
1 Jul 2004	23:52:44	20.221	57.000	0.000
7 Jan 2004	23:16:18	26.434	57.000	180.000
7 Jan 2004	23:16:18	26.434	0.000	0180.000
7 Jan 2004	23:16:18	26.434	57.000	0.000

The tropical atmosphere model was used for the MODTRAN calculations. Below are links to the MODTRAN input files for the simulation for S0 and for the minimal Solar zenith angle simulations:

- station S0, albedo 0.0

- station S0, albedo 0.9
- minimum Solar zenith angle for July and January, albedo 0.0
- minimum Solar zenith angle for July and January, albedo 0.9

Jump to Tropical Summer Results

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2.3 Midlatitudes

Midlatitudes are important for OMI because it is the region where most of the anthropogenic emissions occur. A station N50 was defined at 50N, 0E. Simulations were performed for two time periods : 21 to 23 June 2003 (time of year with smallest Solar Zenith angles), and 21 to 23 December (time of year with highest Solar zenith angles). At these latitudes 1-2 measurements by OMI are available per day, see Figure 2.3. Table 2.5 list the Sun/satellite geometries for the Midlatitude scenario.

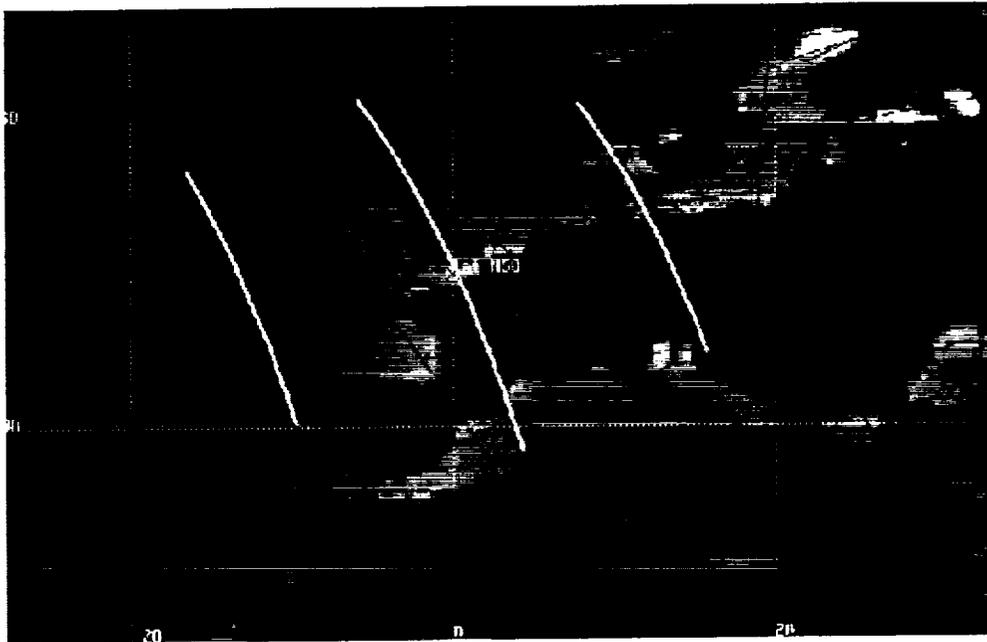


Fig 2.3. OMI daytime coverage over station N55 between 21 September 13:45 GMT and 22 September 13:45 GMT.

Red lines indicate OMI swath middles and swath extremes. White lines indicate the orbits when OMI observations of station N50 are possible. At the midlatitudes, the OMI swath for one day show considerable overlap.

Table 2.5. Sun/satellite geometry for station N55 (N55, 0E).

Date	Time	Sun zenith angle	LOS zenith angle	Sun-LOS azimuth angle
21 Jun 2003	13:58:28	28.096	40.983	138.426
22 Jun 2003	13:04:51	29.188	1.217	-43.758
23 Jun 2003	12:11:39	31.412	49.510	-47.449
23 Jun 2003	13:49:26	28.181	45.294	138.012
21 Dec 2003	14:09:11	73.439	53.230	122.121
22 Dec 2003	13:15:31	74.581	10.552	121.756
23 Dec 2003	12:22:15	76.986	45.521	-58.841
23 Dec 2003	14:00:09	73.492	49.656	121.87

For the Midlatitude scenario simulations a midlatitude summer model atmosphere was used for the June days, and a midlatitude winter model atmosphere used for the December days. Below links to the MODTRAN input files are given:

- station N50, June 2003, albedo 0.0
- station N50, June 2003, albedo 0.9
- station N50, December 2003, albedo 0.0
- station N50, December 2003, albedo 0.9.

[Jump to Midlatitude Results](#)

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2.4 Nominal Radiances

The above described scenario's were used to determine the minimum and maximum radiances. For optimization of S/N calculations also nominal radiances are needed. The radiances vary strongly with solar zenith angle. Therefore three latitudes and four dates were used for the simulations of the nominal radiances. The latitudes are the same as used for the scenario's described above: Antarctic (station S85), Tropical (station S0), and Midlatitude (station N50). Simulations were performed for 1 January, 1 April, 1 July, and 1 October. For the antarctic case 1 July is not used, since there is no sunlight in this time of the year at this location. For the Tropical and Midlatitude cases a surface albedo of 0.30 is used. For the Antarctic case a higher albedo of 0.50 is used, to account for sea/land ice. These albedo's account for the surface reflectivity, as well as for reflectivity contributions by clouds. For each case the radiance was computed for nadir, as well as for the two extreme swath angles of OMI.

Below are links to the MODTRAN input files:

- Antarctic (station S85)
- Tropical case (stations S0)
- Midlatitude (station N50)

[Jump to Nominal Radiances Results](#)

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3. Results

3.1 Antarctic Scenario

The radiance spectra for station S75 and S85 under normal ozone conditions, are shown in Figure 3.1 and 3.2. For the normal ozone hole conditions, the minimum radiance is $1.2\text{E}+08$ photons/cm²/s/sr/nm at 279.56 nm and occurs for station S85 for the largest Solar zenith angle. The maximum radiance for these conditions is $6.0\text{E}13$ at 496.15 nm, and occurs for station S85 for the minimum Solar zenith angle.

The following are links to the data of Figure 3.1 and 3.2 in ASCII format:

- Figure 3.1, station S75, albedo 0.0
- Figure 3.1, station S75, albedo 0.9
- Figure 3.1, station S85, albedo 0.0
- Figure 3.1, station S85, albedo 0.9

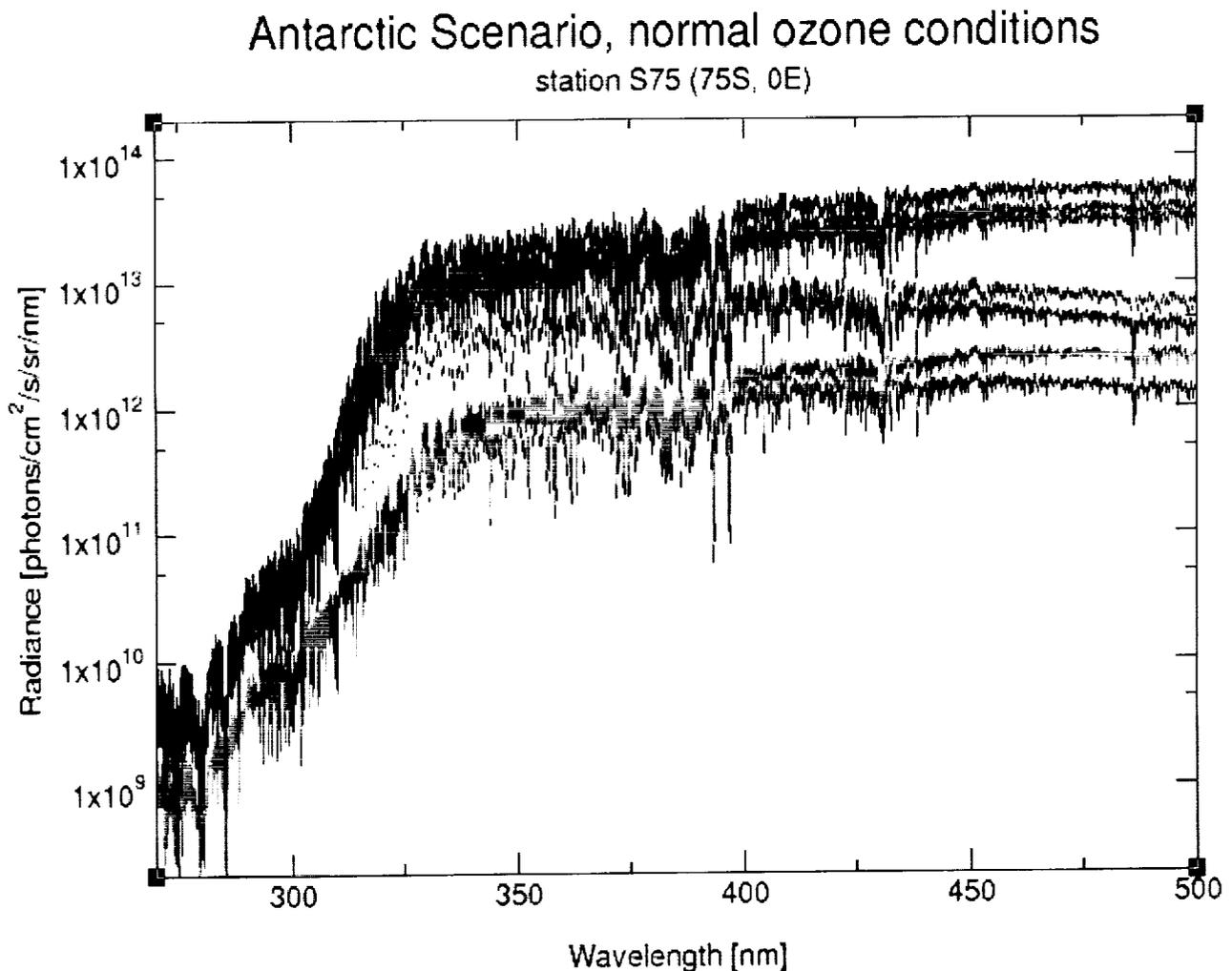


Figure 3.1. Radiance spectra for the Antarctic scenario for station S75, under normal ozone

conditions.

Antarctic Scenario, normal ozone conditions

station S85 (85S, 0E)

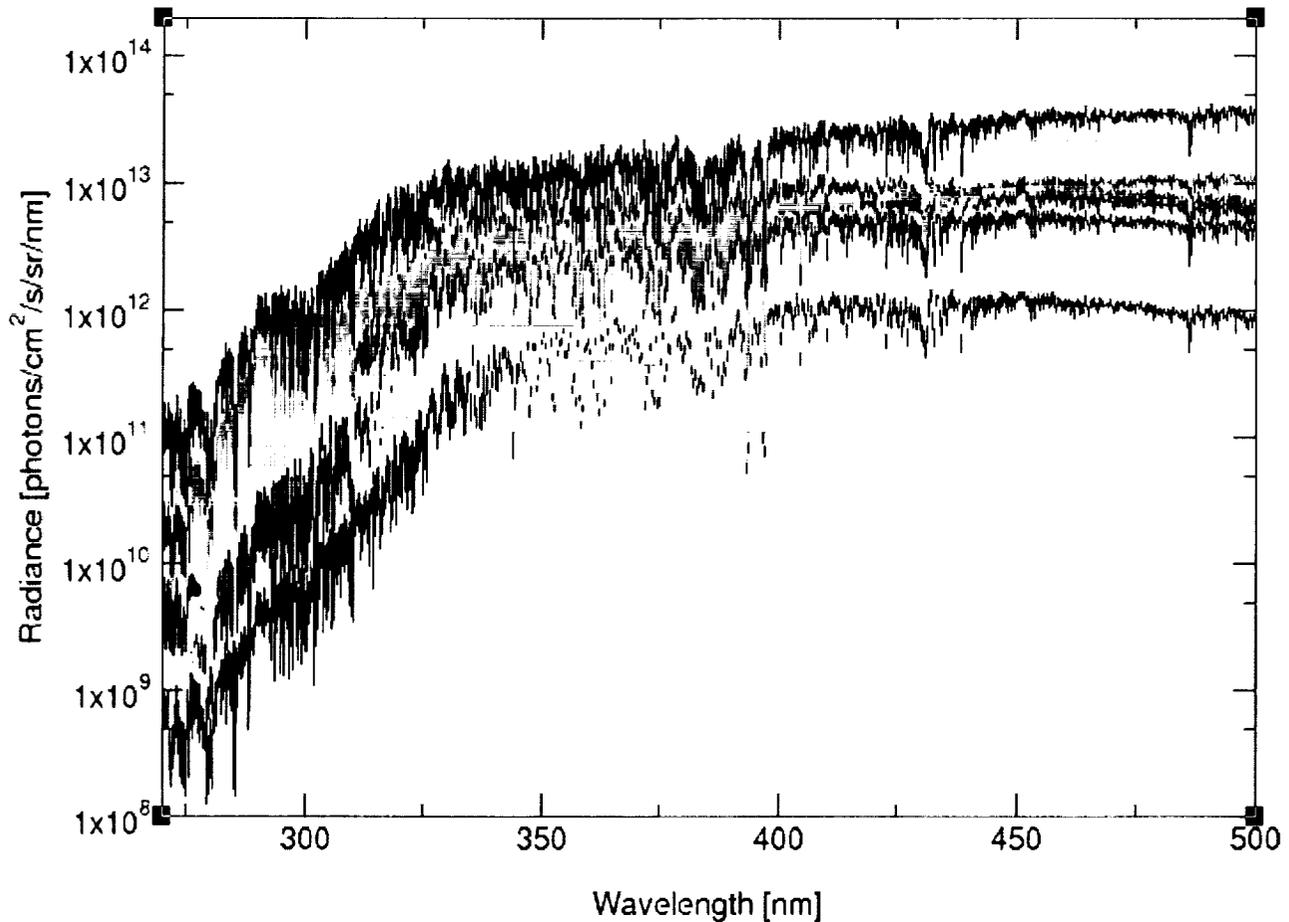


Figure 3.2. Radiance spectra for the Antarctic scenario for station S85, under normal ozone conditions.

Figure 3.3 and Figure 3.4 show the radiance spectra for ozone hole conditions for station station S75 and station S85, respectively. The minimum radiance for ozone hole condition is 3.7E+8 photons/cm²/s/sr/nm at 272.0 nm for station S85. The maximum radiance is 6.2E+13 photons/cm²/s/sr/nm at 496.15 nm for station S75.

The difference between normal ozone conditions (Figures 3.1 and 3.2) and ozone hole conditions (Figures 3.3 and 3.4) is large at wavelengths below approximately 340 nm. Due to the low total column ozone (100 DU), the radiances for ozone hole conditions are much higher in this wavelength range.

