



Scientific Requirements Document

Draft, Revision 1

January 1998

The SCIAMACHY Science Advisory Group



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 1/49

SCIAMACHY - Scientific Requirements

1 EXECUTIVE SUMMARY	3
2 INTRODUCTION	4
2.1 Historical Background	4
2.2 Scope of this Document	5
3 SCIENTIFIC NEEDS	6
3.1 Tropospheric Chemistry	6
3.2 Stratosphere-Troposphere Exchange	6
3.3 Stratospheric Chemistry	7
3.4 Stratospheric Dynamics	7
3.5 Mesospheric Chemistry and Dynamics	8
4 MISSION OBJECTIVES	9
4.1 Primary Mission Objectives	9
4.1.1 Tropospheric Chemistry	9
4.1.2 Stratosphere-Troposphere Exchange	10
4.1.3 Stratospheric Chemistry	10
4.1.4 Stratospheric Dynamics	10
4.1.5 Mesospheric Chemistry and Dynamics	10
4.2 Secondary Mission Objectives	10
4.2.1 Aerosol and Cloud Measurements	10
4.2.2 Pressure and Temperature Measurements	11
4.2.3 Land and Ocean Measurements	11
4.2.4 Climate and Earth Radiation Budget	12
4.3 Required precision	12
5 MEASUREMENT PRINCIPLE AND OBSERVATIONAL MODES	13
5.1 Measurement Principle	13
5.2 Observational Modes	17
6 RETRIEVAL METHODS	19
6.1 General Considerations	19
6.2 Differential Optical Absorption Spectroscopy	20
6.3 Optimal Estimation	21
6.4 Retrieval of Tropospheric Information	21
6.5 Retrieval of Temperature, Pressure, Cloud and Aerosol Information	22



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 2/49

6.5.1 Aerosol	22
6.5.2 Cloud	22
6.5.3 Temperature and Pressure	22
6.6 Summary of Retrieval Approach	23
7 IMPLICATIONS FOR THE INSTRUMENT REQUIREMENTS	24
7.1 Basic Design Assumptions	24
7.2 Viewing Geometries	24
7.2.1 Scan Mirror, Telescope, Sun Sensor and Pointing	24
7.2.2 Limb Scanning	25
7.2.3 Nadir Scanning	25
7.2.4 Combined Limb-Nadir Scanning	25
7.2.5 Solar and Lunar Occultation and Calibration Modes	26
7.2.6 Eclipse / Nighttime Mode	26
7.3 Optical Requirement Implications	26
7.3.1 Wavelength Ranges	26
7.3.2 Spectral Resolution	29
7.3.3 Spectral Knowledge	30
7.3.4 Signal-to-Noise	30
7.3.5 Straylight	31
7.3.6 Radiometric Accuracy / Polarisation Measurement	31
8 FULFILMENT OF MISSION OBJECTIVES	33
8.1 Covered height ranges and retrieval precision	33
8.2 Spatial Resolution	36
9 CALIBRATION STRATEGY	37
9.1 Pre-Launch Calibration	37
9.2 In-Flight Wavelength Calibration	37
9.3 In-Flight Radiometric Calibration	37
10 VALIDATION STRATEGY	38
11 REFERENCES	40
12 SCIAMACHY ADDRESS BOOK	44



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 3/49

1 Executive Summary

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartography) is a space based spectrometer designed to measure sunlight transmitted, reflected and scattered by the Earth atmosphere or surface. SCIAMACHY measures simultaneously and contiguously radiation in the wavelength range from 240 to 1750 nm at moderate spectral resolution (0.2 nm - 1.5 nm). In addition it measures simultaneously in two short infrared bands around 2.0 μm and 2.3 μm . The absorption, reflection and scattering characteristics of the atmosphere are determined by measuring the up welling earthshine radiance observed in nadir, limb and occultation geometry and the extraterrestrial solar irradiance. Up welling radiance can be inverted to provide information about the amounts and distribution of important atmospheric constituents.

The SCIAMACHY project was conceived to improve our knowledge and understanding of a variety of issues of importance for the chemistry and physics of the Earth atmosphere (troposphere, stratosphere and mesosphere) and potential changes resulting from either anthropogenic behaviour or natural phenomena such as:

- tropospheric pollution arising from industrial activity and biomass burning;
- troposphere - stratosphere exchange processes;
- stratospheric ozone chemistry: the emphasis being on the understanding of the ozone depletion in polar regions and at mid-latitudes;
- special events such as volcanic eruptions, solar variability and related regional and global phenomena.

SCIAMACHY measurements provide amounts and/or distribution of O_3 , BrO, OClO, ClO, SO_2 , H_2CO , NO_2 , CO, CO_2 , CH_4 , H_2O , N_2O , p, T, aerosol, radiation, cloud cover and cloud top height from atmospheric measurements in nadir, limb and occultation geometry. From the Limb and Solar/Lunar Occultation atmospheric observations vertical distributions of the atmospheric trace constituents are derived. This provides information about the stratospheric and upper tropospheric composition, yielding important information about stratospheric chemistry and physics as well as exchange between the stratosphere and troposphere. The combination of the near simultaneous limb and nadir observations yields unique information about tropospheric and lower stratospheric constituents (gases, aerosol and cloud). SCIAMACHY is one of a limited number of instruments which is able to detect tropospheric column amounts of O_3 , NO_2 , CO, CH_4 , H_2O , N_2O , SO_2 and H_2CO down to the planetary boundary layer under cloud free conditions. Additionally, accurate profiles of atmospheric constituents having a relatively high vertical resolution result from the solar and lunar occultation measurements.

SCIAMACHY will provide new insight into the global behaviour of the troposphere and the stratosphere. As a result of its versatility and usefulness for a wide range of scientific and operational meteorological applications SCIAMACHY is a good candidate instrument for any future global monitoring system.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 4/49

2 Introduction

2.1 *Historical Background*

The SCIAMACHY proposal (Burrows et al. 1988a) was submitted in July 1988 by the SCIAMACHY Science Team in response to the ESA Announcement of Opportunity (AO) inviting the proposal of experiments for flight on board the Polar Platform Element of the Columbus Programme, now known as Polar Platform (PPF) as part of the Polar Orbit Earth Observation (POEM-1) / ENVISAT-1 Mission. In spring 1989 SCIAMACHY was selected as part of the payload for ENVISAT-1, and a phase A feasibility study was started in summer 1989. After this phase A study (1989 - 1990) SCIAMACHY was selected for flight by ESA as a so-called AO instrument, which implies a national contribution by member states to the ESA-ENVISAT project. In addition ESA selected in 1990 SCIAMini (Burrows et al. 1988b), now better known as the Global Ozone Monitoring Experiment GOME (ESA 1993), as an instrument that would concentrate on measurements in the ultraviolet and visible portions of the spectrum covered by SCIAMACHY, in the nadir geometry, in order to improve the global measurement of ozone and a number of related constituents. GOME is currently flying on the ERS-2 satellite, which was launched in April 1995.

The SCIAMACHY definition study (phase B) was carried out between 1991 and 1992 ending with the Baseline Design Review (BDR) in November 1992. SCIAMACHY then entered the transition phase to phase C/D ending with a successful Preliminary Design Review (PDR) in spring 1993. After the SCIAMACHY instrument design was completed, the manufacturing and integration phase (phase C/D) commenced and the instrument critical design review (ICDR) was passed successfully in April 1996.

As an so-called AO instrument, SCIAMACHY is a national contribution to the ENVISAT-1 mission funded by the German (DLR Bonn, formerly DARA GmbH) and Dutch (NIVR) space agencies, including a Belgian (IASB) contribution. The SCIAMACHY industrial consortium comprises the prime contractors Dornier Satellite Systems (D) and Fokker Space (NL) and the subcontractors OHB-Systems (D), Jenoptik (D), SRON (NL), TPD-TNO (NL), OIP (B) and EPITAXX (USA).

The SCIAMACHY project is supported in the fields of instrument and algorithm development, calibration and characterisation, and validation by the activities of the SCIAMACHY Science Advisory Group (SSAG), headed by the principal investigators Professor J. P. Burrows (University of Bremen, Germany) and Dr. A. H. P. Goede (Space Research Organisation of the Netherlands). Substantial support in different fields of the project also originates from the activities of the different subgroups of the science advisory group: data and algorithm, headed by Dr. K. V. Chance (SAO, United States); calibration and characterisation, headed by Dr. A. H. P. Goede; and validation and interpretation, headed by Dr. H. Kelder (KNMI, The Netherlands). A SCIAMACHY address book can be found in chapter 12 of this document.

Development of operational algorithms and the operational data processing is to be performed by DLR-DFD within the ENVISAT ground segment. The mission operation



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 5/49

is supported by the SCIAMACHY Operations Support Team SOST, which prepares measurement strategies and in-flight instrument calibration and monitoring activities.

The success of GOME on ERS-2 (ESA 1995) has demonstrated the feasibility and capabilities of this new instrument concept. Much of the experience gained with GOME can be used directly for SCIAMACHY. The accuracy currently achieved with GOME (ESA 1996, ESA 1997) is in agreement with what was predicted (ESA 1993). An overview of first results of the GOME mission can be found in the proceedings of the third ERS symposium (ESA 1997).

2.2 Scope of this Document

This document summarises the scientific objectives of SCIAMACHY and their implications for the instrument design. These goals and requirements were used to formulate the instrument performance requirements within the SCIAMACHY Instrument Requirement Document (DARA 1995) which is a binding contractual document for the industrial development team.

On request of the AO provider DLR Bonn (formerly DARA GmbH) this document has been derived from the Phase A Scientific Requirement Specification document (Burrows et al. 1991) with some modifications providing more information with respect to the scientific background of the SCIAMACHY requirements and taking into account the results from the instrument development phase. This document will be the reference for the AO provider to compare the proposed mission objectives with the reached results and to judge of the success of the mission.

The current document takes into account the current development of our knowledge about the behaviour of the global atmosphere using for example the findings of WMO (WMO 1995), IPCC (IPCC 1996) and the European Commission (1997). In chapter 2 gives an overview of the scientific needs is given. The mission objectives derived from the latter are described in chapter 3. The principles used by SCIAMACHY for the derivation of the amounts and distributions of atmospheric constituents and limiting constraints arising from the orbit selected for ENVISAT are discussed in chapter 4. In chapter 5, the methods foreseen for the inversion of the measurements and the retrieval of trace constituents are briefly summarised. The implications of atmospheric radiative transfer in the wavelength ranges to be used by SCIAMACHY and the retrieval of trace constituents on instrument performance parameters is discussed in chapter 6. Chapter 7 summarises the status of sensitivity studies to demonstrate the capabilities of SCIAMACHY to fulfil the requirements. The critical importance of the characterisation and calibration as well as validation of SCIAMACHY is the subject of chapter 8 and 9.