The following are links to the data of Figure 3.3 and 3.4 in ASCII format: Antarctic

- Figure 3.3, station S75, albedo 0.0
- Figure 3.3, station S75, albedo 0.9
- Figure 3.4, station S85, albedo 0.0
- Figure 3.4, station S85, albedo 0.9

Antarctic Scenario, ozone hole conditions

station S75 (75S, 0E)

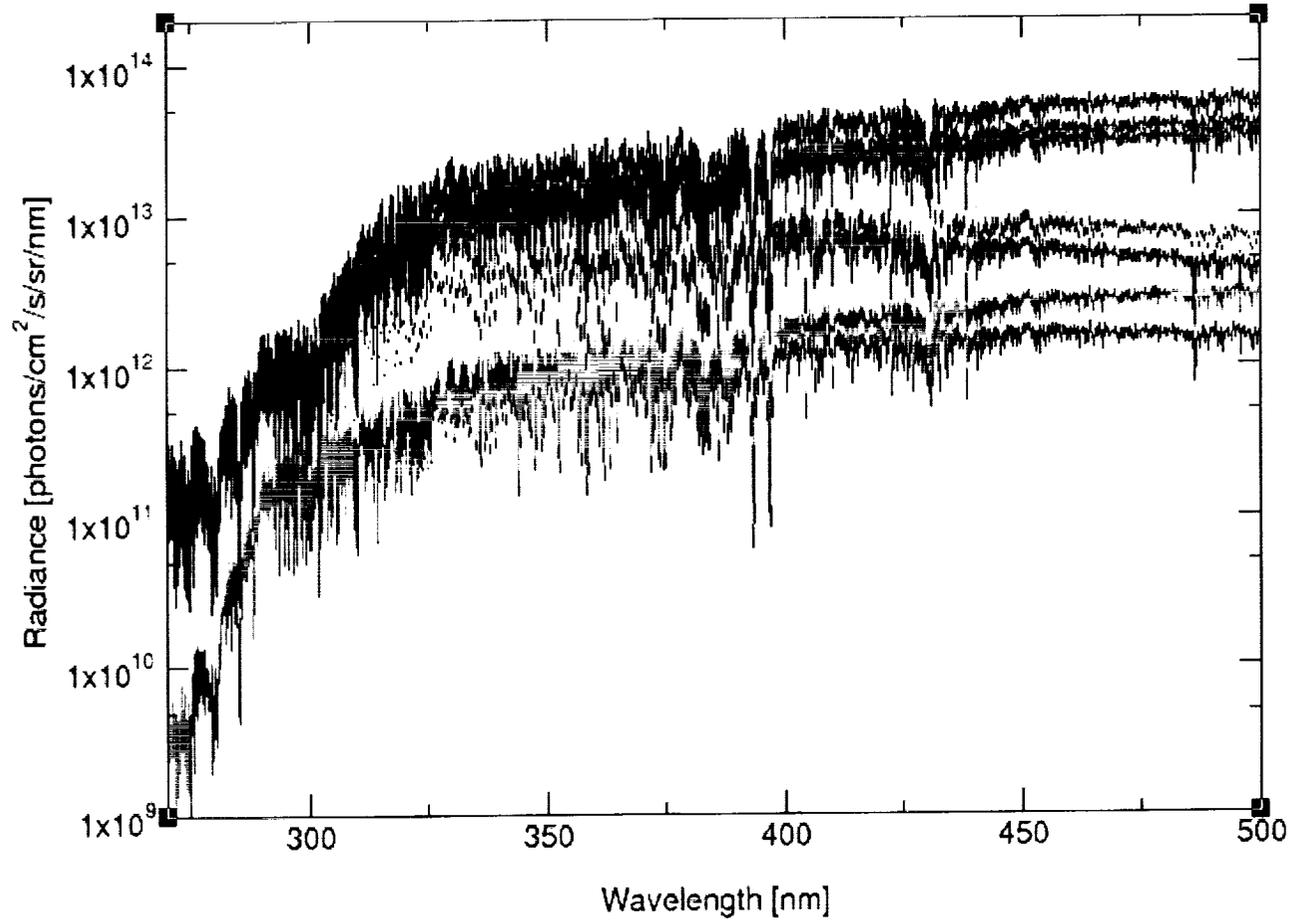


Figure 3.3. Radiance spectra for the Antarctic Scenario for station S75, for ozone hole conditions.

Antarctic Scenario, ozone hole conditions

station S85 (85S, 0E)

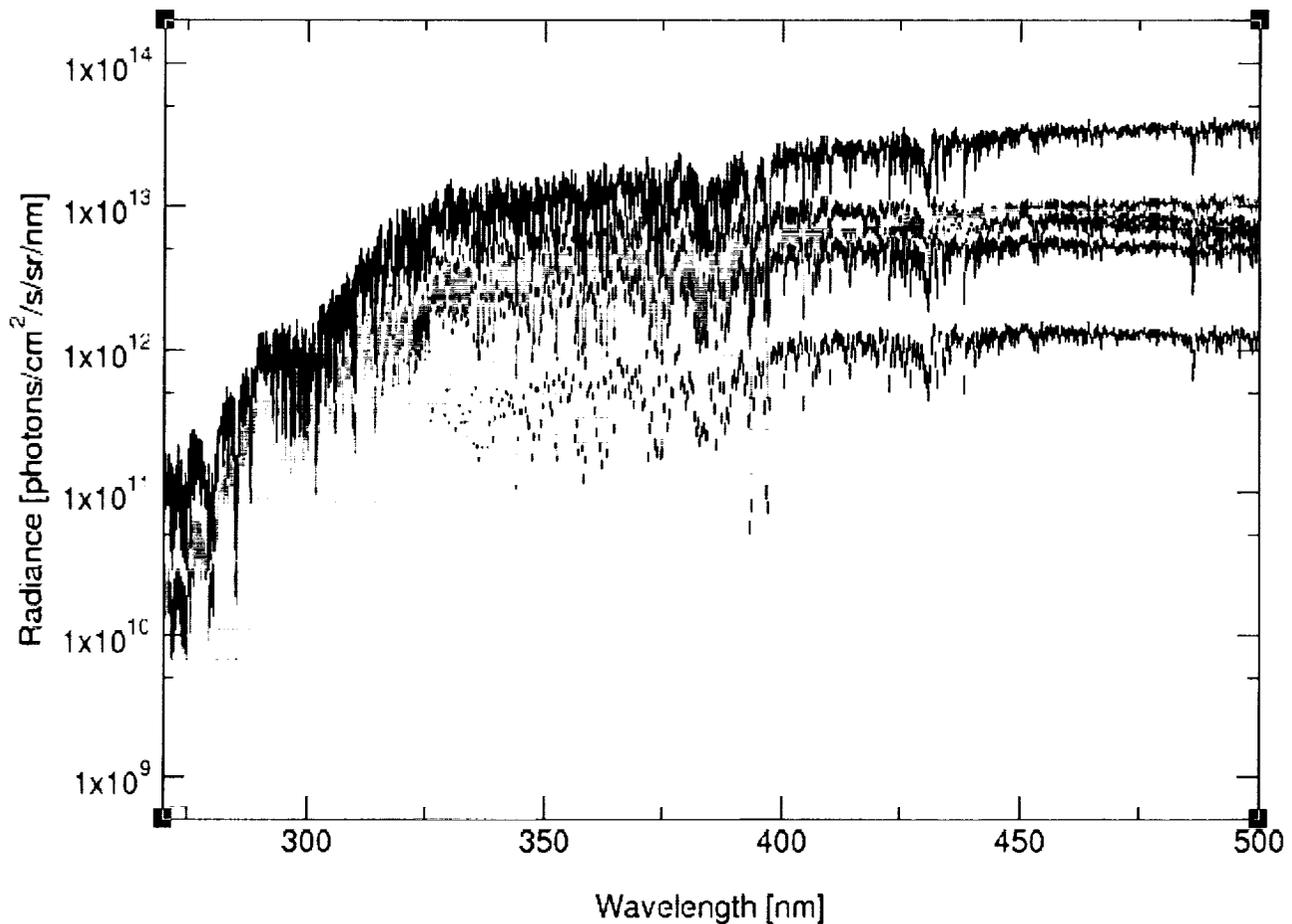


Figure 3.4. Radiance spectra for the Antarctic Scenario for station S85, for ozone hole conditions.

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3.2 Tropical Summer Scenario

The radiance spectra for the Tropical Summer scenario are presented in Figure 3.5 for station S0 and in Figure 3.6 for the minimum Solar zenith angle cases (July and January). The radiances vary from 1.1E+09 photons/cm²/s/sr/nm (at 279.56 nm) and 1.4 E+14 photons/cm²/s/sr/nm (at 496.15 nm) for Figure 3.5, and between 1.4E+09 photons/cm²/s/sr/nm(at 279.56 nm) photons/cm²/s/sr/nm and 1.4E+14 (at 496.15 nm) photons/cm²/s/sr/nm for Figure 3.6. The maximum radiances are reached for the minimum Solar zenith angle case for January, when the Sun-Earth distance is at its minimum.

The following are links to the data for Figure 3.5 and 3.6 in ASCII format.

- [Figure 3.5, station S0, albedo 0.0](#)
- [Figure 3.5, station S0, albedo 0.9](#)
- [Figure 3.6, min Solar zenith angle, albedo 0.0](#)

● Figure 3.6, min Solar zenith angle, albedo 0.9

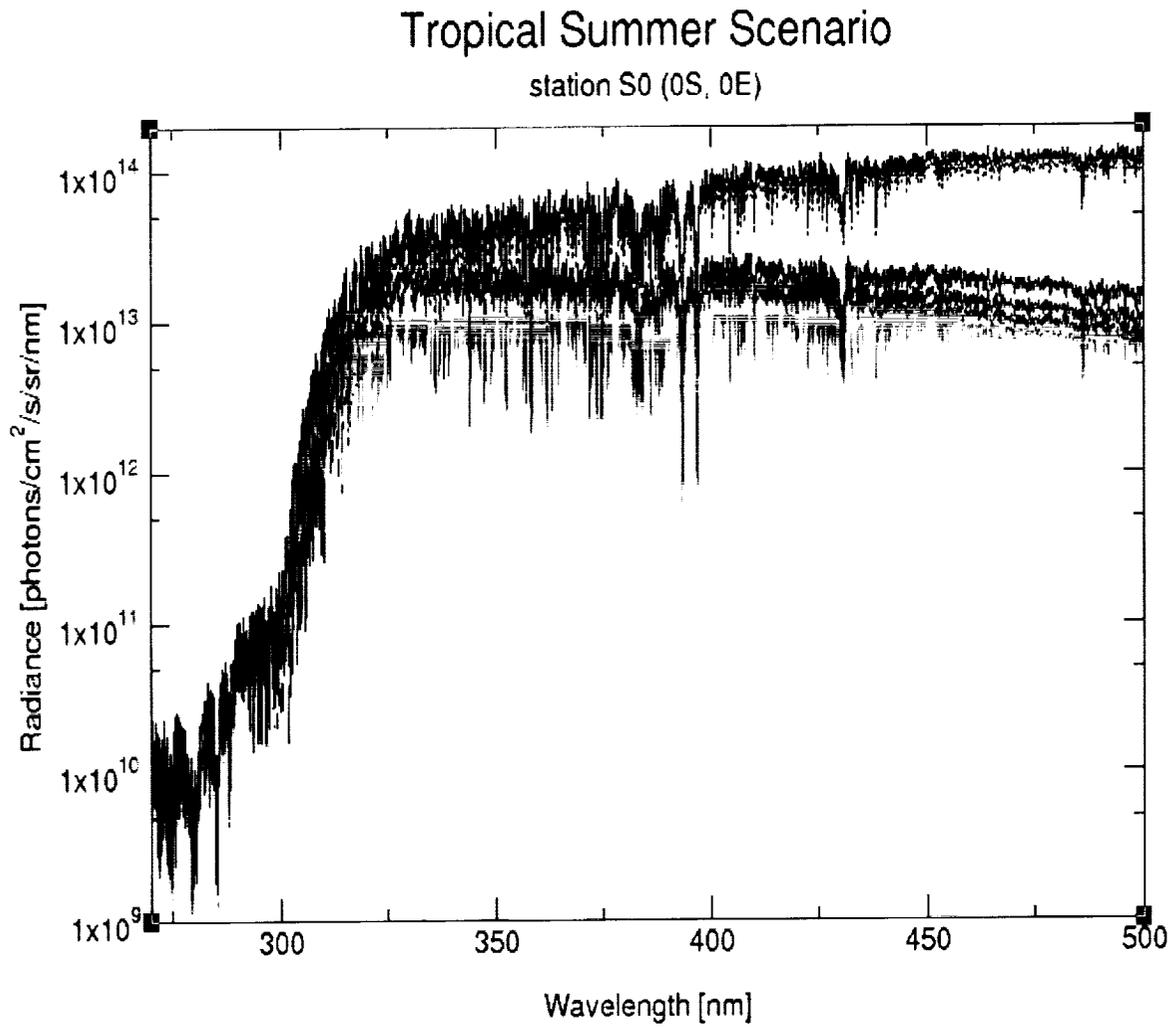


Figure 3.5. Radiance spectra for the Tropical Summer scenario, for station S0.

Tropical Summer Scenario

min Solar Zenith Angle

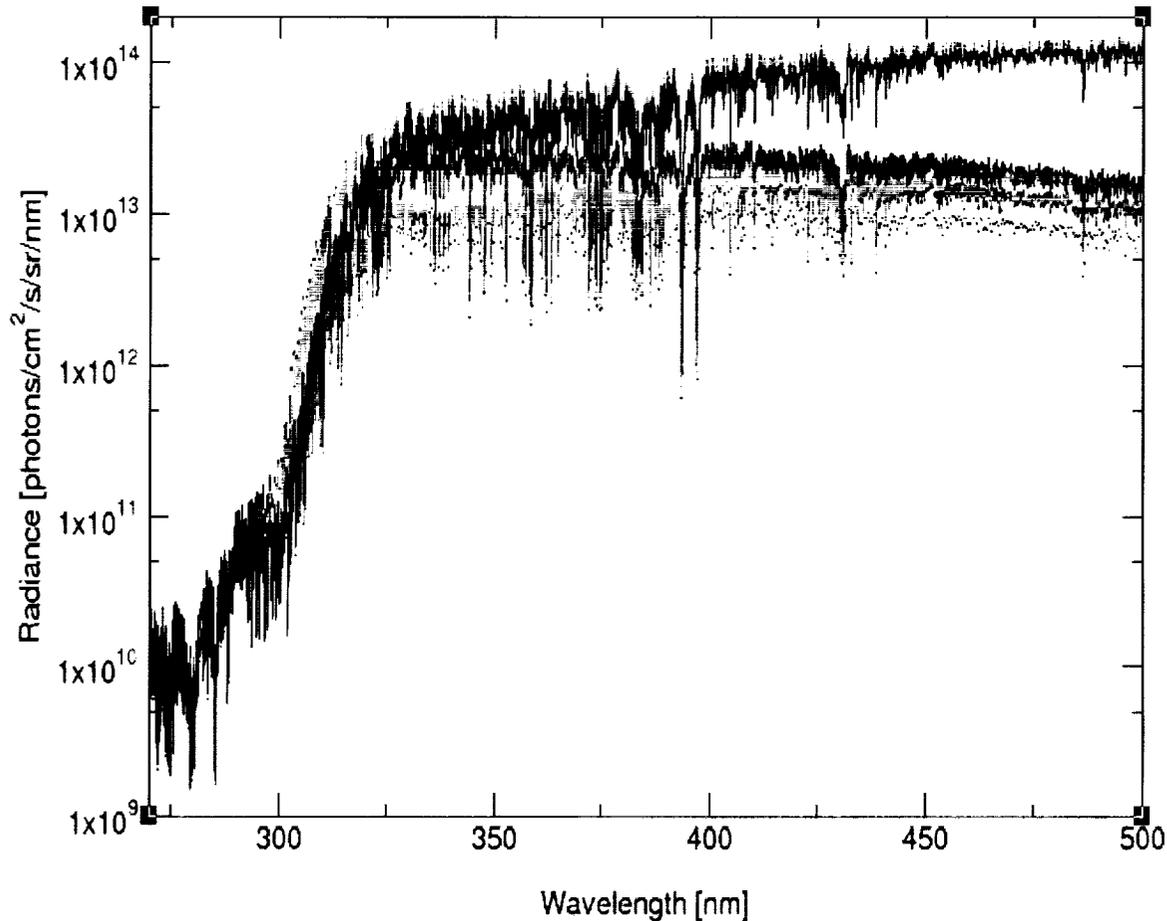


Figure 3.6. Radiance spectra for the Tropical Summer scenario, for the minimal Solar zenith angle case.

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3.3 Midlatitude Scenario

Figure 3.7 and 3.8 show the radiance spectra for the Midlatitude Scenario for station N50, for summer and winter, respectively. For the summer case (Figure 3.7) the radiance is in the range between 1.2E+09 photons/cm²/s/sr/nm (at 279.56 nm) and 1.3E+14 photons/cm²/s/sr/nm (at 496.15 nm). For the winter case (Figure 6) this range is between 1E+09 photons/cm²/s/sr/nm (at 279.56 nm) and 4.3E+13 photons/cm²/s/sr/nm (at 496.15 nm).

The following are links to the data for Figure 3.7 and 3.8 in ASCII format.

- [Figure 3.7, station N50, albedo 0.0](#)

- Figure 3.7, station N50, albedo 0.9
- Figure 3.8, station N50, albedo 0.0
- Figure 3.8, station N50, albedo 0.9

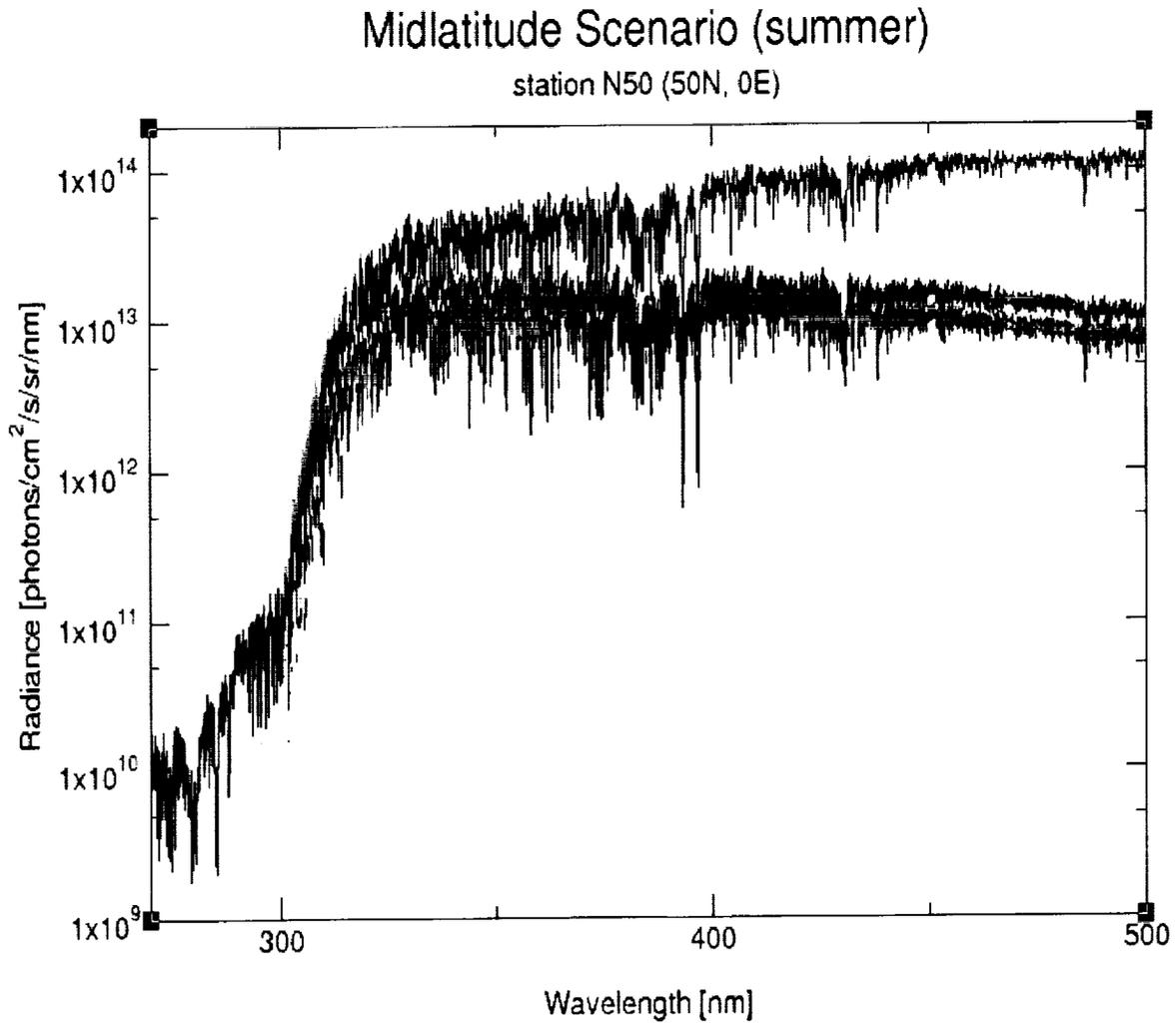


Figure 3.7. Radiance spectra for the Midlatitude summer scenario, for station N50.

Midlatitude Scenario (winter)

station n50 (50N, 0E)

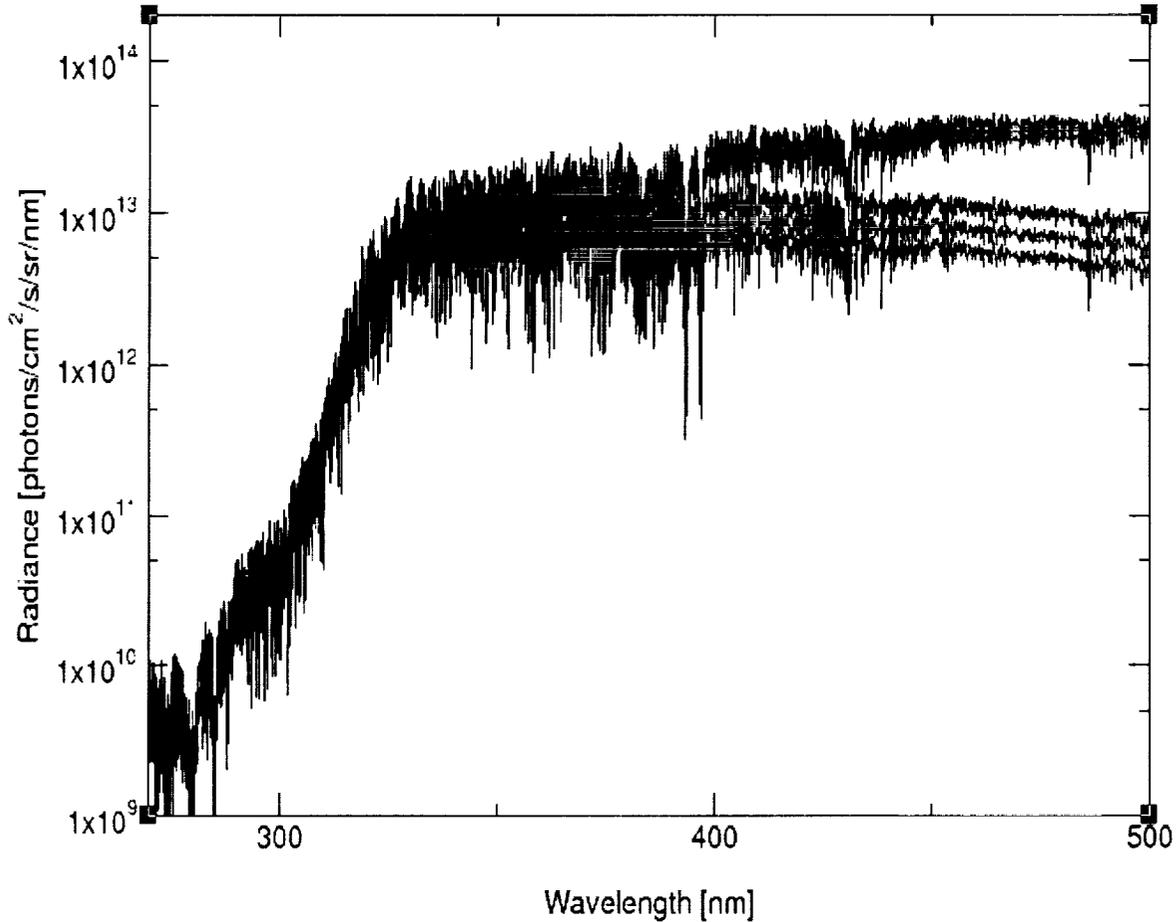


Figure 3.8. Radiance spectra for the Midlatitude winter scenario, for station N50.

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3.4 Nominal Radiances

Figure 3.9 shows the nominal radiances for the Antarctic, Tropical, and Midlatitude stations. These results are averages over the three swath angles and over the four days (three for Antarctic case).

The following are link to the data files in ASCII:

- [Figure 3.9; Antarctic, station S85](#)
- [Figure 3.9; Tropical, station S0](#)
- [Figure 3.9; Midlatitude, station N50](#)

Nominal Radiances

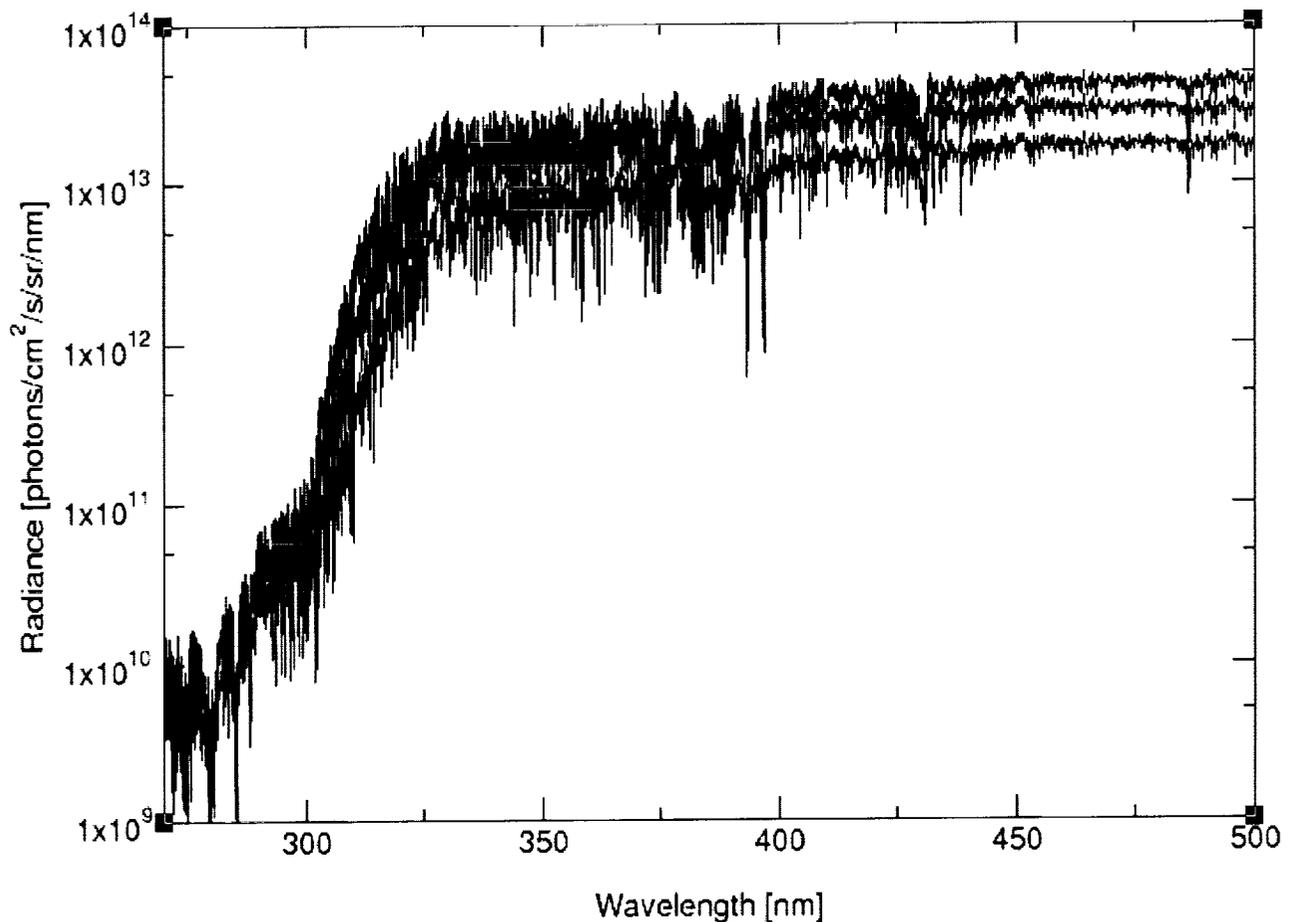


Figure 3.8. Nominal radiance spectra for the Antarctic (black), Tropical (red) and Midlatitude (green) case.

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4. Discussion

4.1 Minimum and Maximum Radiance Spectra

For tuning of OMI, the minimum and maximum expected radiance spectra are important. For each wavelength, the minimum and maximum radiances were determined from all the spectra presented in section 3. Note that this results in spectra that can contain values from different scenario's. Also, separate minimum and maximum spectra were determined for the antarctic, tropical summer and midlatitude scenario. ([link to the data in ASCII](#)).

In Figure 4.1 the minimum and maximum spectra for all data are plotted. For most of the wavelength range of OMI, the difference between the maximum and minimum spectrum is approximately a factor 100. However, around 315 nm this difference reaches a maximum of a factor of 400.

Also plotted in Figure 4.1 are the minimum/nominal/maximum radiances from R1 (link to the data in ASCII). Figure 4.1 shows that the minimum radiances derived in this study are lower than those of R1. Between 360 and 500 nm they are approximately a factor of 10 to 20 lower. Between 270 and 305 nm the difference is less than a factor of 10. The difference at 320 is approximately a factor of 80.

The maximum spectrum and the R1 maximum value correspond well for wavelengths larger than about 300 nm. Below 300 nm the maximum values from this study are higher (more than a factor of 10 at 270 nm). In this wavelength range the maximum range depends strongly on the ozone amount. The high values in this study are for the ozone hole conditions, due to the low ozone amount of 100 DU.

Min/Max Spectra & R1 Radiances

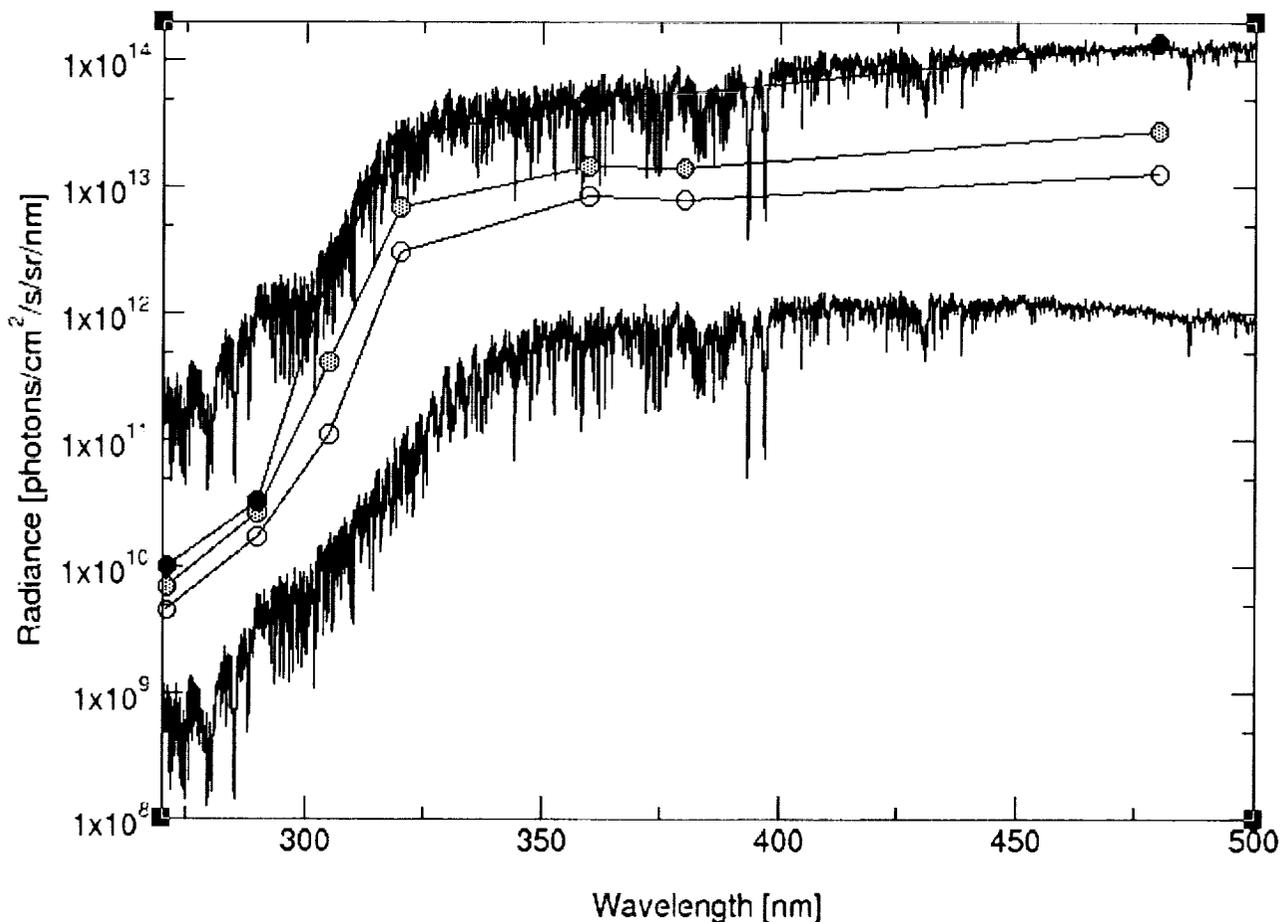


Figure 4.1. Minimum (black) and maximum (red) radiances for all scenario's plotted as a function of wavelength. Also plotted are the minimal/nominal/maximal radiance from R1 (circles).

Figure 4.2 shows a comparison between the minimum and maximum spectra from this study (same as Figure 4.1), and radiance percentile values for small pixel GOME measurements (R2, link to file in ASCII). The minimum spectrum is in between the 1% and 10% percentile values. Below 290 nm and between 300 and 330 nm the minimum are closest to the 1% percentile values.

Above 310 nm, the maximum spectrum is in between the 99 and 100% GOME percentile values. Below 310 nm the maximum values derived in this study are up to approximately a factor of 10 higher than the 100% percentile values. As mentioned above, these simulations are for the ozone

hole scenario. The GOME data are for 4 and 5 February and 4 and 5 May. These GOME orbits did not observe ozone hole conditions.