Additional information about the scientific background relevant to the SCIAMACHY primary objectives is also given in the SCIAMACHY AO proposal, which was submitted to ESA in 1988 (Burrows et al. 1988a). More details about specific issues on calibration and characterisation, data and algorithm, and validation and interpretation can be found in the relevant requirement documents prepared by the three SAG subgroups during the last years.



3 Scientific Needs

The recognition of dramatic changes in the composition and behaviour of the atmosphere (e.g. the precipitous loss of Antarctic stratospheric ozone, known as the 'ozone hole', the decrease in mid-latitude stratospheric ozone, the loss in Arctic stratospheric ozone, and the observed increase of tropospheric greenhouse gases such as CO₂, CH₄, N₂O and O₃) have emphasised the need for global measurements of atmospheric constituents. Since SCIAMACHY was proposed the situation has not improved (Graedel and Crutzen 1993, WMO 1995, IPCC 1995, European Commission 1997). Knowledge about the variability and temporal behaviour of atmospheric trace gases is necessary to test the predictive ability of the theories currently used to model the atmosphere. The accurate assessment of the consequences of present and future anthropogenic activity and natural processes on the behaviour of the atmosphere and the climate-chemistry coupling requires detailed global knowledge of the temporal and spatial behaviour of several atmospheric trace gases.

3.1 Tropospheric Chemistry

Most gases, emitted to the atmosphere by natural processes and anthropogenic activities, are removed from the atmosphere via oxidation initiated by hydroxyl radicals (OH). The concentrations of these are in turn mainly determined by the intensity of solar ultraviolet radiation and the concentrations of O₃, H₂O, CO, CH₄, NO and NO₂. The lack of information on the temporal and spatial distributions of these species, as well as the source strengths of CO, CH₄ and NO_x (NO + NO₂), severely limit the quantitative understanding of the processes involved in tropospheric ozone production and destruction. This is also a pre-requisite for quantitative estimates of the hydroxyl radical distribution and thus of the cleaning power of the atmosphere, which is expected to be changing as a result of increasing emissions and resultant concentrations of O₃, CH₄, NO_x and CO.

3.2 Stratosphere-Troposphere Exchange

Exchange of gases and particles between the stratosphere and the troposphere is of importance for the chemical composition of both regions. For example downward transport of stratospheric ozone is a source of tropospheric ozone, which as a precursor of OH radicals to a large extent determines the oxidising power of the troposphere. In the opposite direction, upward transport of the precursor molecules (e.g. H₂O, N₂O, CFCs) originating from the planetary boundary layer provides the feedstock for ozone-destroying HO_x, NO_x and ClO_x radicals. An adequate knowledge of the meteorological processes that determine stratosphere-troposphere exchange and the distribution of trace gases, especially in the lower stratosphere does not exist.

Photo-chemically stable gases in the troposphere are useful as tracers for transport of tropospheric air into the stratosphere and for stratospheric dynamics, e.g. N₂O, CH₄ and H₂O. Similarly, gases which have relatively high stratospheric, but low tropospheric abundances, such as O₃, can be used as tracers for downward transport from the stratosphere.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 7/49

3.3 *Stratospheric Chemistry*

No part of global environment has been disturbed by human activity as significantly as the stratosphere. A substantial depletion of stratospheric ozone over Antarctica has been observed during spring since the end of the 1970's. This depletion is largely due to the emission of industrial chlorofluorocarbon gases (WMO 1995 and references therein). In the 90's a major (100 DU) depletion of stratospheric ozone over the Arctic has also been observed during spring. Surface reactions on liquid aerosols, nitric acid trihydrate (NAT) particles and ice particles are believed via the activation of chlorine to be primarily responsible for these changes (WMO 1995, European Commission 1997). Although international regulatory measures as the Montreal Protocol have now been taken to eliminate the production of chlorofluorocarbons by the end of this century (WMO 1995), the amount of stratospheric chlorine may not reach its maximum until after the year 2005, due to the relatively slow transport of chlorofluorocarbons into the stratosphere and the manufacturing of chlorine-containing replacement products, such as HCFC-22 (CHF_2Cl).

The loss of ozone on the stratosphere is likely to be affected in a synergistic manner by tropospheric emission of Greenhouse gases. For example, the anthropogenic tropospheric concentrations of nitrous oxide (N_2O) and methane (CH_4) are increasing, leading to additional formation of stratospheric NO_x and water vapour (H_2O) and enhancing the probability for formation of polar stratospheric clouds (PSC's). Reactions on these clouds lead to the activation of chlorine radicals that are responsible for the formation of the 'ozone hole'. Thus, even though the stratospheric chlorine content may be declining 15 years from now, ozone depletion in the lower stratosphere at higher latitudes may not.

As the planned stratospheric aircraft and spacecraft of the future will emit water vapour and nitric oxide into the stratosphere, and as a result of the introduction of advanced supersonic and hypersonic aircraft, serious environmental issues may ensue. For example the emissions of additional H_2O and NO_x may strongly enhance PSC formation. Improved understanding of stratospheric chemical processes and distributions of trace constituents, including aerosol and PSC's, is essential for environmental assessments of future space and aviation activity.

3.4 *Stratospheric Dynamics*

The winter season, in the northern hemisphere, is dynamically active and displays striking phenomena such as the so-called 'sudden warming events'. The middle atmosphere of the southern hemisphere, although more quiescent, is far from being static. Instabilities originating within the deep vortex present in the polar night may alter circulation patterns on a global scale. Comparative studies of the two hemispheres permit the analysis of their dynamically distinct circulation systems, which also have an important effect on the chemistry of the two regions.

Vertical temperature profiles can be used to derive geopotential height profiles, winds and other dynamic quantities (e.g. potential vorticity). The distribution of quasi-conservative constituents (e.g. water vapour, nitrous oxide, methane, CFC's and



ozone) provide valuable tracer information to check the transport of species predicted by the dynamic models.

3.5 Mesospheric Chemistry and Dynamics

The mesosphere extends from the temperature maximum at the stratopause around 50 km altitude to the atmospheric temperature minimum at the mesopause around 85 km, little detailed information about this atmospheric layer is available. Satellites have provided some data about mesospheric temporal and spatial distributions of O₃ and temperature.

In this context, little is known about the dynamics and chemistry at high latitudes. Knowledge about the distribution of H₂O and O₃ is very limited. Ground-based microwave radiometry has been used to investigate the diurnal variation of O₃. Although the results appear qualitatively in agreement with theory, in order to get a clear picture, global data are much required.

The growth in atmospheric CH₄, will lead to an increase in mesospheric H₂O concentrations. It is expected that this will result in enhanced noctiluscent cloud formation around 85 km. Global circulation in the upper mesosphere and lower thermosphere can be monitored using CO and H₂O as tracers.

Measurements of the vertical profile of UV flux plus the retrieval of O₃ and O₂(¹Δ_g) will provide information about the photolysis of O₃ in the mesosphere. Combined with the measurements of NO and NO₂ this will provide a unique set of data for the study of mesospheric chemistry.

Temperature is one of the key parameters needed to improve our understanding of the chemistry and dynamics of the mesosphere. It has been shown by two-dimensional model calculations that, during the polar night, the thermosphere may act as a large source region for mesospheric and stratospheric NO, which may destroy ozone by catalytic reactions. Several mechanisms have been proposed by which the O can be transported downwards. Such downward transport can be investigated by the measurements of CO and H₂O in the mesosphere and lower thermosphere, and by the measurements of NO_y compounds in the stratosphere.



4 Mission Objectives

The main objective of the SCIAMACHY mission is to improve our knowledge of global atmospheric change and the related global issues of importance to the chemistry and physics of our atmosphere (compare WMO 1995 and IPCC 1996) such as:

- the impact of tropospheric pollution arising from industrial activity and biomass burning,
- exchange processes between the stratosphere and troposphere,
- the stratospheric chemistry relevant at polar regions (e.g. under 'Ozone hole' conditions) as well as at mid-latitudes,
- natural modulations of atmospheric composition resulting from volcanic eruptions, lightning, solar output variations (e.g. solar cycle), or solar proton events.

4.1 Primary Mission Objectives

The primary scientific objective of SCIAMACHY is the global measurement of trace gases in the troposphere and stratosphere. In the A.O. Proposal (Burrows et al. 1988a), the following gases were targeted for measurement:

- O₂, O₃, O₄, NO, NO₂, NO₃, CO, CO₂, H₂CO, CH₄, H₂O, SO₂, possibly ClO, OClO.

As a result of the sensitivity analysis performed during the Phase A Study (Chance et al. 1991), N₂O, BrO and O₂(¹Δ_g) have been added to the target list. In addition, the OClO and ClO measurements have been further investigated and, under ozone hole conditions, both are observable. The list of target molecules for SCIAMACHY at the end of Phase A was thus:

- O₂, O₂(¹Δ_g), O₃, O₄, NO, NO₂, NO₃, N₂O, H₂CO, SO₂, CO, CO₂, CH₄, H₂O, BrO, ClO, OClO, HF.

With the exception of HF, this list of targeted molecules was maintained at the end of Phase C/D. In the following subsections the targeted constituents will be specified for the different height ranges on the basis of the scientific needs from chapter 2.

4.1.1 Tropospheric Chemistry

SCIAMACHY measures O₃, CO, CH₄, H₂O and NO₂. Under tropospheric pollution SCIAMACHY shall be able to measure SO₂ and H₂CO. In addition, measuring the magnitude of the backscattered ultraviolet radiation will help to define the active photochemical environments in which the reactions producing O₃ and OH occur. In cloud free regions, the tropospheric measurements of SCIAMACHY includes the planetary boundary layer. When clouds are present the measurements extend downwards to the top of the clouds. To determine cloud top height/pressure it is necessary to measure O₂ and/or CO₂. In addition the observation of the greenhouse gases can be used to monitor the inventories of emissions produced by the various countries in accordance with the measures agreed at the Earth Summit in Kyoto/Japan in 1997.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 10/49

4.1.2 Stratosphere-Troposphere Exchange

SCIAMACHY provides height resolved measurements of O₃, N₂O, H₂O and CH₄ which will strongly enhance our knowledge about the chemical composition of the lower stratosphere, upper troposphere and stratosphere-troposphere exchange processes.

4.1.3 Stratospheric Chemistry

SCIAMACHY measures height resolved profiles of gases that are chemically most relevant in stratospheric processes: O₃, NO₂, H₂O, CH₄, N₂O. In addition SCIAMACHY provides, for the first time, height resolved information on the distributions of BrO and OClO and possibly ClO under 'ozone hole' conditions. To get a detailed picture of stratospheric processes aerosol and/or PSC information is of great importance.

4.1.4 Stratospheric Dynamics

To provide new insight into dynamic and transport processes SCIAMACHY is required to measure constituent data with high height resolution in combination with temperature and pressure fields.

4.1.5 Mesospheric Chemistry and Dynamics

To study the distribution of H₂O and O₃, their global circulation, as well as the ozone destruction due to mesospheric and stratospheric NO, SCIAMACHY is required to measure in the upper stratosphere and lower mesosphere profiles of O₃, H₂O, N₂O, NO, O₂ and O₂(¹Δ).