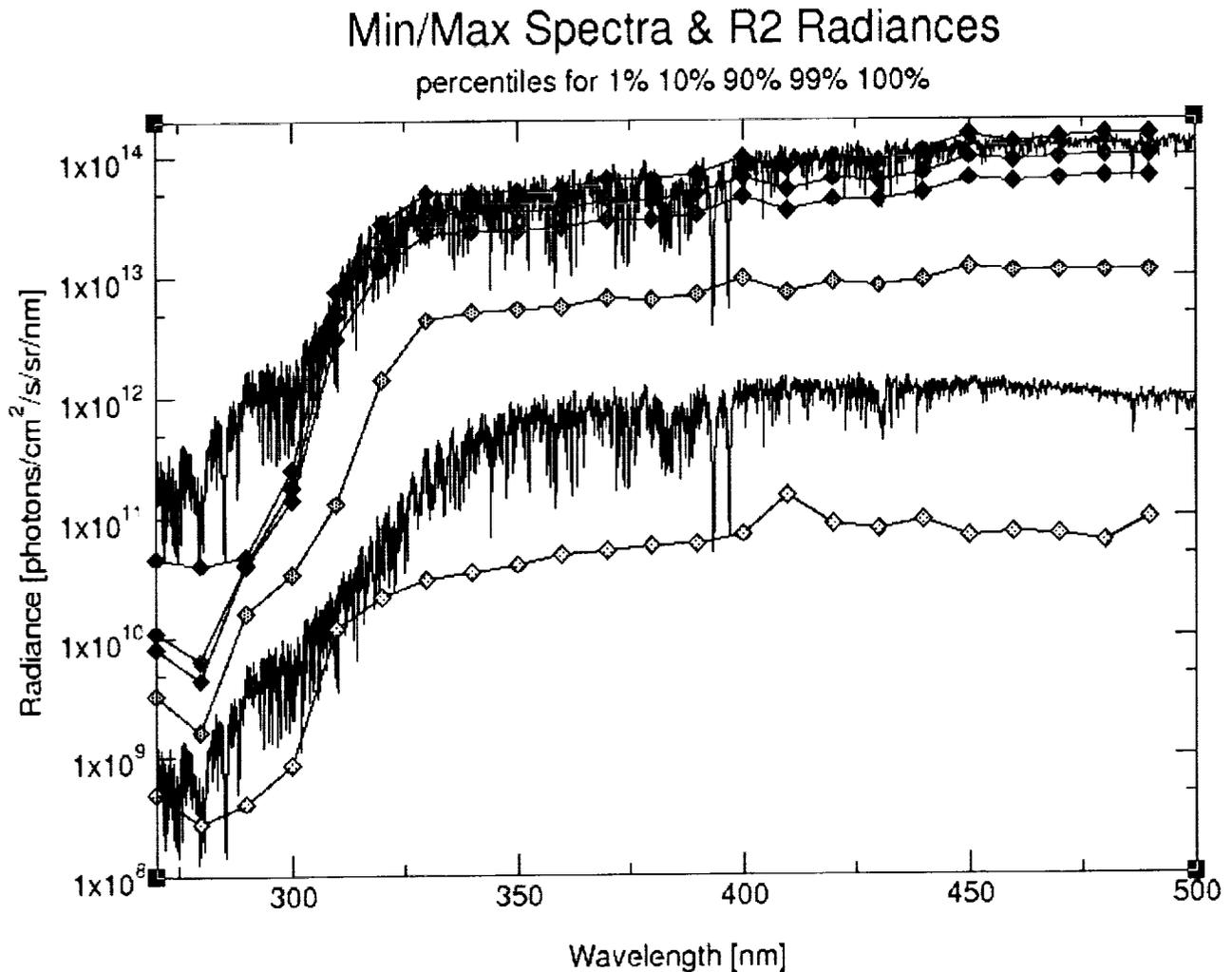


Figure 4.2. Minimum (black) and maximum (red) radiances for all scenario's (same as Figure 4.1). Also plotted are the R2 GOME percentile values for 1%, 10%, 90%, 99%, and 100% (blue diamonds).

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4.2 Minimum and maximum radiances over an orbit

The radiances that will be observed by OMI vary over an orbit due to changes in the Sun satellite geometry and due to the state of the atmosphere. For optimal performance of OMI, it is important to predict the minimum and maximum radiances as a function of orbit position. This information can be used to set the gain switches of the amplifiers of OMI. The radiance variations as a function of orbit position were investigated for two wavelengths: 279.56 nm and 496.15 nm. For most of the simulations described in section 3 the minimum radiance was observed at 279.56 nm. The maximum radiance for the spectra in section 3 was observed for 496.15 nm. For wavelengths above approximately 300 nm the minimum and maximum radiances depend on the

Solar zenith angle and on the surface albedo. In Figure 4.3a and 4.3b the radiances at 496.15 nm for the spectra of section 3 are plotted as a function of the cosine of the Solar zenith angle. Figure 4.3a is for surface albedo 0.0 and Figure 4.3b for surface albedo 0.9. The blue line in Figure 4.3a and the red line in Figure 4.3b are used to model the minimum and maximum radiances as a function of the Solar zenith angle.

For wavelengths below 300 nm the minimum and maximum radiances depend on the Solar zenith angle and the ozone column. Due to the strong ozone absorption and large Rayleigh optical thickness in this wavelength range, very few photons reach the surface. Therefore, the radiance at the top of the atmosphere does not depend on the surface albedo. Figure 4.3c and 4.3.d show the radiances at 279.56 nm plotted as a function of the cosine of the Solar zenith angle. Figure 4.3c is for normal ozone conditions, Figure 4.3d is for ozone hole conditions. The blue and red lines in Figure 4.3c and d are used to model the minimum and maximum radiance at 279.56 nm as a function of the Solar zenith angle.

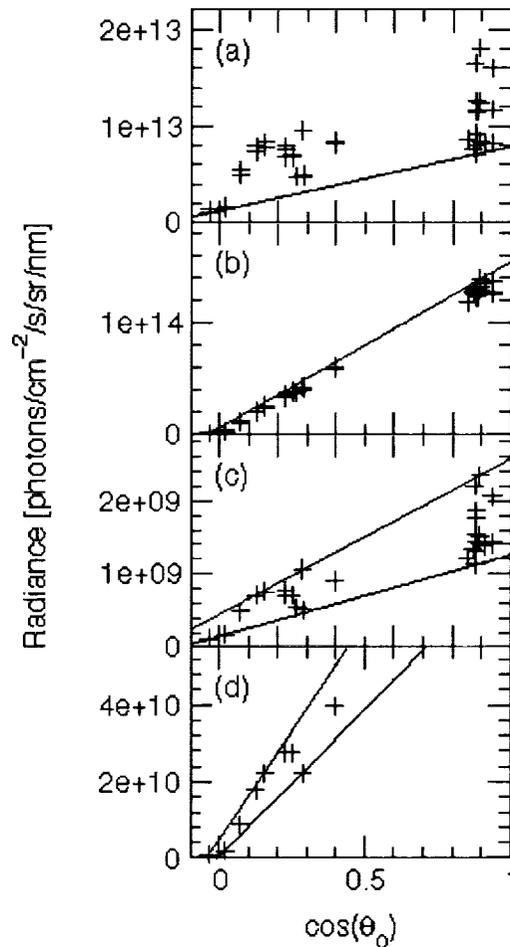


Figure 4.3. Radiance plotted as a function of the cosine of the Solar zenith angle. (a) wavelength 496.15 nm and albedo 0.0; (b) wavelength 496.15 nm and albedo 0.9; (c) wavelength 279.56 nm for normal ozone hole conditions; (d) wavelength 279.56 nm for ozone hole conditions.

Orbit simulations were performed for the EOS-CHEM orbit for four days: 21 March, 21 June, 21 September and 21 December 2003. The Solar zenith angles from the orbit simulations was used to determine the minimum and maximum radiances for 279.56 nm and 496.15 nm, using the blue and red lines of Figure 4.3. For 21 September, ozone hole conditions were used for latitudes between 55S and the South Pole.

Figure 4.4 and 4.5 show the minimum and maximum radiances at 496.15 nm over one orbit for each of the days. The orbits start and end at the Equator on the night side of the Earth. The shift of the pattern is caused by the seasonal variations in the Solar zenith angle.

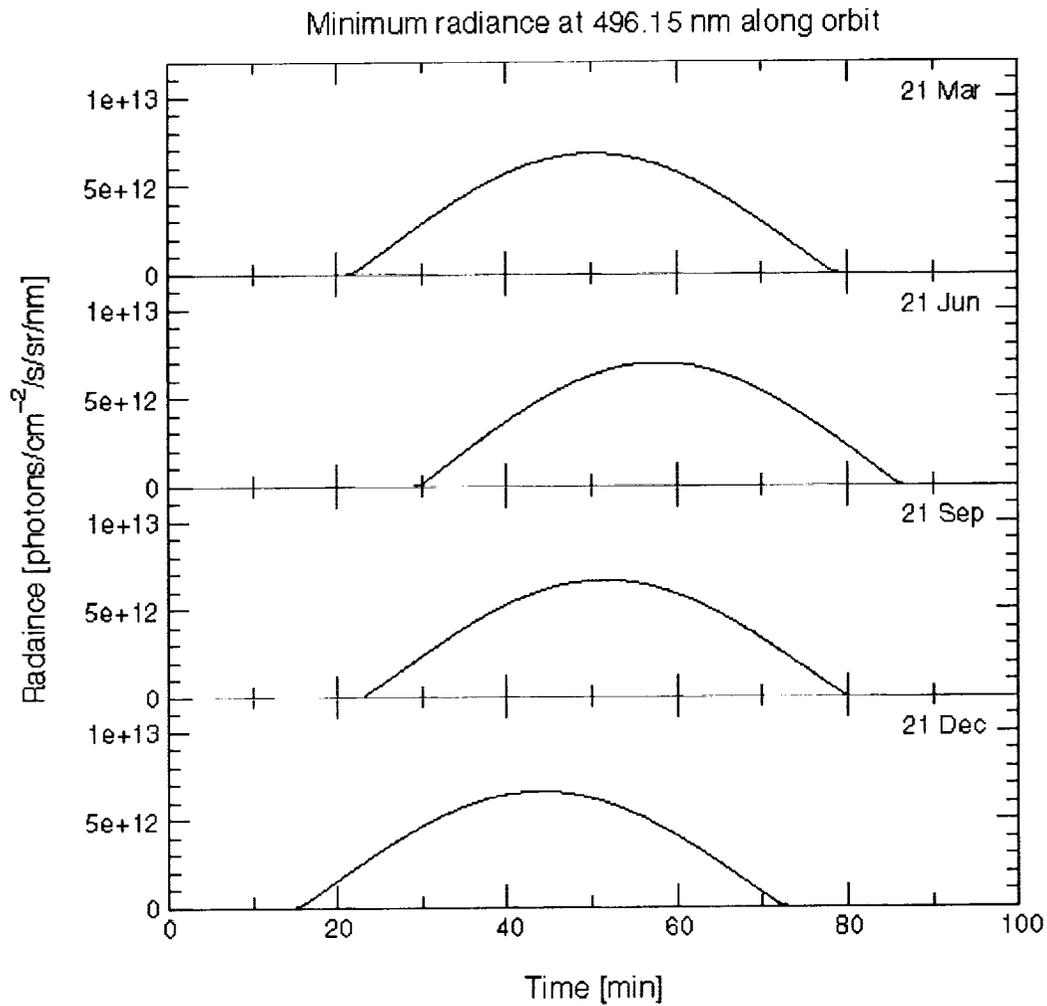


Figure 4.4. Minimum radiance at 496.15 nm over an orbit for four days of the year. The orbits start and end at the Equator on the night side of the orbit (descending direction).

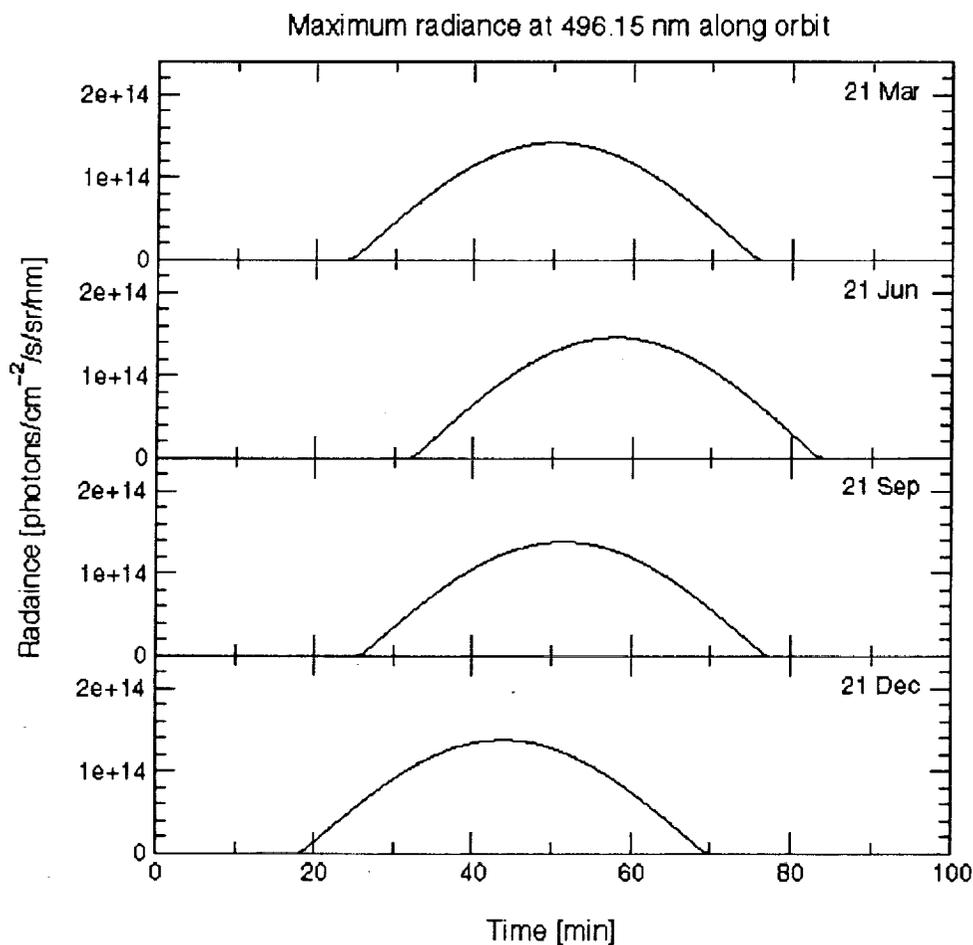


Figure 4.5. same as Figure 4.4, but for maximum radiances at 496.15 nm.

Figure 4.6 and 4.7 show the variations over the orbit of the minimum and maximum radiances at 279.56 nm. For the part of the orbit with ozone hole conditions, the radiances at this wavelength are much higher compared to the normal ozone conditions. This has large impact of the operation of OMI. During the time of the year when ozone hole conditions can be expected, predictions of the ozone hole spatial extend have to be used to schedule the gain settings. Note that ozone holes usually have very sharp edges. Therefore, variations of the order of a factor of 50 can occur in less than one minute of the orbit.

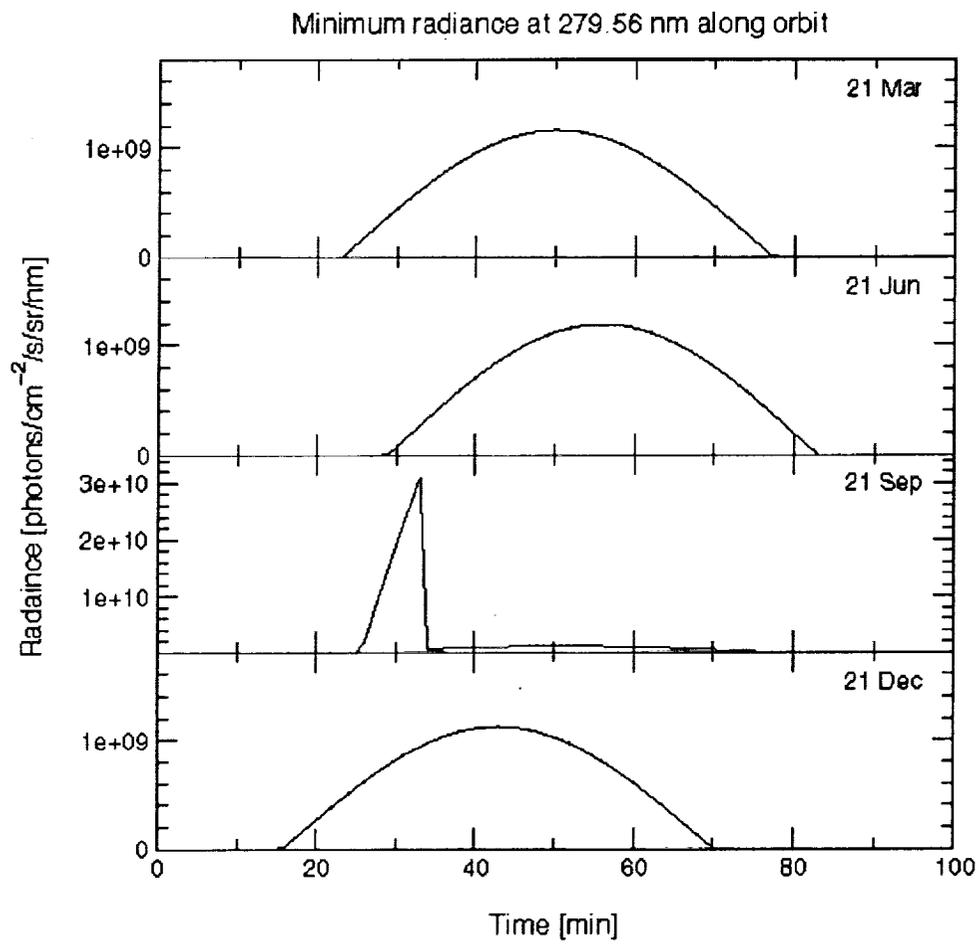


Figure 4.6. Same as Figure 4.4 but for minimum radiance at 279.56 nm.

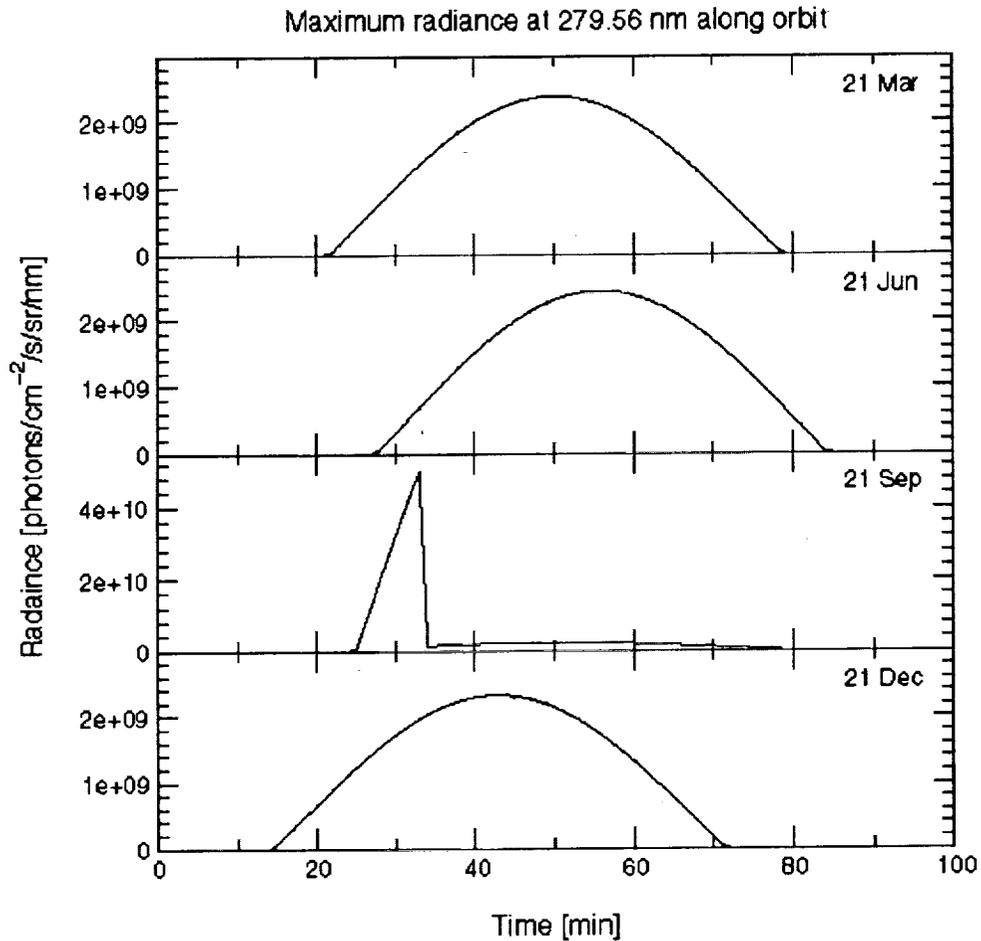


Figure 4.7. Same as Figure 4.4, but for maximum radiance at 279.15 nm.

The following are links to the data for Figure 4.4, 4.5, 4.6 and 4.7 in ASCII format.

- [Figure 4.4 and 4.5](#)
- [Figure 4.6 and 4.7](#)

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4.3 Sun glint, volcanic eruptions and polar stratospheric clouds

In the minimum and maximum radiances described in section 4.1 and 4.2, the following three cases have not been considered:

- Sun glint
- Large volcanic eruptions
- Polar stratospheric clouds (PSCs).

Sun glint will be observed frequently in part of the OMI swath. For sun glint, radiances at wavelengths larger than approximately 300 nm can be higher than the maximum radiance described

above. It is questionable if sun glint scenes can be used for retrieval of data products. If OMI goes into saturation for part of the swath, it is important if other swath angles are affected (for example due to 'blooming' on the CCD). Also, the recovery time after saturation is important.

Major volcanic eruptions can bring large amounts of aerosols into the stratosphere. Due to scattering and absorption by these aerosols the radiance observed by OMI are affected. For the shortest wavelengths the effects are not important, since only a small part radiation penetrates to the altitude of these aerosol layers. For wavelengths larger than 330 nm the effect is much larger. MODTRAN simulations for extreme volcanic conditions show that the minimum radiances at large solar zenith angles can be up to a factor of two lower than before the eruption. For high volcanic aerosol load minimum radiances can be 20% lower. Recovery after a major volcanic event can take several years.

PSCs occur at high latitudes in the winter at altitudes between 15 and 25 km. Most of the PSCs have very low optical depths (<0.02). However, in some cases the optical depth can be up to 1. The effect of PSCs on the radiance depends strongly on the wavelength, Sun/satellite geometry and surface albedo. As most PSCs occur over the polar ice caps, the surface albedo is high. Simulations were performed for PSCs with optical depth 0.2 at an altitude of 20 km. These simulations were performed for Solar zenith angles of 70 and 80 degrees and for relative azimuth angles of 0, 60, 120 and 180 degrees. The surface albedo was set to 0.8. The following was concluded from these simulations:

1. At 300 nm PSC will cause a small increase of the radiance ($<1\%$)
2. For wavelengths between 330 and 500 nm, the radiance can be increased by 30-50%, when looking into the direction of the sun.
3. For wavelengths between 330 and 500 nm, the maximum decrease of the radiance is 14%.

It should be noted that the optical depth of most PSCs is much smaller (typical a factor of 10) than the worst case tested here.

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4.4 Nominal Radiances

To compare the nominal radiances as presented in section 3.4 with data from R1 (link to the data in ASCII) and R2 (link to file in ASCII), an average spectrum was computed from the nominal data for the Antarctic, Tropical, and Midlatitude cases. This spectrum (link to the data in ASCII), the nominal radiances from R1 and the percentile data from R2 are shown in Figure 4.8. Percentile data for 40%, 50% and 60% is used. Figure 4.8 shows that the nominal radiance spectrum from this study compares well both with the nominal radiances from R1 as well as with the 50% percentile values from R2.

Nominal Radiances

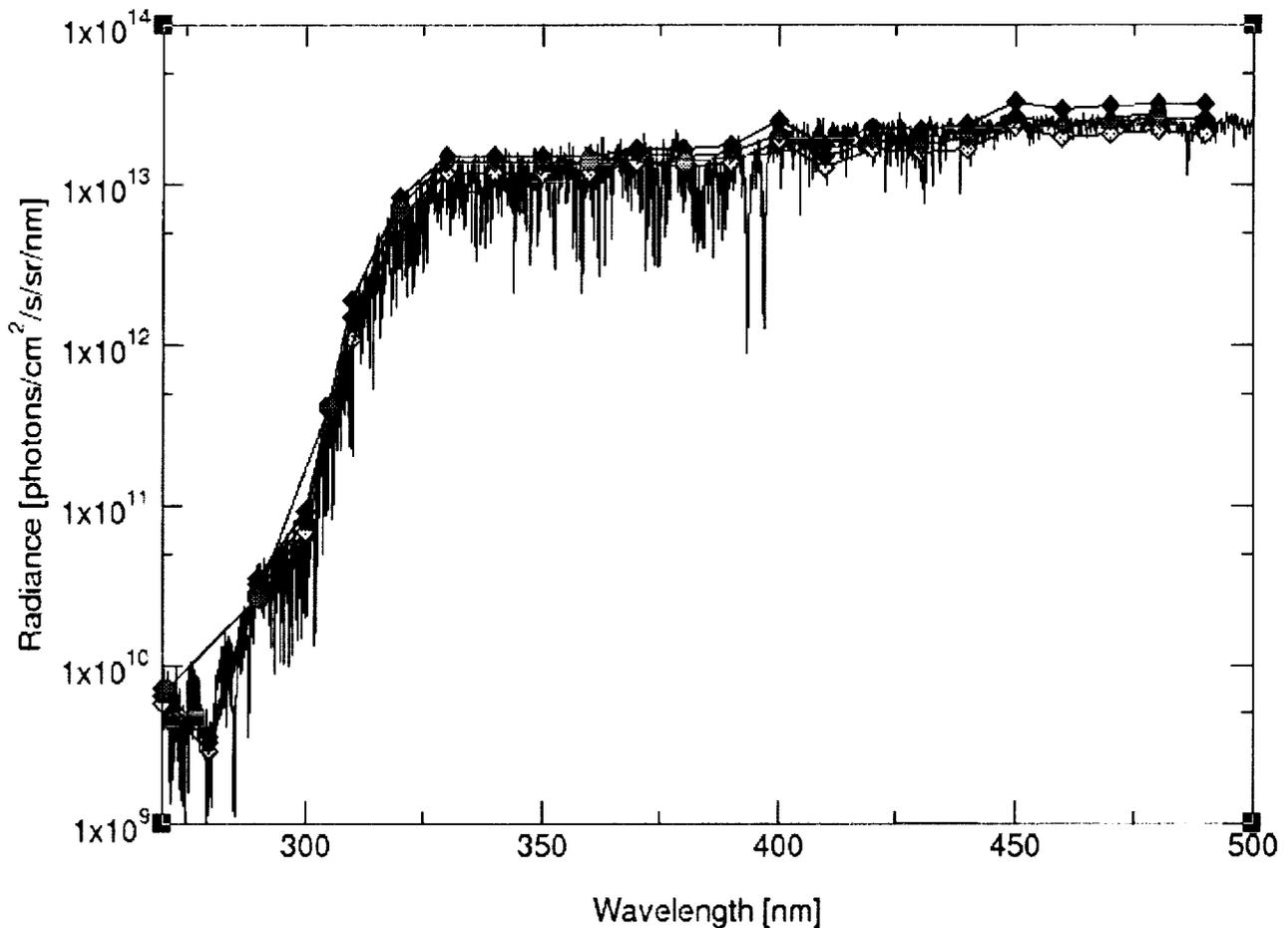


Figure 4.8. Average nominal spectrum from this study (magenta), nominal radiances from R1 (circles), and Percentile radiances for 40, 50 and 60% from R2 (blue diamonds).

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5. Conclusions

Radiance spectra representative for OMI orbits were generated. Three scenario's were considered: ozone hole conditions, tropical summer conditions, and midlatitude conditions. From the simulated spectra, minimum and maximum values were determined for each wavelength. These minimum and maximum spectra were compared to two other sets of spectra that are used in the OMI documentation: the R1 minimum/nominal/maximum values and the R2 GOME percentiles. The following are the conclusions of these comparisons:

1. The minimum radiances from this study are lower than the R1 minimum values
2. The minimum spectrum is in between the 1% and 10% R2 GOME percentile spectra
3. Above 300 nm there is good comparison between the R1 maximum values and the maximum spectrum from this study.
4. Above 310 nm the maximum spectrum compares well to the 99% and 100% R2 KNMI

- GOME percentile spectra.
5. For small wavelengths (below 300 nm for R1 and below 310 nm for R2) the maximum radiances from this study are larger than the other data sets. These large values occur during ozone hole conditions.
 6. Ozone hole conditions can cause variations in the radiance at 279.56 nm of the order of a factor of 50 in less than one minute of OMI observations.
 7. The nominal radiances derived in this study compare well with R1 nominal radiances and R2 50% percentile values.

It is noted that effects of sun glint, major volcanic eruptions and polar stratospheric clouds were not considered in the computations. Sun glint will cause radiances larger than those computed in this study. For wavelengths larger than approximately 330 nm, volcanic eruptions and polar stratospheric clouds can cause decreases up to 50% in the minimum radiances.

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6. References

R1: OMI-EOS Instrument Specification Document, issue 2.

R2: Radiance percentile values for small-pixel GOME earthshine measurements, R. van Oss, 25 June 1999.

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ID: SN-OMIE-KNMI-236
 Title: Effect of spectral structures on DOAS retrieval
 Author: J.P. Veefkind
 Version: 1 of 28 November 2000
 Checked: J. de Haan
 Approved: P.F. Levelt

Effect of spectral structures on DOAS retrieval

History

Action item on KNMI to investigate the effect of spectral structures similar to those of gaseous absorbers on the DOAS retrieval of O₃ (UV and VIS), NO₂, BrO and SO₂. This action originated from the OMI Instrument Preliminary Design Review (I-PDR), held at TNO-TPD, Delft in The Netherlands from 2 to 4 December 1998 and was formulated in Review Item Description (RID) NIVR-192 (originator P. Levelt).

This study replaces the draft version of 17 June 1999. Only a few minor corrections were made with respect to the draft version of 17 June 1999 (most important ones: the maximum error for the O₃ column is now 2% instead of 1% and in Table 1, "Maximum dl" is corrected to "Maximum dl/I").

Description of the action

The effect on the DOAS retrieval is investigated of spectral structures similar to the absorption structures of the retrieved gases. The maximum value for these structures is calculated, for given error levels and slant column densities.

Method

In the DOAS method the slant column density *scd* of a gaseous absorber is derived from the following formula:

$$-\ln\left(\frac{I_e(\lambda)}{I_s(\lambda)}\right) = f(\lambda) + scd \cdot \sigma(\lambda), \quad (1)$$

where $I_e(\lambda)$ is the earthshine radiance, $I_s(\lambda)$ is the solar irradiance, $f(\lambda)$ is a low order polynomial function and $\sigma(\lambda)$ is the absorption cross section for the given absorber. DOAS uses the fine spectral structure in the absorption cross section to derive the *scd*. Equation (1) can be rewritten as:

$$-\ln\left(\frac{I_e(\lambda)}{I_s(\lambda)}\right) = f'(\lambda) + scd \cdot \sigma'(\lambda), \quad (2)$$

where $\sigma'(\lambda) = \sigma(\lambda) - g(\lambda)$ and $g(\lambda)$ is a polynomial fit of $\sigma(\lambda)$ of the same (or lower) order as $f(\lambda)$. To investigate the effect of instrumental spectral features similar to those of the gaseous absorbers, $I_e(\lambda)$ is perturbed with a signal with the spectral structure of $\sigma'(\lambda)$. This case reflects a worst case scenario. When the perturbation does not exactly fit the gas absorption structures, the effects on the DOAS retrieval are much smaller. For the perturbed radiance $I_e'(\lambda)$ Equation (2) can be written as:

$$-\ln\left(\frac{I_e'(\lambda)}{I_s(\lambda)}\right) = f'(\lambda) + scd \cdot \sigma'(\lambda) \cdot (1 + \varepsilon), \quad (3)$$

where ε is the systematic error in the retrieved *scd* due to the perturbation of the earthshine radiance.

Combining Equations (2) and (3) the error can be expressed in terms of the perturbation $dI(\lambda)$.

$$\frac{dI_e(\lambda)}{I_e(\lambda)} = \left| \frac{I_e'(\lambda)}{I_e(\lambda)} - 1 \right| = \left| e^{(-scd \cdot \sigma'(\lambda) \cdot \varepsilon)} - 1 \right| \approx |scd \cdot \sigma'(\lambda) \cdot \varepsilon|, \quad (4)$$

Given a required maximum error ε , the corresponding maximum value for $\frac{dI_e(\lambda)}{I_e(\lambda)}$ is computed by solving Equation (4) for the maximum value of $|\sigma'(\lambda)|$. It is noted that this also depends on the scd .

Results

For O₃ (UV and VIS), NO₂, BrO and SO₂ the maximum amplitude of instrumental spectral structures can be computed from Equation (4). $\sigma'(\lambda)$ was computed by subtracting a second order polynomial function from $\sigma(\lambda)$. A third order polynomial was tested as well, but the differences with the second order polynomial were small. The maximum amplitude of $\sigma'(\lambda)$ was computed as half the peak-to-peak variation of $\sigma(\lambda)$, see Table 1.