4.2 Secondary Mission Objectives

4.2.1 Aerosol and Cloud Measurements

From the dependence of the scattered light intensity on wavelength, the atmospheric aerosol abundance can be determined from SCIAMACHY observations. Aerosol scattering has a first order wavelength dependence (Mie scattering cross-section $\propto \lambda^{-1}$), whereas molecular scattering has a fourth order wavelength dependence (Rayleigh scattering cross-section $\propto \lambda^{-4}$). The large wavelength range of SCIAMACHY makes it ideally suited to the determination of atmospheric aerosol properties. To analyse the scattering properties of back scattered light, including contributions from aerosols and clouds, measurements of the polarisation properties of the scattered light are necessary and the measured signal should be corrected for the instrument dependent polarisation effects.

The nadir and limb viewing strategies of SCIAMACHY will yield global aerosol total column amount and stratospheric profiles. This will enable the stratospheric and tropospheric abundances to be estimated.

In nadir viewing, the O₂, O₄ and CO₂ absorptions will enable the penetration depth of light in the atmosphere and therefore the cloud top height to be estimated. In addition, the spectral reflectance (i.e. albedo) in the range 0.33-2.4 μm will enable the cloud cover to be estimated. The following cloud physical parameters can be determined by



SCIAMACHY: optical thickness, average particle size and cloud top altitude.

Polar Stratospheric Clouds (PSCs) were first discovered by SAM II (McCormick and Trepte 1986) and will be readily measured by SCIAMACHY. These clouds play a very important role in the 'ozone hole' depletion mechanism.

4.2.2 Pressure and Temperature Measurements

Stratospheric density / pressure profiles along the limb can be determined from the limb and occultation profiles of the well mixed gases O₂ and CO₂. There are two methods to determine temperature profiles:

(a) stratospheric density profiles can be readily inverted from the measurements to yield stratospheric temperature profiles;

(b) via the Boltzmann distribution of the CO₂ vibrational-rotational features.

Under cloud-free conditions, the surface pressure can be determined from the O₂ and/or CO₂ measurements in nadir viewing.

4.2.3 Land and Ocean Measurements

SCIAMACHY is required to monitor broad-band surface absorptions in the range 0.33-2.4 μm. These measurements are relevant for the Ocean and Land-Usage scientific communities. However, the typical spatial resolution of 30 km x 60 km of SCIAMACHY in nadir viewing, is not as high as that of dedicated imaging devices such as MERIS on ENVISAT. Nevertheless, SCIAMACHY will provide useful global information on the surface spectral reflectance in the range 0.33-2.4 μm for large scale processes with a much higher spectral resolution as for example MERIS.

Oceanographic measurements: Ocean colour can be determined from broad-band visible absorptions under cloud-free conditions. This can be used to estimate the abundance of near-surface phytoplankton biomass, which in turn is correlated to water column primary productivity. An example of a large scale event to be studied is the El Niño southern oscillation phenomenon in the pacific ocean, which is thought to have a large impact on global weather patterns.

Terrestrial measurements: The surface spectral reflectance will be measured in cloud-free areas by SCIAMACHY. Broad-band absorption due to the presence of chlorophyll in plants will be measured. This enables the following parameters to be determined globally at low spatial resolution: vegetation index and ground classification and state (desert etc.). This leads to knowledge about deforestation and the extent of biomass burning in savannah regions which are extremely important parameters in global change considerations.

Studies of the usefulness of SCIAMACHY observations for these applications and synergism with other instruments (e.g. dedicated surface instruments such as MERIS on ENVISAT) shall be undertaken in future.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 12/49

4.2.4 Climate and Earth Radiation Budget

In the context of climate and global change SCIAMACHY measurements yields the distribution of 'Greenhouse' gases O₃, H₂O, CH₄, N₂O, CO₂, aerosol and cloud data, surface spectral reflectance (320 nm - 2380 nm), the incoming and outgoing short wave flux (240 nm - 2380 nm), as well as profiles of p and T (via O₂ and CO₂). As SCIAMACHY observations are to be performed globally for several years and provided that the record is large enough, its observations are well suited for the study of the variations of the solar output on climate change and the interaction between chemical processes and climate change.

The observations made by SCIAMACHY are also of interest to scientists studying the earth's radiation budget. SCIAMACHY measures 95% of the incoming solar radiation and outgoing short wave (SW) flux directly. There is currently a long-term satellite programme (the earth radiation budget experiment ERBE) which focuses on this issue. However, the ERBE sensors typically have much lower spectral resolution than SCIAMACHY in the range 0.24-2.4 μm . SCIAMACHY spectral observations shall also be made available to the ERBE community.

4.3 *Required precision*

From the scientific point of view, without taking into account any instrumental limitations, it is required to retrieve at least the total column amount of prominent atmospheric trace gases with an accuracy of 1 - 5 % as a design goal. An accuracy of 5 - 10% should be the design goal for atmospheric profiles.

Since more realistic precision estimates and calculations base upon instrument parameters which are subject to change during instrument development phases and will only be given precisely after instrument characterisation (end of 1998), corresponding uncertainties have to be considered. Therefore simulations of the expected precision were performed in parallel to the instrument development (compare e.g. Burrows et al. 1988, Chance et al. 1991, ESA 1993, Schrijver et al. 1995). A summary of the expected precision for the different targeted trace gases is shown in Table 5 (chapter 8).

5 Measurement Principle and Observational Modes

5.1 Measurement Principle

SCIAMACHY will retrieve the atmospheric amounts of trace gases from observations of transmitted, back-scattered and reflected light from the atmosphere in the wavelength range 240 - 2380 nm. Trace gases, aerosols, clouds and the surface of the Earth attenuate the solar output observed by SCIAMACHY via absorption, emission and scattering processes as can be seen in Figure 1. The ratio of the upwelling radiance and the extraterrestrial solar irradiance can be inverted to provide information about the amounts and distribution of important atmospheric constituents, which absorb or scatter light, and the spectral reflectance (or albedo) of the Earth's surface.

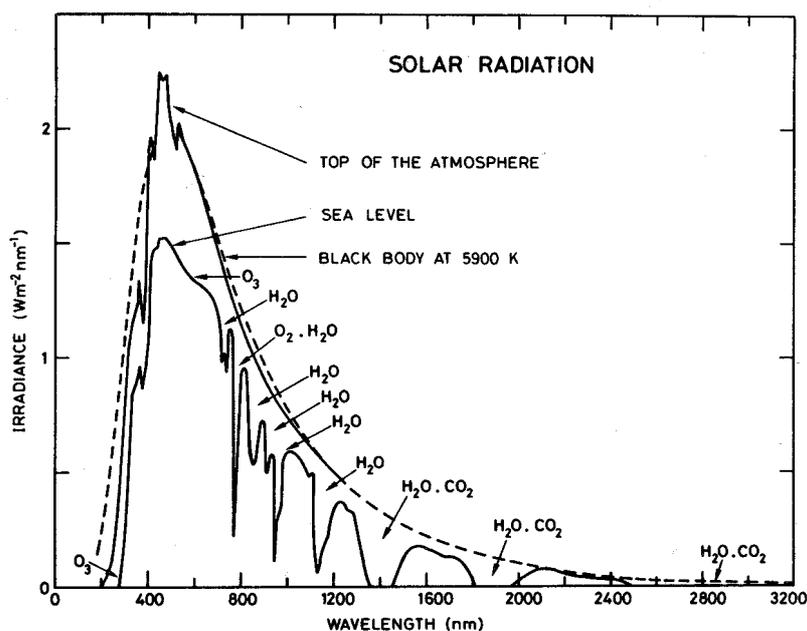


Figure 1 Spectrum of solar spectral irradiance from the UV to the near infrared (NIR) outside the earth's atmosphere and at sea level (from Brasseur and Solomon 1995).

Inversion of the ratio of the upwelling radiance and the solar irradiance measurements enables the amounts and distributions of a significant number of constituents to be retrieved from their spectral signatures. To detect all constituents identified in chapter 3, SCIAMACHY has to observe the relevant spectral. Table 1 summarises the spectral regions where the targeted constituents may be detected. These constituents absorb in spectral regions ranging from the ultraviolet (UV) to the near infrared (NIR). In Figure 2 a schematic overview of these spectral regions is given and for comparison the spectral range covered by GOME on ERS-2 is also shown.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
 Issue: Draft, Rev. 1
 Date: Jan. 1998
 Page: 14/49

Constituent	Wavelength Range [nm]
O₃	
Hartley	240-300
Huggins	300-350
Chappuis	400-700
O₂ A-Band	680-762
O₄	380-1400
O₂(¹Δ)	1270
NO, γ-band emission	240-300
NO₂	300-700
NO₃	600-700
N₂O	2250-2350
CO	2300-2380
CO₂	1980-2020
CH₄	2250-2380
BrO	300-450
H₂O	400-2380
ClO	260-320
OCIO	300-440
H₂CO	300-350
SO₂	300-320
NO₃	600-700
Aerosol	240-2380
Albedo	240-2380

Table 1 Wavelength ranges where the targeted constituents can be detected.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
 Issue: Draft, Rev. 1
 Date: Jan. 1998
 Page: 15/49

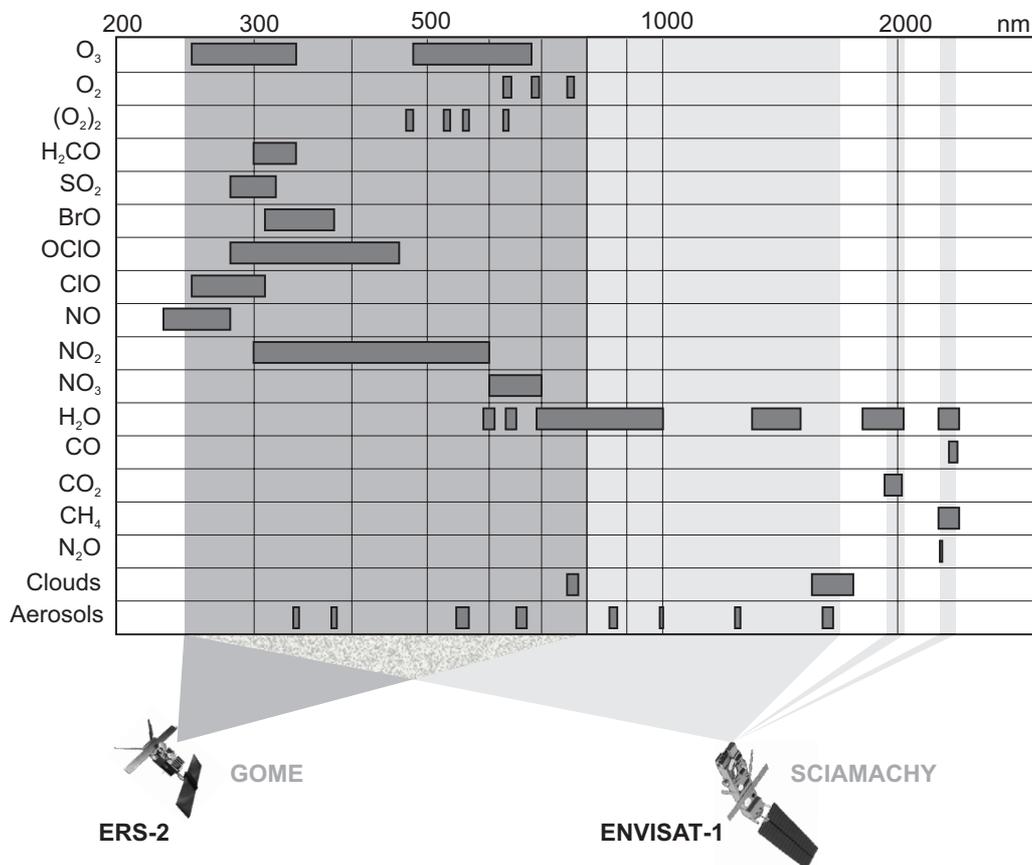


Figure 2 Wavelength range covered by GOME and SCIAMACHY including the absorption windows of the targeted constituents