	O ₃ UV	O ₃ VIS	NO ₂	BrO	SO ₂
Slant column density	400 DU	400 DU	$2 \times 10^{15} \text{ cm}^{-2}$	$3 \times 10^{13} \text{ cm}^{-2}$	$3 \times 10^{16} \text{ cm}^{-2}$
Fit window [nm]	320 – 335	450 – 500	425 – 450	345 – 360	314– 327
Amplitude of $\sigma'(\lambda)$ [cm^{-2}]	4.7×10^{-21}	1.2×10^{-22}	1.7×10^{-19}	4.1×10^{-18}	3.0×10^{-20}
Maximum error ε [%]	2	2	10	10	20
Maximum dI/I	1×10^{-3}	5×10^{-5}	3×10^{-5}	1×10^{-5}	2×10^{-4}

Table 1 Minimal detectable scd , fit window, amplitude of $\sigma'(\lambda)$, maximum error ε , and resulting value of the amplitude dI/I .

As mentioned above, the error of instrumental spectral structures depends on the slant column density scd . To compute the maximum value of $\frac{dI_e(\lambda)}{I_e(\lambda)}$ for a given error level, the minimal expected scd or the minimal detectable scd should be used. For O₃ 400 DU is expected the minimum scd . For the other gases the detection limit for the GOME instrument is used. For NO₂ this limit is 2×10^{15} molecules cm^{-2} [Burrows *et al.*, 1999]. For BrO and SO₂ the detection limit is estimated as 3×10^{13} molecules cm^{-2} (1×10^{13} molecules cm^{-2} vertical column [Richter *et al.*, 1998]) and 1×10^{16} molecules cm^{-2} (0.4 DU vertical column [Eisinger and Burrows, 1998]), respectively. For the maximum error the required accuracy as listed in Table 3.1 of the OMI-Science Requirements Document version 2 (SRD) was used.

Table 1 shows the maximum amplitude of instrumental spectral structures for the slant columns and error levels are also listed in Table 1. Instrumental spectral structures will give the largest problems for O₃ VIS, BrO, and NO₂ retrieval. Spectral structures of the order of 10^{-5} or smaller are needed not to exceed the maximum error. The same values for the maximum error are used for the UV as VIS windows in Table 1. The value for the maximum error for O₃ VIS (2%) is very strict. However, note that OMI does not intend to use the Visual channel for the retrieval of the O₃ column. For O₃ UV and SO₂ the effects of instrumental spectral structures on the DOAS retrieval are much smaller. For spectral structures of the order of 10^{-4} the maximum error is not exceeded.

Conclusions

The effects on DOAS retrieval of an instrumental spectral structure was investigated for a worst case scenario when these structures exactly match the spectral features of the retrieved gases. The maximal tolerable error was set to the required accuracy. The maximum instrumental spectral structure was calculated for O₃ for retrieval in UV and VIS for the expected minimum slant column density, and for NO₂, BrO and SO₂ for minimal detectable slant columns reported for the GOME instrument. The effect is largest for O₃ VIS, BrO and NO₂, for which the



spectral structures should be of the order of 10^{-5} , or smaller. For O_3 UV and SO_2 the effects are smaller. The maximum amplitude of instrumental structures for these gases should be of the order of 10^{-4} , or smaller. In practice, this means that instrumental structures with amplitudes smaller than 10^{-5} are tolerable. Structures with larger amplitudes should be investigated in the appropriate spectral windows.

References

- Burrows, J.P., and co-authors, *The Global Ozone Monitoring Experiment (GOME): Mission concept and first scientific results*, J. Atmos. Sci, 56, 151-175, 1999.
- Eisinger, M and J.P. Burrows, *Tropospheric Sulfur Dioxide observed by the ERS-2 GOME Instrument*, Geophys. Res. Lett., Vol. 25, no. 22, 4177-4180, 1998
- Richter, A., F. Wittrock, M. Eisinger and J. P. Burrows, *GOME Observations of Tropospheric BrO in Northern Hemispheric Spring and Summer 1997*, Geophys. Res. Lett., 25, no. 14, p. 2683-2686, 1998.

Effects of Scrambler on NO₂ and BrO DOAS retrieval

document: KNMI-OMI-2000-005
version: 1.0
date: 18 February 2000
author: J.P. Veefkind
approved: G.H.J. van den Oord
checked: F. Boersma

1. Introduction

The scrambler of OMI causes spectral structures in the radiance, which affect DOAS retrieval of gases. The largest errors in the retrieved vertical column density can be expected for NO₂ and BrO [R1, R2].

Results of the scrambler breadboard confirmed the spectral structures as expected by the TNO-TPD analytical model. The maximum amplitude of the structures for OMI were estimated as < 0.1% for the VIS, < 0.03% for UV-2, and < 0.01% for UV-1 [R3]. These results are used to estimate the error in NO₂ and BrO retrievals due to the scrambler effects. The errors due to scrambler effects are compared with errors due to noise.

2. OMI simulations

OMI measurements were simulated for wavelengths between 425 and 455 nm for NO₂ and between 340 and 365 nm for BrO. Radiative transfer computations were performed with the Doubling Adding KNMI (DAK) model. The DAK model was used to compute both the radiance and the linear polarization. The OMI instrument was simulated by accounting for scrambler effects, convolution with the slit function and spectral sampling.

Simulations were performed for 36 Sun/satellite geometry's and two values for the surface albedo: 0.0 and 0.8. The scrambler effects were accounted for by using the TNO-TPD analytical model, with an amplitude of 1E-3 (0.1%) in the VIS at 500 nm, and 3E-4 (0.03%) in UV-2 at 380 nm. To account for off axis effects, two versions were used for the scrambler effect function. For these functions, the phase of the rapid varying mode differs by $\frac{1}{2}\pi$, see Figure 1.

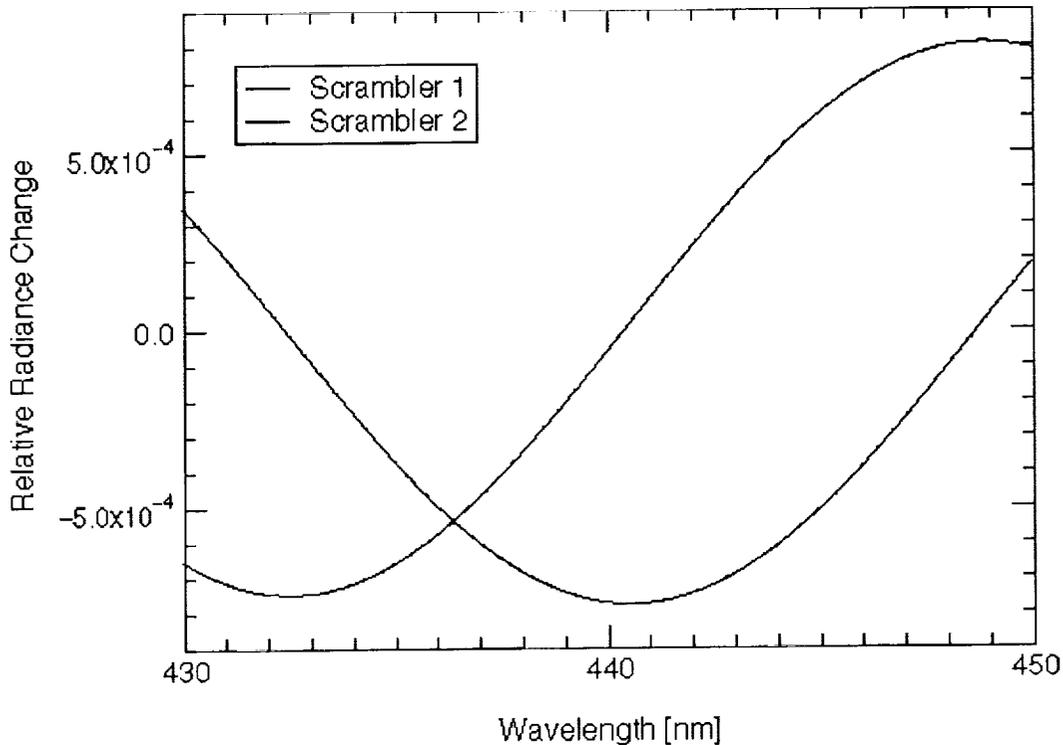


Figure 1. Scrambler effects on radiance as a function of wavelength for the VIS channel. Scrambler 1 and 2 differ by a phase shift of the rapid varying mode.

3. Results for NO₂

From the OMI VIS channel simulations the NO₂ slant column density (SCD) was computed in the wavelength region between 430 and 450 nm, using standard DOAS methods. The SCD was computed for simulations without scrambler effects, and for the two versions of the scrambler. The relative error due to scrambler effects was computed by comparing the SCD with and without scrambler effects.

The largest errors for three NO₂ concentrations are given in table 1 for vertical column densities of 2.0E15, 6.0E15 and 1.2E16 molec/cm². As expected, the largest error occurs for the smallest concentration. The error is almost linearly with the inverse of the concentration. For scrambler 2 the effect is larger than for scrambler 1. This illustrates the effect on DOAS retrieval of the exact shape of the perturbation.

Table 1. Maximum error on NO₂ SCD due to effects of the scrambler.

NO ₂ [molec/cm ²]	scrambler 1 [%]	scrambler 2 [%]
2.0E15	0.96	-2.5
6.0E15	0.32	-0.84
1.2E16	0.16	-0.42

An earlier study reported an error of maximum 4 % on NO₂ retrieval due to 1E-3 scrambler effects [R1]. This study used concentrations of 6.0E15, and 1.2E16 molec/cm² and assumed 100%

polarization of the incoming radiance. When in the present study the same assumption on the polarization is made, the maximum error in the SCD due to scrambler residual polarization is 2 %.

To assess the accuracy of the NO₂ slant column retrieval, the effect of the scrambler should be compared to errors due to signal to noise. Therefore, effects of signal-to-noise of 1000 were added to the OMI simulator described above. Simulations were performed for a vertical column density of 6.0E15 molec/cm² and a surface albedo of 0.0. Figure 2 shows the error due to scrambler effects alone and for the combined scrambler and noise effects. As can be seen in Figure 2, the effects of noise are generally larger than the effects of the scrambler. It should be noted that the scrambler errors are systematic (but vary over the swath), whereas noise causes random errors.

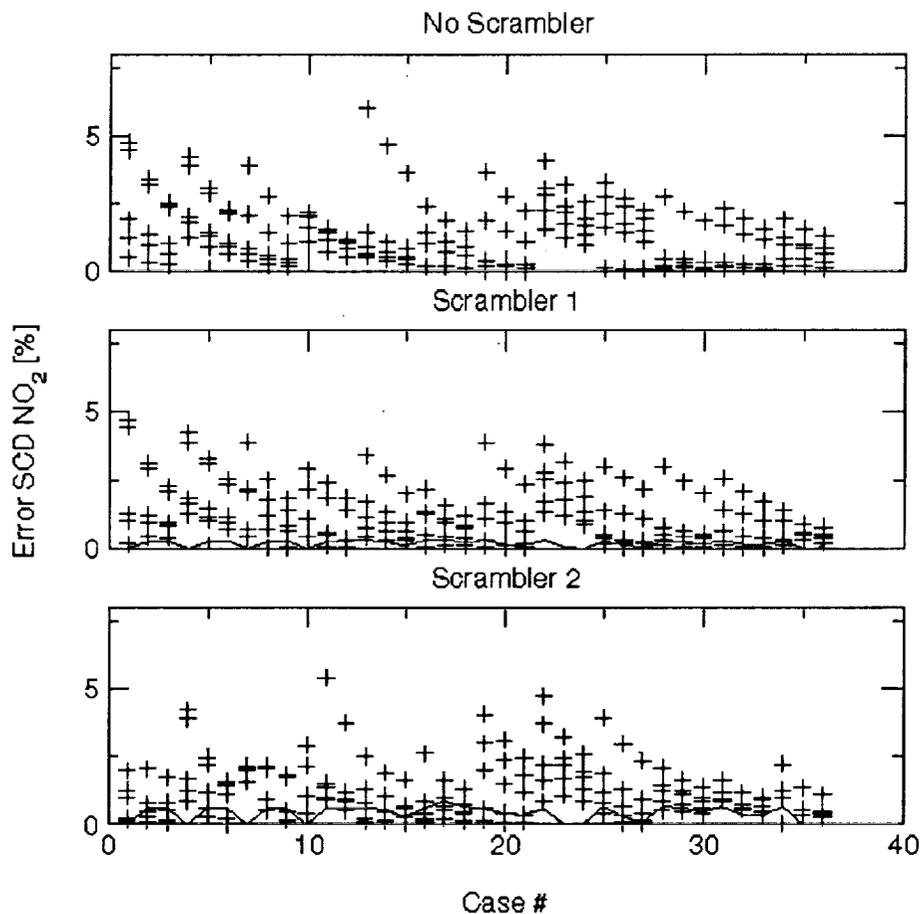


Figure 2. Error due to scrambler effects (line) and due to combined scrambler and noise effects (plusses), for no scrambler (upper plot), scrambler 1 (middle plot), and scrambler 2 (lower plot). For each case 5 simulations with (random) noise were performed.

4. Results for BrO

The SCD of BrO was computed from the simulated spectra between 345 and 360 nm, using a standard DOAS method. The error due to the scrambler was determined from the simulations with and without the scrambler effects. The vertical column density was 4.0E13 molec/cm². The scrambler effects were -1.1 and -1.5 %, for scrambler 1 and 2, respectively.

An earlier study [R2] reported errors in the VCD of $< 5\%$ for 100% polarized light and a VCD of $6.3E13$ molec/cm². For simulations using these assumptions the maximum error is 4%.

To assess the effects of noise, the simulations were repeated with a signal-to-noise level of 1200. Figure 3 shows the effects of the scrambler and the effect of the combined scrambler and noise effects. As can be seen in Figure 3, the effects of the scrambler are much smaller than the noise effects.

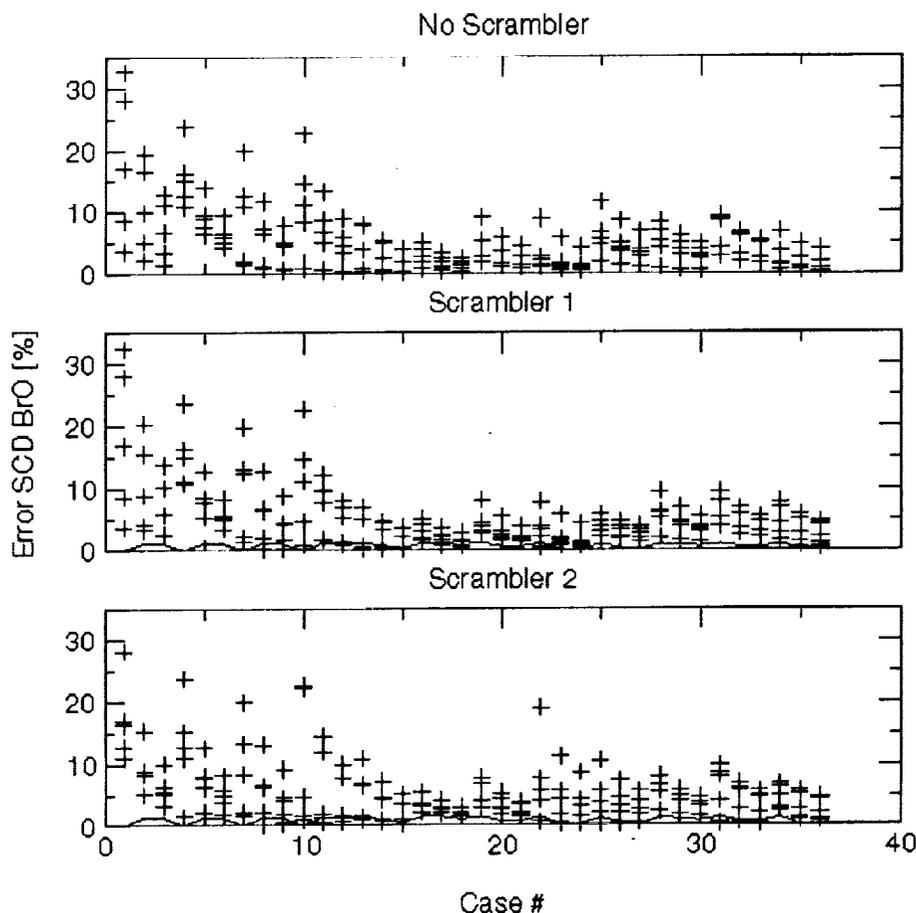


Figure 3. Error due to scrambler effects (line) and due to combined scrambler and noise effects (plusses), for no scrambler (upper plot), scrambler 1 (middle plot), and scrambler 2 (lower plot). For each case 5 simulations with (random) noise were performed.

5. Conclusions

Simulations were performed to assess the error in NO₂ and BrO DOAS retrievals due to the scrambler residual polarization effects. Radiative transfer calculations included linear polarization. For the scrambler effects the expected amplitudes from the breadboard results were used [R3]. Errors due to the scrambler were compared to errors due to noise. The following is concluded from the simulations:

1. For a NO₂ vertical column density of $6.0E15$ molec/cm² the error in the SCD is $< 1\%$.

Scrambler effects were found to be smaller than effects of noise for a signal-to-noise value of 1000.

2. For a BrO vertical column density of 4.0×10^{13} molec/cm² the scrambler error in the SCD was < 1.5 %. The error due to the scrambler is smaller than due to noise for a signal-to-noise level of 1200.
 3. Including realistic values for the degree of polarization, strongly reduces the error due to the scrambler.
-

6. References

R1. Spectral structures similar to absorption features + optical test scrambler: consequences for DOAS column retrievals of ozone and trace gases and ozone profile retrieval. R van Oss, KNMI, 23-07-1999.

R2. Effects of scrambler distortions of 10×10^{-3} on DOAS retrieval. J.P. Veefkind and R. van Oss, KNMI, 29-07-1999.

R3. Proposal for requirement specifications on the polarization sensitivity of the OMI signal levels. H. Visser, TNO-TPD, 8-12-1999.

Reference cross-sections for the OMI Data product

Introduction

Due to the fact that DOAS retrieval is extremely sensitive to spectral structures that resemble absorption structures of the trace gas of interest, the following requirement is defined in the OMI Science Requirements Document:

SR 5.2.2.8 *The effect of spectral structures similar to absorption structures caused by the instrument and/or its calibration in the reflectivity spectra shall be less than 10^{-4} at all wavelengths and swath angles.*

The figures in this Annex show the relevant absorption structures for the OMI-instrument in the retrieval windows as specified in the Table 4.1 of the SRD.

References

For O₃, NO₂, BrO, SO₂, as used in the MODTRAN 4.1 model:

Berk, A., L.S. Bernstein, and D.C. Robertson, *MODTRAN: A Moderate Resolution Model for LOWTRAN 7*, GL-TR-89-0122, Geophysics Directorate, Phillips Laboratory, Hanscom AFB, MA 01731 (April 1989) ADA214337.

For HCHO, see:

C.A. Cantrell, J.A. Davidson, A.H. McDaniel, R.E. Shetter, and J.G. Calvert, *Temperature-dependent formaldehyde cross sections in the near-ultraviolet spectral region*, J. Phys. Chem. 94, 3902-3908, 1990.

For OCIO, see:

- 1) H. Kromminga, J. Orphal, S. Voigt, J. P. Burrows, to be published.
- 2) H. Kromminga, *Diploma Thesis*, IUP, University of Bremen, 1999.
- 3) H. Kromminga, S. Voigt, J. Orphal, J. P. Burrows, *UV-Visible FT Spectra of OCIO at Atmospheric Temperatures*, Proceedings of the 1st European Symposium on Atmospheric Measurements from Space, ESA Special Publication, 1999.

For O₂-O₂, see:

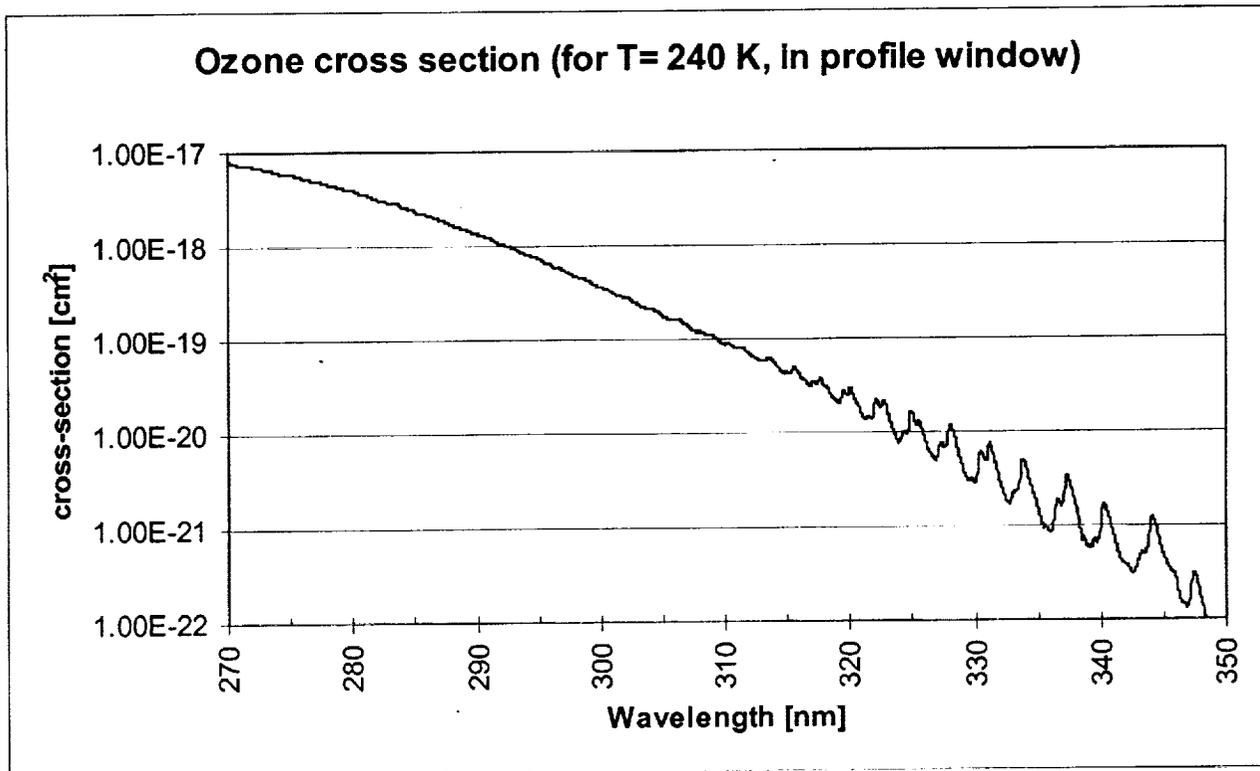
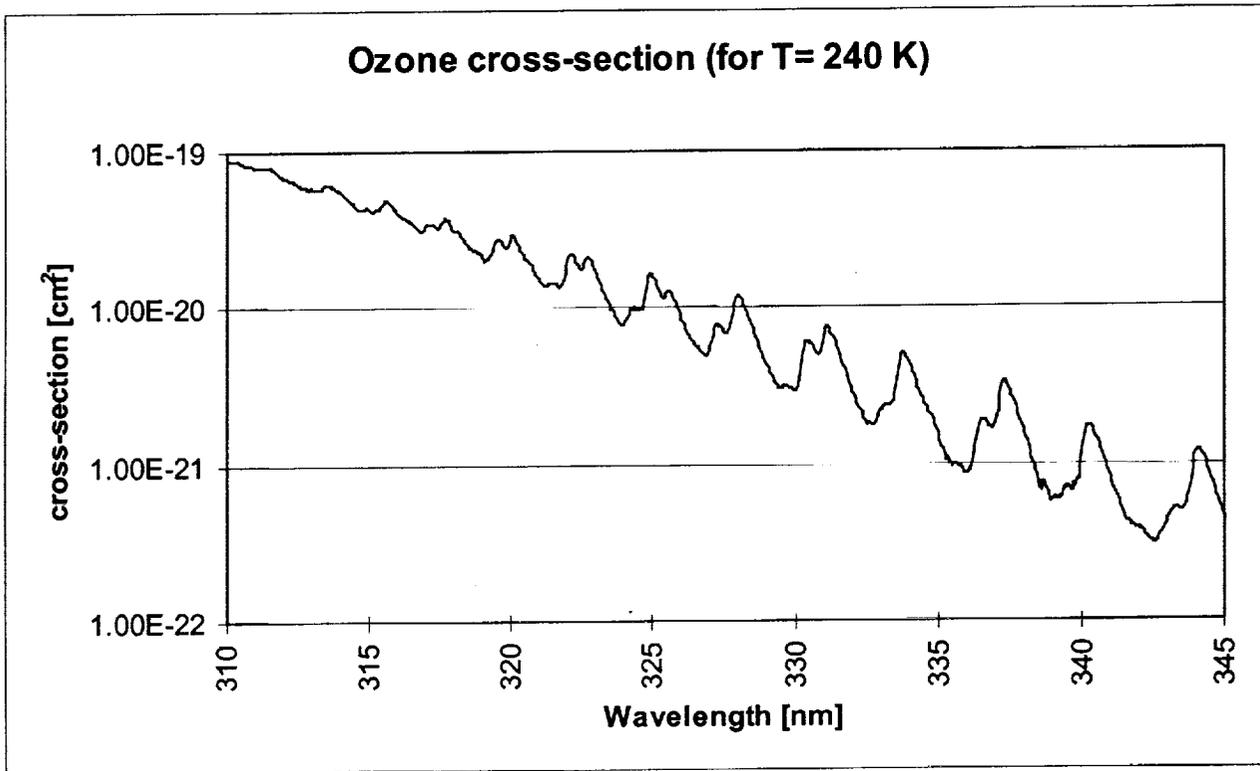
Greenblatt, G.D., J.J. Orlando, J.B. Burkholder and A.R. Ravishankara, , J. Geophys. Res., 95, 18577 – 18582.

For the Ringspectrum, see:

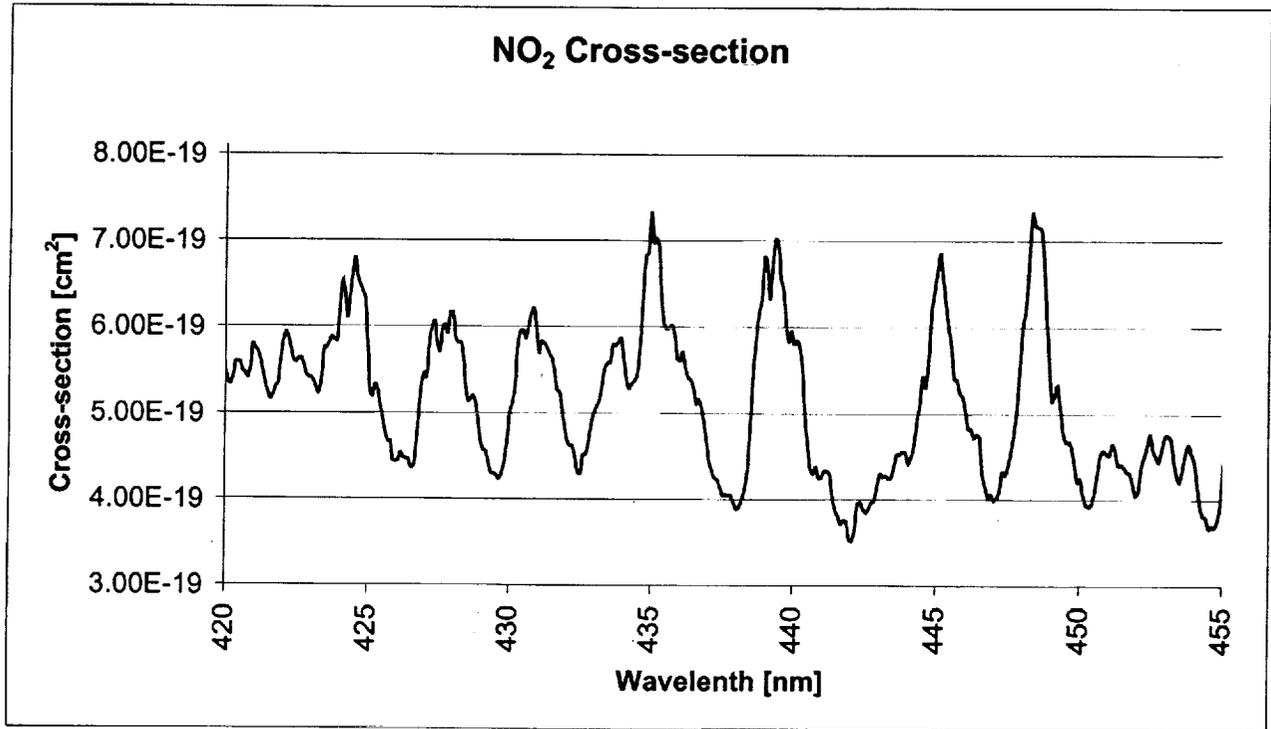
K. Chance and R.J.D. Spurr, *Ring Effect Studies: Rayleigh Scattering, Including Molecular Parameters for Rotational Raman Scattering, and the Fraunhofer Spectrum*, Applied Optics 36, 5224-5230, 1997.