As can be seen from Table 1 or Figure 2, to detect all constituents identified in chapter 3, it is essential that SCIAMACHY observes continuously the wavelength ranges 240 - 1750 nm, 1940 - 2040 nm and 2265 - 2380 nm.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 16/49

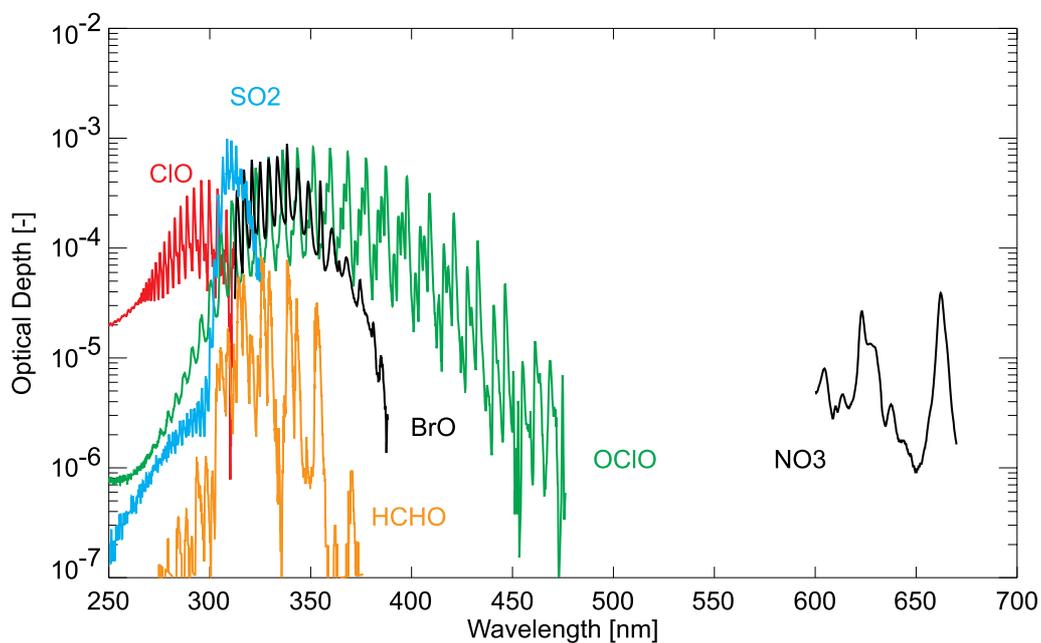
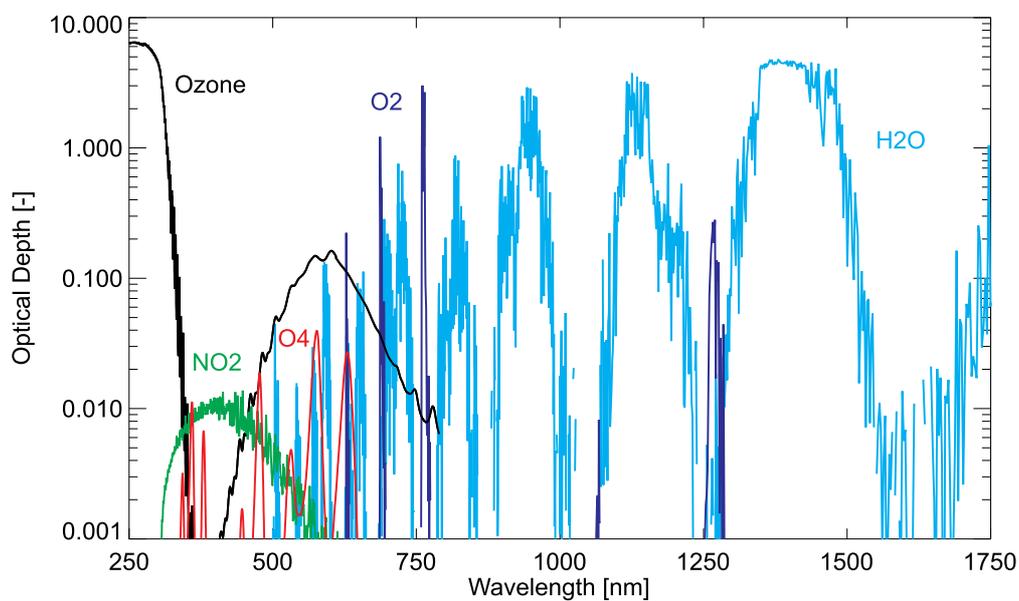


Figure 3 Typical optical depth as function of wavelength for SCIAMACHY targeted constituents for nadir view (SZA= 60°, albedo=0.1, MPI atmosphere 55 N).

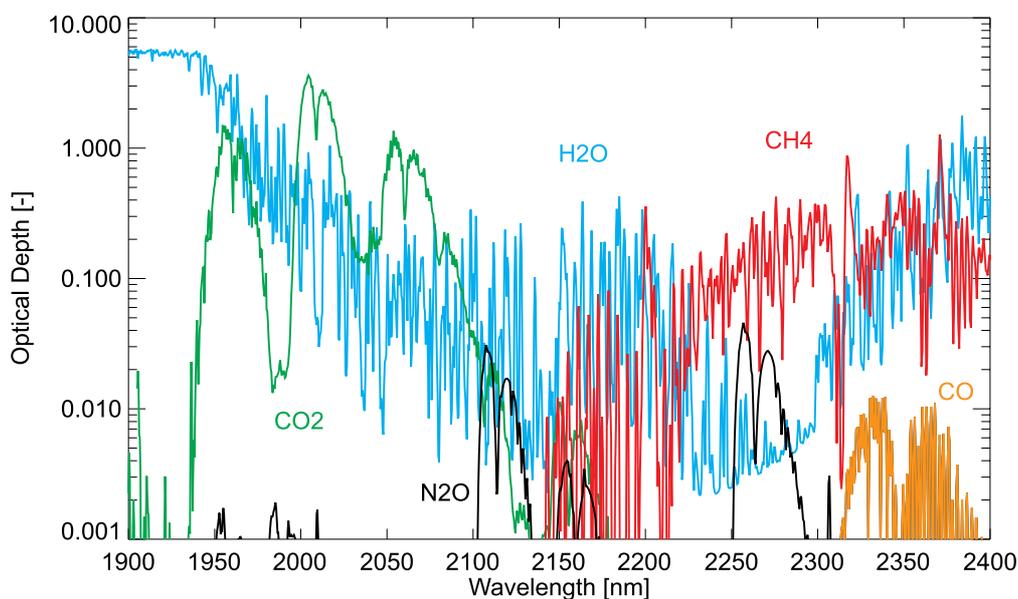


Figure 4 Typical optical depth as function of wavelength for SCIAMACHY targeted constituents (SZA= 60°, albedo=0.1, MPI atmosphere 55 N).

The retrieval of the amounts of constituents depends on the ability of SCIAMACHY to measure their absorptions accurately. This is of course dependent on the photon flux and the design of the instrument and the detectors. Typical optical depth for the targeted trace gases are depicted in Figure 3 and Figure 4. Atmospheric trace gases can be divided into 'strong' absorbers (large optical depth, e.g. O₃, O₃, H₂O) and 'weak' absorbers (e.g. NO₂, BrO, HCHO etc.). To detect the minor trace gases, SCIAMACHY needs to be able to measure intensity changes in the optical depth of 10⁻³ - 10⁻⁴.

5.2 Observational Modes

To fulfil the mission objectives with respect to spatial resolution and coverage, SCIAMACHY it is required to combine the measurement principles and observational modes of the nadir scattered sunlight measuring instruments such as TOMS and SBUV (Heath et al. 1975), the solar occultation instrument SAGE (Maudlin et al. 1985) and the limb scattered sunlight measuring instrument SME (Barth et al. 1983) within one instrument. This requires measurements of the following:

- the scattered and reflected solar photons in nadir and limb geometry,
- the light transmitted through the atmosphere in solar and lunar occultation geometry,
- the extraterrestrial solar and lunar irradiance.

As total column amounts and height resolved profiles are required, SCIAMACHY shall



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 18/49

alternately observe the atmosphere in limb and nadir viewing and solar occultation measurements shall be made during each orbit. Solar occultation is only possible over the northern hemisphere for SCIAMACHY's location on ENVISAT. It is therefore required to observe regions over the southern hemisphere by lunar occultation measurements where feasible. SCIAMACHY aims to obtain global coverage within 3 days at the equator in limb or nadir mode. The combined limb/nadir mode will consequently achieve global coverage in around 6 days at the equator. Data assimilation and convection schemes may allow to interpolate global maps with a higher time resolution.

Nadir viewing measurements should be used to retrieve total column amounts with high horizontal resolution. Vertical profiles can be obtained for species for which the absorption changes significantly with altitude, as it is the case for O_3 , NO_2 and H_2O .

Limb viewing geometry is particularly suited for the retrieval of stratospheric profiles. As a result of the long light path through the atmosphere and long integration times, the horizontal resolution is only moderate, and tropospheric profiles are often corrupted by the presence of clouds.

In **solar occultation** measurements, absorption spectra of the atmosphere are recorded having the Sun as an extremely bright light source. With the high solar irradiance and an in-built Sun scanning option, solar occultation measurements are expected to have the highest vertical resolution coupled with the best S/N values. The major disadvantage is that solar occultation measurements are restricted to about 60 seconds viewing time after sunrise and therefore to specific geographical positions between $65^\circ N$ and $90^\circ N$ for SCIAMACHY on ENVISAT.