K. Chance, private communication

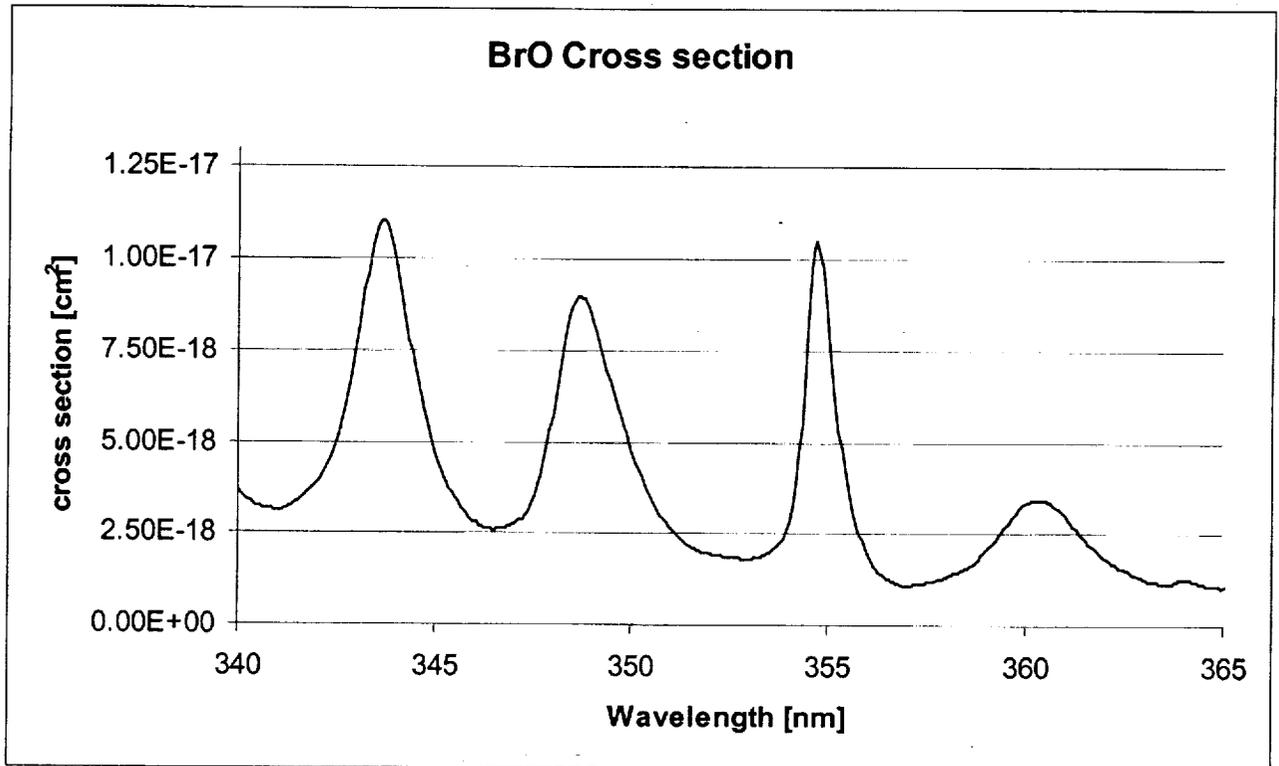
Ozone



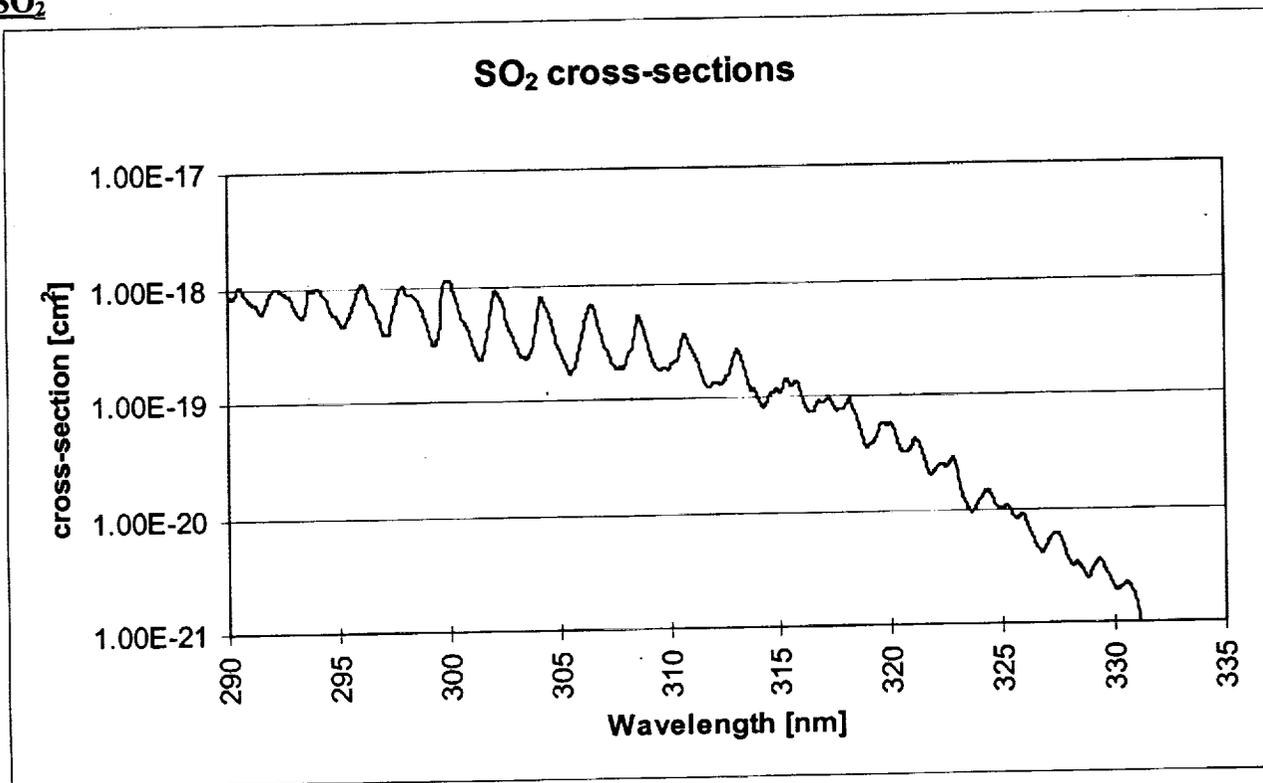
NO₂



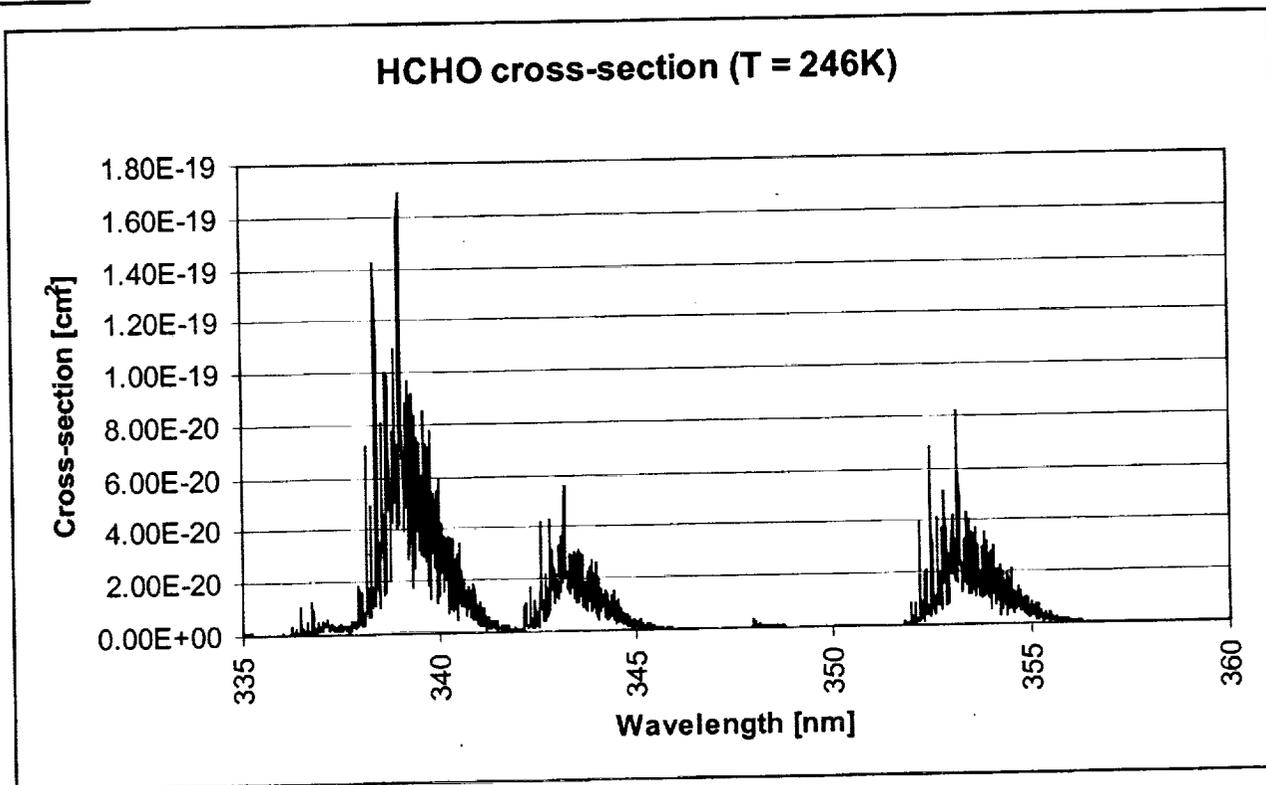
BrO



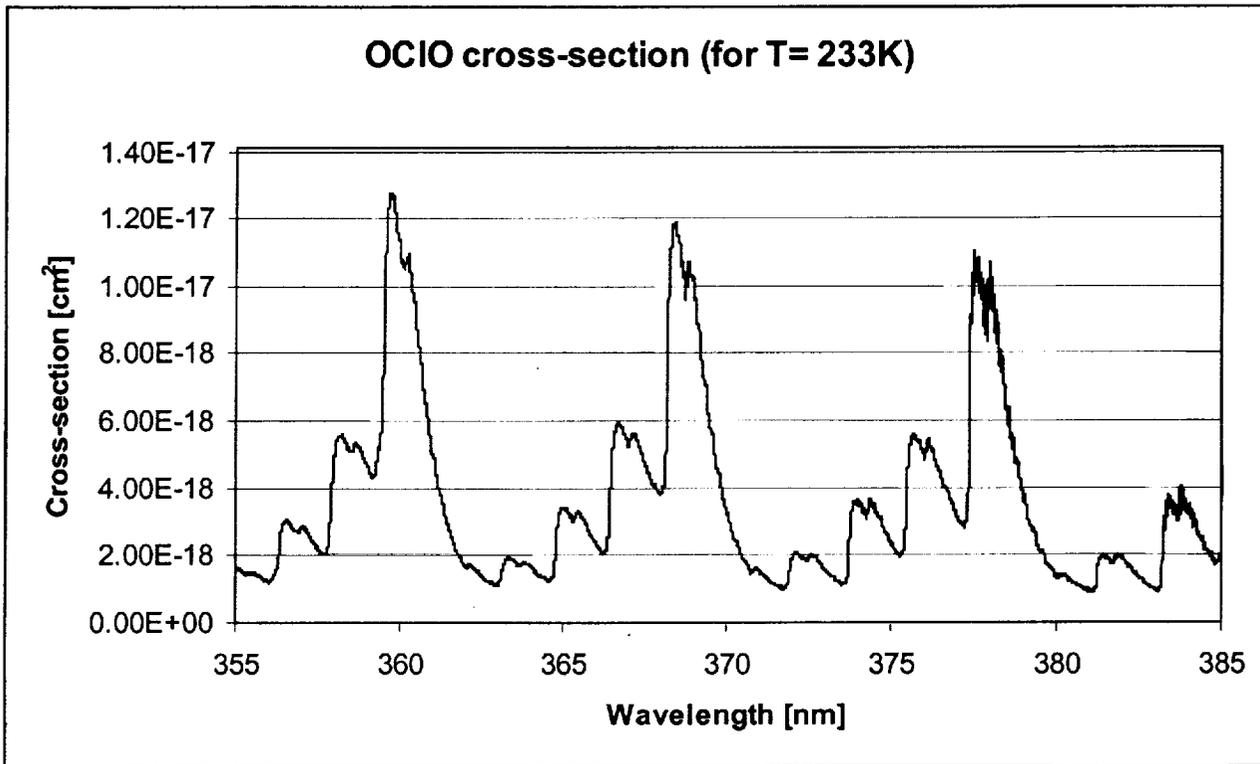
SO₂



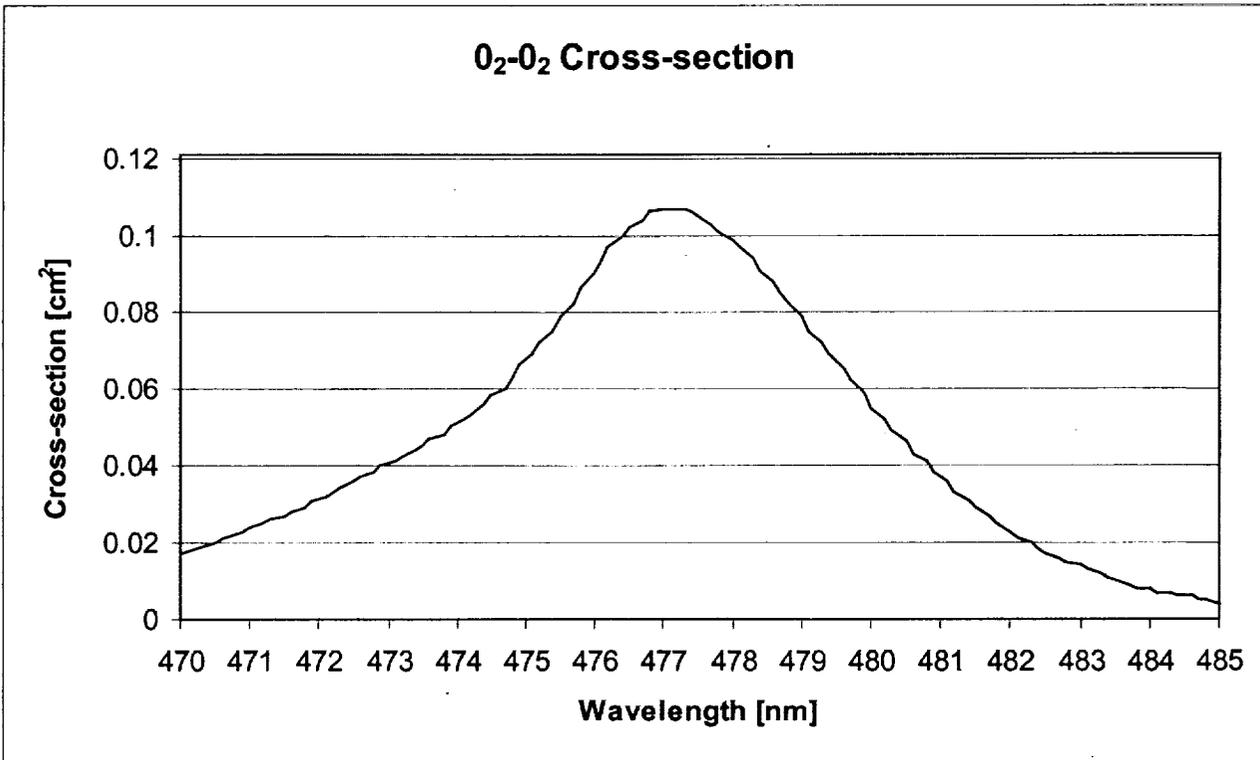
HCHO



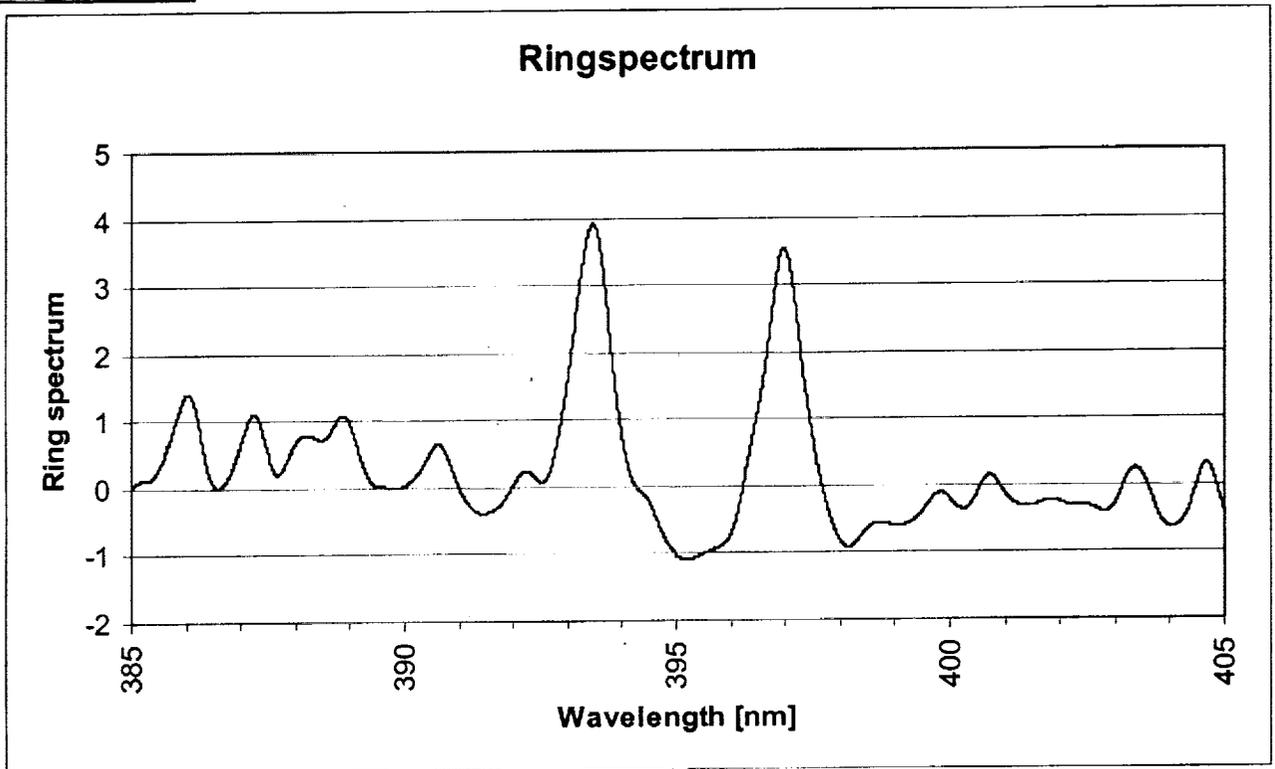
OCIO



O₂-O₂



Ring spectrum



The effect of a non-linearity in the radiometric response of the OMI instrument

Prepared by : Ronald van der A
 Date: 8 December 1999

Subject: Non-linearity
 Approved: G.H.J. van den Oord

Definition

The non-linearity of the radiometric response is defined as the relative deviation of the instrument response from the radiometric input. Note that any requirement for the non-linearity has to be valid for the complete dynamic range.

Method

A typical non-linearity occurs when the instrument response is a quadratic function of the radiometric input, while a linear dependence is assumed. In this study such situation is considered in all simulations.

Then, for a certain maximum non-linearity μ , radiometric input signal x , minimum signal x_{\min} , maximum signal x_{\max} , the instrument response y can be written as

$$y(x) = a \left(\frac{x - x_{\min}}{x_{\max} - x_{\min}} \right)^2 + b \left(\frac{x - x_{\min}}{x_{\max} - x_{\min}} \right) + c, \quad [1]$$

where

$$a = 2 \cdot (1 + \mu - p) \cdot (x_{\max} + x_{\min}),$$

$$b = (1 + \mu) \cdot (x_{\max} - x_{\min}) - a,$$

$$c = (1 + \mu) \cdot x_{\min}.$$

The deviation $z(x)$ of the response from a linear response is given by

$$z(x) = \frac{y(x) - x}{x}. \quad [2]$$

The parameter p is calculated from the following set of conditions :

$$\begin{aligned} z(x_{\min}) &= \mu \\ z(x_{\max}) &= \mu \\ z(x_e) &= -\mu \quad \text{where} \quad \frac{\partial z(x_e)}{\partial x} = 0 \end{aligned} \quad [3]$$

From this conditions follows the parameter p (calculated by Bert van den Oord) :

$$p = 1 - \mu \sqrt{1 - \left(\frac{x_{\max} - x_{\min}}{x_{\max} + x_{\min}} \right)^2}. \quad [4]$$

A set of 13 simulated GOME spectra is distorted according to equation 1 and the non-linearities in Table 1. For all these spectra profiles are retrieved and compared to the reference profile retrieved from the spectra without non-linearity. The deviations between these profiles are given in the Figures for each of the 13 spectra.