Lunar occultation measurements provide, in addition to O_3 and NO_2 , the possibility for the detection of photolytically sensitive species such as NO_3 or ClO . These species are nighttime reservoirs for NO , NO_2 and ClO respectively, which are involved in the catalytic cycles destroying stratospheric ozone. However the lunar intensity levels are low and results in requirements on the S/N ratio and/or on the spatial resolution being less demanding than those of the solar occultation measurements. In addition, lunar occultation is restricted to about 60 seconds before Moonset, and is possible only for approximately 8 days around full Moon.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 19/49

6 Retrieval Methods

Detailed requirements on retrieval algorithms are specified in the Scientific Requirements Document for SCIAMACHY Data and Algorithm Development (SCIAMACHY Data and Algorithm Subgroup 1996) prepared by the data and algorithm subgroup, headed by of Dr. K. V. Chance.

6.1 General Considerations

Retrieval methods for SCIAMACHY should be able to cover a wide range of demands: they should be able to invert trace gas amounts from their narrow spectral absorption features in one extreme and for example aerosol information from their broad band scattering characteristics on the other extreme.

A robust retrieval method for the derivation of trace gas column amounts from measured UV-vis spectra is the differential optical absorption spectroscopy DOAS (Platt et al. 1979, Perner and Platt 1979). Within the last decade DOAS developed to a well established method for environmental remote sensing of the troposphere and the stratosphere (Roscoe and Clemithshaw 1997 and references therein) and has been applied to the retrieval of trace gases from space borne spectral measurements for the first time by GOME (an overview of results from GOME can be find in ESA 1997)

A second well established method to retrieve trace gas concentrations and profiles from satellite measurements is based on the optimal estimation OE procedure (Rodgers 1979). OE is able to use full spectral and radiometric information contained in the measurement in combination with a-priori information and has been applied for example to the inversion of stratospheric ozone profiles from SBUV measurements (Bharthia et al. 1996).

As SCIAMACHY is a radiometric calibrated multi-channel spectrometer, which has a much larger spectral coverage than the existing instruments, especially the retrieval of the NIR absorbers H₂O, CO₂, CO, N₂O and CH₄, and the NIR scattering characteristics of clouds and aerosols requires adaptations of existing retrieval methods to the relevant spectral range, taking into account the physical nature of the absorption and scattering processes.

There are several advantages in having different retrieval methods, the most important being:

- data continuity (i.e. data obtained from SCIAMACHY can be compared with TOMS/SBUV or SAGE instruments which have been operating for some years) and
- self-validation (i.e. the different approaches used to determine constituent amounts can be internally compared thereby improving overall retrieval precision).

As DOAS and optimal estimation will have somewhat different requirements on the instrument performance it is instructive to separate the retrieval of column amounts and stratospheric profiles from the nadir, limb and occultation measurements into two distinct categories: differential optical absorption spectroscopy (DOAS) and back-



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 20/49

scattered ultra-violet and visible radiometry, here summarised as optimal estimation.

6.2 *Differential Optical Absorption Spectroscopy*

For DOAS the retrieval process can be split into four steps. These steps can be partly combined, when implementing the DOAS scheme. In a first step, the measured spectrum I is divided by the un-attenuated spectrum of the light source, the extra-terrestrial solar spectrum I_0 : $OD_\lambda = \ln(I_0/I)_\lambda$. In the second step, broad band spectral features resulting from atmospheric effects like broad band absorption, Rayleigh and Mie scattering, and surface reflection are separated from the measured OD by fitting and subtracting a low-order polynomial to/from OD_λ . This process generates the so-called differential optical depth. In the next step, the effective slant column densities of the target trace gases are determined by fitting the differential optical depth with laboratory absorption cross-section spectra. In the fourth step, the slant column densities are converted to vertical column densities by dividing the slant column densities by appropriate air mass factors. Air mass factors describe the enhancement of trace gas absorptions due to the slant path of the sunlight through the atmosphere; their value depends on the trace gas, its vertical distribution, solar zenith angle and wavelength. Contrary to slant columns, vertical column densities are independent of the specific viewing geometry of the instrument and the position of the sun. Note that the ground based DOAS methods where not be able to measure I_0 , which results in an additional error source. This error source will be definitely be avoided by using space based instruments like SCIAMACHY and GOME which obtains I_0 by direct observation of the sun. One implicit assumption used in DOAS for satellite measurements is that the optical depth is less than approx. 5%. For these candidates the air mass factor is constant over a given DOAS spectral window (Diebel et al. 1995).

DOAS was introduced for ground based measurements of tropospheric stratospheric gases (Noxon 1975, Noxon et al. 1979, Platt et al. 1979, Perner and Platt 1979) but was effectively applied to zenith sky scattered light and solar and lunar transmitted light for the ground based measurements of tropospheric and stratospheric constituents (Brewer et al. 1973, Solomon et al. 1987). In recent years, ground-based, balloon-borne and aircraft-borne single channel as well as multi channel spectrometers have successfully observed a variety of atmospheric trace gases using the DOAS approach: O_3 , O_2 , O_4 , NO_2 , NO_3 , HCHO, BrO, and OCIO (see for example Roscoe and Clemithshaw 1997 and references therein). The application of DOAS to the retrieval of trace gases from space borne spectral measurements has been successfully demonstrated for the first time by GOME for O_3 , NO_2 , BrO, OCIO, SO_2 and HCHO (an overview of results from GOME can be find in ESA 1997).

As SCIAMACHY is a multi-channel spectrometer, which has a much larger spectral coverage than the existing instruments, it will be able to probe more species (compare Figure 2). Especially the retrieval of the NIR absorbers H_2O , CO_2 , CO, N_2O and CH_4 requires an adaptation of the retrieval method.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 21/49

6.3 *Optimal Estimation*

The optimal estimation (OE) iterative least-squares fitting procedure is a well established method for solving illposed inversion problems by using a-priori information. An optimal estimation algorithm consists mainly of two parts:(i) a forward model calculation of the measured radiance (more general the measured quantity), based on a radiation transfer model, which calculates at the relevant geometry the radiance for a given state of the atmosphere and, (ii) an inversion scheme which matches in iterative steps the calculated radiance compared to the measured radiance by modifying model atmospheric parameters such as for example the vertical distribution of ozone using appropriate weighting functions as provided by the radiative transfer model. The well known scheme of Rodgers (1976) can be used to invert the data.

Optimal estimation has been applied for example to the inversion of stratospheric ozone profiles from SBUV measurements (Bharthia et al. 1996). The successful retrieval of ozone profile information with optimal estimation from GOME nadir measurements has also been demonstrated (Siddans et al. 1997, DeBeek et al. 1997).

A retrieval method which uses the intercomparison of the measured radiance to the simulated radiance requires an accurate radiometric calibration of the instrument .

6.4 *Retrieval of Tropospheric Information*

Electromagnetic radiation in the majority of the wavelength range selected for SCIAMACHY (0.33-2.4 μ m) penetrates the atmosphere down to the earth's surface. This enables the column amounts down to the planetary boundary layer to be retrieved from nadir measurements under cloud free conditions.

As it is required that SCIAMACHY measures the same volume of air in limb and in nadir, tropospheric amounts of trace gases will be determined by subtracting total column amounts and stratospheric profiles of atmospheric constituents. This approach is known as tropospheric column residual method. The feasibility of this method has been investigated for tropospheric ozone by subtracting SAGE stratospheric ozone columns from TOMS total ozone columns (Fishman et al. 1990) or by subtracting SBUV stratospheric ozone columns from TOMS total ozone columns (Fishman et al. 1996). Up to now the main limitations of the method has been the inadequate spatial and temporal overlap between measurements. SCIAMACHY will overcome this problem by using a dedicated limb-nadir observation strategy where subsequent limb and nadir measurements of the same air volume are performed. Using SCIAMACHY data, the residual method is to be applied to tropospheric column retrieval of O₃, SO₂, H₂O, H₂CO, N₂O, CO, CH₄, NO₂ and aerosol. MOPITT on EOS-AM-1 uses a similar technique to derive tropospheric CO and CH₄ concentrations (Drummond et al. 1997).

In the special case of O₃, a profile including the troposphere can be determined from the temperature dependence of the Huggins bands: the simultaneous observation of the T-dependent Huggins bands and the T-independent Hartley and Chappuis bands enables tropospheric ozone to be retrieved from nadir measurements directly (Chance



et al. 1996). First results on tropospheric ozone retrieval using Hartley- and Huggins band from nadir measurements of GOME were presented at the third ERS symposium (Siddans et al. 1997).

6.5 Retrieval of Temperature, Pressure, Cloud and Aerosol Information

6.5.1 Aerosol

SCIAMACHY aerosol vertical profile retrieval from limb and occultation measurements have some similarities with the SAGE retrieval procedure (McCormick and Trepte 1986, Woodbury and McCormick 1986), providing some continuity of the two aerosol data series. The aim of this retrieval is the determination of the vertical distributions of size and density of the aerosols. The SCIAMACHY spectral coverage may also be used, after careful gas retrieval, to investigate the composition of the aerosols. The wavelength coincidence between SO₂ and ozone spectra, and between the NO₃ and NO₂ spectra, does not allow this possibility to be used at the lower spectral resolution of SAGE II. Both stratospheric and tropospheric aerosol abundances can be determined from the different atmospheric viewing geometries. In nadir viewing, tropospheric aerosols will be dominant.

6.5.2 Cloud

SCIAMACHY can play a unique role in cloud studies, because it is designed to detect near infrared absorption by water and ice clouds in channel 6. Water and ice each have a broad absorption band near 1.6 μm , but the band shapes are different. Therefore, discrimination between the two phases of water will be possible. By combining the reflectivity of clouds at non-absorbing wavelengths in the visible with the reflectivity at absorbing wavelengths in the near infrared, the cloud optical thickness and particle size can be found. Near infrared absorption is thought to be one of the possibilities to explain the so-called anomalous absorption by clouds. SCIAMACHY could contribute significantly to cloud-radiation studies, as it measures almost all shortwave radiation. Combined with cloud properties derived from specific wavelengths, such as optical thickness, particle size, and cloud top height, the integrated shortwave radiation from SCIAMACHY would be an important product for cloud studies.

The measurement of penetration depth and therefore cloud-top height was described in the SCIAMACHY proposal. It can be retrieved by using either the CO₂ absorption around 2.0 μm or the O₂ A-band absorption around 760 nm (Kuze and Chance 1994). This approach actually measures an effective scattering height and deduces the cloud top from this measurement.

6.5.3 Temperature and Pressure

SCIAMACHY will determine atmospheric temperature and pressure profiles from the limb and occultation measurements of the well-mixed atmospheric gases O₂ and CO₂. The use of the O₂ A-band absorption about 762 nm in nadir viewing for the determination of surface pressure in cloud-free regions was proposed by Barton and

 <p>SCIAMACHY</p>	<h1>SCIAMACHY</h1> <p>Scientific Requirements</p>	Doc.No.:SCIA-SRD Issue: Draft, Rev. 1 Date: Jan. 1998 Page: 23/49
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Scott in 1986 with an estimated accuracy of 0.2%. SCIAMACHY is able to use both O₂ and CO₂ absorptions to determine the surface pressure in cloud-free regions. The temperature can independently be determined from the Boltzmann distribution of the CO₂ vibrational-rotational absorptions.

6.6 Summary of Retrieval Approach

It is important to point out that the information content of the SCIAMACHY measurements is much more than could be simply retrieved by currently existing DOAS type or OE type methods on their own. The algorithms which retrieve the different atmospheric parameters and constituents from SCIAMACHY measurements shall therefore recognise the high spectral resolution and enormous wavelength coverage intrinsic to SCIAMACHY which differentiates it from previous satellite remote sensing instruments using UV or visible spectroscopy, such as SBUV/TOMS, SAGE or SME. Consequently, much more information (especially on the troposphere) will be retrievable from SCIAMACHY measurements than has been possible with previous devices.



7 Implications for the Instrument Requirements

7.1 Basic Design Assumptions

The SCIAMACHY instrument is a passive remote sensor for atmospheric constituents, comprised of one imaging spectrometer (instead of two, as originally proposed) which will observe transmitted, reflected and scattered light from the atmosphere in the UV, visible and near infrared wavelength regions. The spectrometer will be equipped with state-of-the-art photodiode array detectors which can integrate 'on-chip' the collected photons. This allows small optical absorptions of the order of 10^{-3} to 10^{-4} to be detected. The design of the SCIAMACHY instrument shall enable atmospheric spectra to be recorded at moderate spectral resolution. During phase A and B several trade-offs between scientific requirements and technical feasibility were discussed (e.g. Goede et al. 1993, 1994). The result is the current instrument design and mission profile as described in (Burrows et al. 1995 and Bovensmann et al. 1997). The major requirements on the instrument design are summarised in the following. A more detailed discussion of the relation between scientific objectives and the instrument requirements can be found in (Burrows and Blindauer 1993).

7.2 Viewing Geometries

Ideally, SCIAMACHY should provide accurate information on atmospheric constituents with high spatial resolution in both vertical and horizontal direction. However, depending on the viewing geometry, the requirement in one direction is usually fulfilled at the expense of that in the other direction (compare 5.2). With the various advantages and disadvantages inherent in the various viewing modes, a comprehensive viewing strategy is required. It is clearly desirable from the scientific point of view that SCIAMACHY should perform:

- simultaneous limb and nadir viewing measurements (two separate spectrometers) thus enabling the tropospheric amount and the stratospheric profiles of the important trace gases to be clearly differentiated.
- solar and lunar occultation measurements over both the Northern and Southern hemispheric polar regions.

This approach was originally proposed for SCIAMACHY but was scaled down during Phase B. Instead, viewing options were reduced to :

- alternate limb and nadir measurements (one spectrometer only).
- solar occultation only over the northern and lunar occultation measurements only over the southern hemisphere.

7.2.1 Scan Mirror, Telescope, Sun Sensor and Pointing

The scan mirror system is capable of observing the atmosphere in nadir and limb geometries, as well as monitoring the sun and moon in occultation and calibration. A sun/moon sensor is included to position the scan mirror on the centroid of the sun and



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 25/49

moon. The SCIAMACHY telescope is a simple off-axis parabolic mirror which, together with the entrance aperture, defines the f-number of the instrument. The width of the entrance slit defines the instrument field-of-view of $0.045^\circ \times 1.8^\circ$.

The required knowledge of the pointing system is determined from the requirement that, in limb and occultation, the imaging system (scan mirror and telescope) must be able to resolve an atmospheric layer of 3 km height.

7.2.2 Limb Scanning

The present baseline limb measurement strategy divides the atmosphere into 30 partially overlapping layers of roughly 3 km height. As the azimuth scan takes 1.5 s for every elevation step, the satellite moves by approximately 300 km during a complete limb measurement. The SCIAMACHY scanning mirror system is specified in such a way that the limb is scanned horizontally (in azimuth direction) as well as vertically (in elevation direction). This is to ensure that the volume of air observed in the limb scan matches that observed in subsequent nadir viewing. For the largest scan option, limb measurements are therefore typically (integration time of 0.375s) averaged over a distance of 240 km perpendicular to the satellite track.

With the present design, the imaging system of SCIAMACHY achieves a vertical resolution of approx. 3 km in limb scanning mode and 2,5 km in solar occultation mode. However, the effective vertical resolution may be slightly degraded by the spacecraft pointing capability which limits the pointing accuracy to approx. 2 km in limb viewing, yielding an overall vertical resolution of 4-5 km. Global coverage at the equator is achieved within 3 day for the limb only measurements.

7.2.3 Nadir Scanning

For the ENVISAT-1 orbit, complete longitudinal coverage at the equator can be achieved by SCIAMACHY in three days for an across-track scan range of approx. 960 km on the ground. At higher latitudes, complete longitudinal coverage is achieved more rapidly. By varying the scan angle range of the scan mirror, the swath width can be adapted. For a given scan range, the time interval between successive read-outs (integration time) determines the horizontal resolution. To monitor important products such as cloud cover, ozone and NO_2 with a high spatial resolution in the global scan mode special spectral windows should be read out at a rate of 8 Hz (125 ms) or higher which corresponds to an image of approx. $30 \times 30 \text{ km}^2$ on the earth's surface.

7.2.4 Combined Limb-Nadir Scanning

To derive tropospheric information it is required that SCIAMACHY is capable to observe the same atmospheric volume first in limb and thereafter in nadir mode. This requires the synchronization of integration times, scan ranges and viewing directions for all limb and nadir measurements. With a dedicated limb-nadir scanning strategy and a swath width of 960 km global coverage is reached after 6 days at the equator for the combined limb nadir strategy.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 26/49

7.2.5 Solar and Lunar Occultation and Calibration Modes

Solar occultation and calibration measurements can be made at sunrise in each orbit. Lunar occultation and calibration measurements can be made for approx. 8 days around full moon. The accommodation of SCIAMACHY on ENVISAT-1 does not allow both sunrise and sunset and moonrise and moonset observations. The combination of solar occultation at sunrise over the north pole and lunar occultation at moonrise over the south pole near full moon is a compromise. For the ENVISAT-1 orbit, solar occultation is restricted to latitudes between 65°N and 90°N. Lunar occultation can be performed from half moon to full moon, provided that the moon is visible for SCIAMACHY. For periods of 5 to 8 days per month lunar occultation measurements will provide latitudinal coverage from 30°S to 90°S maximum.

The solar scanning strategy should be similar to the SAGE II scanning (Maudlin et al. 1985): during sunrise SCIAMACHY scans several times over the full solar disc. When the sun is above the atmosphere several calibration measurements shall be performed. However for the lunar measurements a 'stare' mode similar to that used on HALOE (Russel et al. 1993) is required.

During solar occultation and calibration measurements, it is mandatory to down-link the measurement data at a high rate to achieve the best vertical resolution. A data rate of 1.8 Mbps has recently been granted for the time period of SCIAMACHY solar occultation and calibration measurements of approx. 2 minutes.

7.2.6 Eclipse / Nighttime Mode

During eclipse, only low-level light sources like lunar radiation, stars, airglows, fires are available. The necessity to average over long time intervals to achieve a reasonable signal-to-noise level reduces dramatically the spatial resolution and the data rate of SCIAMACHY during the eclipse.

7.3 *Optical Requirement Implications*

7.3.1 Wavelength Ranges

The measurement concept of SCIAMACHY relies on the observation of the solar radiation, which is transmitted or scattered through the atmosphere and reflected from the ground. Provided the spectral resolution of SCIAMACHY is appropriately chosen, characteristic 'fingerprint' spectra of molecular features can be identified.

As described in chapter 4, it is essential that SCIAMACHY channels 1 to 6 shall observe the entire spectrum from 240 to 1750 nm. Channel 7 and 8 will measure the selected regions 1.94 - 2.04 μm and 2.265 - 2.38 μm . To minimise the number of channels, no measurements have been planned for the wavelength range from 1.75 to 1.94 μm . As it is required to cover the whole wavelength range at moderately high spectral resolution 8 array detectors (= 8 'channels'), each comprising 1024 photodiodes, shall be used. Table 2 and Table 3 summarise the channel definition. The channel wavelength definitions listed below represent a compromise between the need to have a small light-weight instrument with as low a data rate as possible, and



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 27/49

the scientific objectives of SCIAMACHY. The exact wavelength limits chosen to separate channels 1 to 6 results from both scientific and technical considerations. For example, channel 1 has the lowest photon flux, and its separation from channel 2 was chosen such as to minimise the straylight.

- Channel 1: 240-314 nm. Due to the fall-off in the solar source function and the absorption of O_3 , light levels are relatively small in this channel. It is used to observe the O_3 Hartley band maximum and the NO γ -band emission. Under high ClO and low O_3 conditions, the strongest ClO absorptions might also be observed.
- Channel 2: 309-405 nm (UV-B and UV-A radiation). A variety of molecules have banded absorption features in this region: O_3 , O_4 , NO_2 , ClO, OCIO, BrO, SO_2 , and H_2CO .
- Channel 3: 394-620 nm. The following molecules have identifiable banded visible absorption features: NO_2 , NO_3 , OCIO, H_2O , O_2 , O_3 , and O_4 .
- Channels 4 and 5: 604-805 nm and 795-1050 nm. The following species absorb significantly in this region: NO_3 , O_2 , O_4 , and H_2O .
- Channel 6: 1000-1750 nm. Features due to $O_2(^1\Delta_g)$, CH_4 , O_4 and H_2O are monitored in this near-infrared channel.
- Channel 7: 1940-2040 nm. This region was specifically chosen for CO_2 measurements. H_2O also absorbs in this region.
- Channel 8: 2265-2380 nm. Absorptions due to CO, CH_4 , N_2O , and H_2O are observed in this atmospheric window.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
 Issue: Draft, Rev. 1
 Date: Jan. 1998
 Page: 28/49

Optical Channel	Wavelength Range [nm]	Pixel Resolution [nm]	Atmospheric Constituent	Spectral Feature
1	240 - 314	0.12	O ₃ NO (ClO) Aerosol Albedo Rayleigh	A Hartley E γ -bands A A-bands S A, E, S S
2	309 - 405	0.13	O ₃ O ₄ NO ₂ ClO OCIO BrO H ₂ CO SO ₂ Aerosol Albedo Rayleigh	A Huggins A A A A A A A S A, E, R, S S
3	394 - 620	0.22 -	O ₃ O ₄ NO ₂ BrO OCIO H ₂ O Aerosol Albedo Rayleigh	A Chappuis A A A A A S A, E, R, S S
4	604 - 805	0.24	O ₂ O ₃ NO ₂ NO ₃ H ₂ O Aerosol Albedo Rayleigh	A A-band A B-band A Chappuis A A A S A, E, R, S S

Table 2 SCIAMACHY Optical Channels 1-4. Abbreviations: A - absorption, E - emission, S - scattering, R - reflectance



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 29/49

Optical Channel	Wavelength Range [nm]	Pixel Resolution [nm]	Atmospheric Constituent	Spectral Feature
5	785 - 1050	0.27	H ₂ O Aerosol Albedo Rayleigh	A S A, E, R, S S
6	1000 - 1750	0.74	O ₂ (¹ Δ) O ₂ O ₄ H ₂ O Aerosol Albedo Rayleigh	E A A A S A, E, R, S S
7	1940 - 2040	0.11	CO ₂ H ₂ O Aerosol Albedo Rayleigh	A A S A, E, R, S S
8	2265 - 2380	0.13	CO CH ₄ N ₂ O H ₂ O Aerosol Albedo Rayleigh	A A A A S A, E, R, S S

Table 3 SCIAMACHY Optical Channels 5-8. Abbreviations: A - absorption, E - emission, S - scattering, R - reflectance

7.3.2 Spectral Resolution

In every spectroscopic experiment, the spectral resolution should be sufficient to distinguish unambiguously all absorption, emission or scattering features of the species to be observed. For the broad-band scattering features and atmospheric absorptions of aerosols and some atmospheric trace gases, this instrument requirement can be readily attained. However, rotational-vibrational transitions of diatomic molecules often exhibit narrow absorption and emission lines that require a moderately high resolution. This is especially important for the NIR channels of SCIAMACHY. In addition, it is desirable to resolve the sharp Fraunhofer structure of the solar spectrum to correct for thermal shifts taking place in SCIAMACHY. Consequently the highest spectral resolution is required in the UV and the NIR channels.

On the other hand high spectral resolution over a large spectral interval requires a high data rate. As a result of the relatively high data rate obtained from a globally monitoring imaging spectrometer such as SCIAMACHY, one of the objectives of the Phase A



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 30/49

Study was to reduce where possible the data rate of SCIAMACHY without compromising its scientific objectives. It was decided to limit the spectral coverage of SCIAMACHY to 8 channels with diode array detectors of 1024 pixel elements each. In order to avoid spectral aliasing problems mainly due to the strong and narrow Fraunhofer features in the UV and visible spectral ranges, the spectrometer slit needs to be designed such that the resulting spectral resolution (FWHM without binning) matches the Nyquist limit of approximately twice the pixel resolution. The required pixel resolution for the different channels is given in Table 2 and Table 3. The detector pixel resolution in SCIAMACHY varies between 0.1 and 0.8 nm, resulting in spectral resolutions between 0.2 and 1.6 nm. The values of spectral pixel resolution listed in Table 1 and 2 represent a compromise between the scientific ideal required to resolve completely the spectroscopic lines of all atmospheric trace gases, and the need to obtain reasonable S/N values and high spatial resolution under the constraint of limited data transmission rates.

7.3.3 Spectral Knowledge

The nadir, limb and occultation spectra as observed by SCIAMACHY will be analysed by comparison with the relevant simulated spectra. All wavelength shifts between these measured and simulated spectra appear as an additional noise in the resulting fit residuals and deteriorates the retrieval precision. As a result of the narrow features in the Fraunhofer lines and absorption structures, even small shifts resulting from thermal variations can generate significant retrieval errors.

For GOME, the error resulting from a wavelength shift of 1/50 pixel, i.e. 0.002 nm below 400 nm and 0.004 nm above (valid for both GOME and SCIAMACHY), has been estimated (Diebel et al. 1995). Two high-resolution solar spectra were convoluted with a realistic GOME slit function, then shifted against each other and divided. The resulting noise was typically one order of magnitude *larger* than the sum of the noise contributions from photon statistics, dark current and ADC read-out in the case of a 1.5 s integration time. This amounts to about 1% of the signal in the ultraviolet region. Therefore, the nominal wavelength of any pixel should be known with an accuracy of 1/50 pixel over one orbit. High spectral stability of the instrument in combination with a dedicated spectral calibration strategy is therefore required.

7.3.4 Signal-to-Noise

The precision of any retrieved concentration profile or total column abundance of any atmospheric constituent is restricted by the signal-to-noise values in the absorption spectra (Burrows and Blindauer 1993, Roscoe et al. 1994). From the required accuracy a constituent should be retrieved, the S/N can be derived. Therefore the signal-to-noise value (S/N) was selected as a measure of the instrument performance of SCIAMACHY. It is defined as the ratio of the signal produced by the instrument (in electrons) to the noise on this signal. The signal depends on the amount of light-reaching the instrument (determined by viewing geometry and atmospheric conditions) and on instrumental properties such as FOV, instrument throughput and conversion efficiency. The noise is given by the root sum square of shot noise and various



electronic noise sources.

As the SCIAMACHY signal-to-noise ratio is dependent on the number of photons reaching the detector, the light throughput of the instrument should be as high as possible. S/N should be typically in the order of some 10^3 . A detailed specification of the required S/N in the different channels can be found in the Instrument Requirement Document (DARA 1995).

7.3.5 Straylight

Good straylight performance is an important characteristic of any spectrometer. As SCIAMACHY is a double monochromator which uses prisms as predispersers and gratings for the secondary dispersion, it has good straylight rejection capabilities. However, straylight is likely to be a problem in the UV channels 1a and 1b (240-314 nm), where light levels are low compared to the photon flux at longer wavelengths (the photon flux at 400 nm is four orders of magnitude larger than at 240 nm).

Straylight originates from two sources (inside or outside the spectrometer):

- Optical straylight is unwanted radiation external to the FOV, originating either from poor telescope imaging quality (astigmatism, etc.) or unbaffled reflections from SCIAMACHY or ENVISAT.
- Spectral straylight is radiation which is reflected or scattered within the spectrometer and is picked up by detector array pixels having different nominal wavelengths.

Straylight is critical to the performance of SCIAMACHY and must be suppressed for three reasons

- It represents an additional source of noise and thus affects the retrieval precision adversely.
- As spectral straylight contributes to the regular signal in an additive manner, absorbances are systematically underestimated in the same proportion as the magnitude of the straylight.
- Optical straylight enhances the effective FOV and thus corrupts the spatial resolution of the instrument. If optical straylight originates from solar reflections from SCIAMACHY or ENVISAT and has not been attenuated by the atmosphere, it adds to the systematic error in the determination of absorbances.

Since straylight enters the measurements in the same proportion as it contributes to the detected signal, its percentage should be as small as possible, and definitely below 1% of the light within a given detector pixel.

7.3.6 Radiometric Accuracy / Polarisation Measurement

Relative Radiometric Accuracy

Atmospheric light of radiance $R_{\text{abs}}(\lambda)$ as observed by SCIAMACHY in nadir, limb or occultation viewing may be polarised to a considerable extent through Rayleigh scattering and surface scattering effects. In contrast, the extra-terrestrial solar light of



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 32/49

radiance $R(\lambda)$ is unpolarised. Due to the polarisation sensitivity of SCIAMACHY, the radiances $R_{\text{abs}}(\lambda)$ and $R(\lambda)$ are related to electronic signals $S_{\text{abs}}(\lambda)$ and $S(\lambda)$ through different instrument transfer factors $T_{\text{pol}}(\lambda)$ and $T_{\text{unpol}}(\lambda)$:

$$S(\lambda) = T_{\text{unpol}}(\lambda) * R(\lambda)$$

$$S_{\text{abs}}(\lambda) = T_{\text{pol}}(\lambda) * R_{\text{abs}}(\lambda)$$

The information about the retrievable atmospheric parameters is contained in $\ln(R/R_{\text{abs}})$, the ratio of the incoming radiances. However, electronic signals S_{abs} , and S are the only measurable quantities, and $\ln(R/R_{\text{abs}})$ can be computed from $\ln(S/S_{\text{abs}})$ only if the ratio $T_{\text{pol}}/T_{\text{unpol}}$ is accurately known. For DOAS retrieval, however, it suffices that the value of $\ln(R/R_{\text{abs}})$ is known apart from a wavelength-independent factor - constant factors are easily accounted for in the retrieval algorithm. This requirement is fulfilled if the ratio $T_{\text{pol}}/T_{\text{unpol}}$ does not depend on the wavelength ('relative radiometric accuracy'). On the other hand, instrument transfer functions $T_{\text{pol}}(\lambda)$ and $T_{\text{unpol}}(\lambda)$ that vary over the range of absorption bands can corrupt the retrieval process. The relative radiometric precision goal is 1%. This value is not impossible even in the UV as the sun has been shown to be a stable light source beyond 240 nm (WMO 1985).

Absolute Radiometric Accuracy

In order to derive absolute values of the input radiance from the detector signal (number of electrons), the conversion (instrument transfer) factor must be known. Except for the optical throughput, all parameters determining the conversion factor (FOV, telescope area, detector QE and pixel resolution, integration time) can be calibrated prior to flight. The radiometric accuracy of the measurements depends on the state of polarization of the incoming light as well as on the polarization properties of the instrument. An ideal instrument should have a similar high efficiency for all states of polarisation over the whole wavelength range. To achieve a high radiometric accuracy, dedicated on-ground and in-flight calibration measurements have to be performed in combination with measurements of the polarization properties of the atmosphere. For the latter purpose SCIAMACHY shall be equipped with seven polarization measurement devices PMD's (Slijkhuis and Stammes 1993, Buchwitz et al. 1993). In order to measure the degree of polarisation of the incoming light, a well-defined ratio of the vertically polarised component is selected at the predisperser prism and measured by PMD's in six regions of the SCIAMACHY wavelength range. To derive the angle of polarisation χ , one additional PMD, tilted by 45° with respect to the so-called linear PMD's, is placed in the spectral region where the largest error due to polarisation sensitivity of the instrument is expected to occur. In the correction algorithm, χ will be assumed constant over the SCIAMACHY spectral range, and the circularly polarised component of the incoming light is assumed zero.

Using this approach, an absolute radiometric accuracy of better than 2-3 % for unpolarised and 3-4 % for polarised light should be achieved. These values might be improved by in-flight calibration of the polarisation response of SCIAMACHY by viewing the unpolarised Sun or the partly polarised limb at higher altitudes, where the degree of polarisation is known from simulations.

8 Fulfilment of Mission Objectives

To assess the expected retrieval precision and the sensitivity of SCIAMACHY in the different height ranges and observing modes (nadir, limb, occultation), several sensitivity studies were performed by members of the SCIAMACHY Science Advisory Group and their institutes (Burrows et al. 1988a, Chance et al. 1991, Burrows et al. 1992a, Burrows and Chance 1992, Rozanov et al. 1992, ESA 1993, Burrows et al. 1994, Schrijver et al. 1995). In the above mentioned studies noise and instrument performance were estimated using different variants of a SCIAMACHY instrument model or simulator. The radiation entering SCIAMACHY was simulated using a radiative transfer model coupled, with a line by line model of the atmospheric absorptions where necessary. Table 5 summarises the current status of the sensitivity studies.

8.1 Covered height ranges and retrieval precision

Figure 5 summarises the targeted constituents and the height ranges where SCIAMACHY will detect the targeted constituents. Details of the information which can be retrieved in the different height ranges are summarised in Table 4.

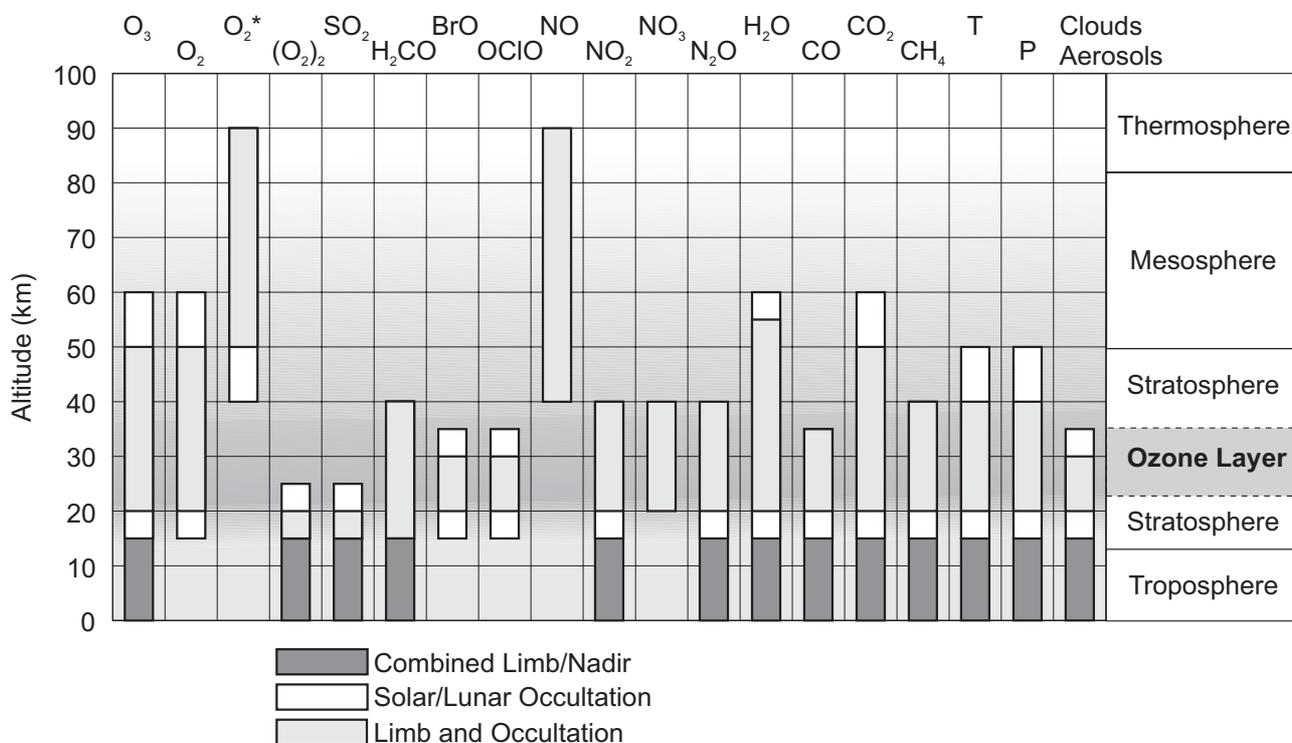


Figure 5 Altitude ranges of atmospheric constituents targeted by SCIAMACHY. Retrieval from the occultation measurements yield information over a wider altitude range than the limb measurements, due to its higher S/N.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 34/49

	Wavelength Range [nm]	Nadir	Limb	Occultation	
				Solar	Lunar
O₃ Hartley Huggins Chappuis	240-300				
	300-350	TC/VP T,S	VP T,S,M	VP T,S,M	VP T,S,M
	400-700				
O₂	680-762	TC	VP T,S,M	VP T,S,M	VP T,S,M
O₄	380-1400	TC	VP T,S	VP T,S	VP T,S
O₂(¹Δ)	1000-1400		VP S,M		
NO γ-band emission	240-300	TC ≥40km	VP S,M		
NO₂	300-700	TC	VP S	VP T,S	VP T,S
NO₃	600-700				VP S
N₂O	2250-2350	TC	VP T,s	VP T,S	VP T,S
CO	2300-2380	TC	VP T,s	VP T,S	VP T,s
CO₂	1980-2020	TC	VP T,S,M	VP T,S,M	VP T,S,M
CH₄	2250-2380	TC	VP T,s	VP T,S	VP T,S
BrO	300-450	TC	VP s	VP S	VP s
H₂O	400-2380	TC	VP T,S	VP T,S,M	VP T,S
Aerosol	240-2380	TC	VP T,S	VP T,S,M	VP T,S
Albedo	240-2380	SR			
<u>Ozone Hole</u>					
ClO	260-320	TC	VP s		
OCIO	300-440	TC	VP s	VP s	VP s
BrO	300-390	TC	VP s	VP S	VP s
<u>Trop. Pollution</u>					
H₂CO	300-350	TC			
SO₂	300-320	TC			
<u>Volcanic eruptions</u>					
SO₂	300-320	TC	VP s	VP s	VP s
<u>Twilight</u>					
NO₃	600-700	TC			VP S

Table 4 Summary of information about SCIAMACHY targeted constituents in the different height ranges and observational modes: TC - total column amount; VP - vertical profile; SR - surface reflectance; T - troposphere; s - lower stratosphere; S - upper stratosphere; M - mesosphere;



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
 Issue: Draft, Rev. 1
 Date: Jan. 1998
 Page: 35/49

Table 5 represents a summary of the expected precision of trace gas measurements in the different measurement modes. Values for the limb and occultation retrievals depends strongly on the tangent height.

Molecule	Nadir Column	Vertical Profiles			Nadir - Limb Tropospheric Column
		Occultation		Limb	
		Solar	Lunar		
O₃	~1 %	~1 %	2 %	10 %	10 %
NO₂	2 % ^{##}	~1 %	5 %	10 %	10 %
NO₃	5 %	50 % (day)	10 % (twilight)	?	-
BrO	5 % ^{##}	5 %	?	50 %	?
OCIO^{&}	5 % ^{##}	2 %	5 %	?	?
ClO^{&}	20 %	50 %	?	50 %	-
H₂CO^{!#}	20 % ^{##}	-	-	?	25 %
SO₂[!]	10 % ^{##}	-	-	?	10 %
H₂O	1 %	~1 %		10 %	~ 5 %
N₂O	5 %	~1 %	5 %	10 %	~10 %
CO	5 %	1.5 %		10 %	~10 %
CO₂	1 %	~1 %		10 %	~ 5 %
CH₄	1 %	~1 %		10 %	~ 5 %
NO[§]	20 %	~1 %		10 %	-
O₄	5 %	10 %		20 %	10 %
O₂	~1 %	~1 %		10 %	~10 %
O₂ (¹Δ_g)	~1 %	~1 %		10 %	-

Table 5 Precision estimates of the SCIAMACHY trace gas measurements. Summary of the precision estimates of targeted trace gases. Note that values for limb profiles depends strongly on altitude. (!) polluted tropospheric conditions or volcanic emission, (#) biogenic emissions and biomass burning, (§) estimated knowledge of column above 40 km, (&) under Ozone hole conditions, (##) feasibility of the retrieval of SO₂, BrO, OCIO, H₂CO and NO₂ total column amount was already shown by GOME (ESA 1997), (?) feasible, but a study is necessary to determine retrieval precision.

The reason for the higher uncertainty on the limb measurements arises mainly from the uncertainty in the scattered light path through the atmosphere rather than from the uncertainty in the optical density, which is rather small.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
 Issue: Draft, Rev. 1
 Date: Jan. 1998
 Page: 36/49

8.2 Spatial Resolution

The current instrument design will result in the spatial resolution and coverage as shown in

Table 6.

		Geometrical FOV	Coverage	Typ. Spatial Resolution
Nadir	along track	25 km	continuous	30 km
	across track	0.6 km	+/- 480 km	240 (60 [#]) km
Limb	azimuth	110 km*	+/-480 km*	240 km*
	elevation	2.5 km*	0 - 150 km*	3 km*
Solar Occultation	azimuth	40 km*	N.A.	30 km*
	elevation	2.5 km*	0 - 150 km*	2,5 km*

Table 6 Spatial coverage and resolution (*) at tangent point (#) for selected spectral windows



9 Calibration Strategy

The retrieval of aerosol parameters, cloud cover, surface spectral reflectance and the abundances of absorbing and fluorescence trace gases requires an excellent radiometric (6.3.6) as well as a accurate spectral calibration (6.3.3) of the SCIAMACHY instrument. Special attention has therefore been paid to calibration issues in the Phase A Study. The approach to be used was described in the A.O. One major change in the meantime was the rejection of the use of a spare flight model of SCIAMACHY for calibration issues for cost reasons. This fact strengthens the need for extensive on-ground and in-flight calibration activities.

Detailed requirements for the calibration and characterisation of SCIAMACHY on-ground and in-flight are laid down in the document Scientific Requirements for Calibration and Characterisation (Dobber and Goede 1995) prepared by the calibration and characterisation subgroup, headed by Dr. A. H. P. Goede.

9.1 Pre-Launch Calibration

Great care needs to be taken to calibrate the SCIAMACHY spectrometer before launch. A hollow-cathode lamp has been selected to provide a set of atomic emission lines for the wavelength calibration. A white light source is available for the radiometric calibration of the instrument. The effective Ring cross-section for SCIAMACHY will have to be measured on the ground. Reference spectra of the relevant trace gases need to be recorded at various temperatures and pressures using the SCIAMACHY FM, and the performance of the instrument will be thoroughly investigated. Observation of the line source and the white light source will enable the calibration of the instrument to be regularly tested prior to launch. It is essential to monitor the response of the instrument with the same procedures throughout its working life.

9.2 In-Flight Wavelength Calibration

Two independent approaches are available. The first method uses the internal line source. The second method uses the well-known solar Fraunhofer structure from the direct observation of the sun and the moon or from selected regions of the earth radiance spectra.

9.3 In-Flight Radiometric Calibration

The radiometric calibration of SCIAMACHY will be achieved from observations of the sun, the moon and an on-board lamp. The calibration approach uses the observation of the sun and the moon as described in the AO Proposal: using the scan mirror and the sun/moon sensor, SCIAMACHY will obtain sun and full moon spectra with an excellent and reasonable signal-to-noise, respectively. Calibration will be regularly repeated to monitor any changes in SCIAMACHY. The second calibration method uses the internal white light source which will have been calibrated on ground. With this light source the response of the instrument can be monitored on-ground as well as in-flight.



10 Validation Strategy

The activity of validation is that process by which operational and scientific data products derived from their respective algorithms are shown to be valid. This necessitates estimating the overall precision and accuracy of these data products. Without the ability to assign both random and systematic errors to satellite data - as with any other data - it is not possible to exploit such data sets scientifically. Therefore the final objective of validation of SCIAMACHY data products is to provide data sets for atmospheric and climate change scientific studies, which are reliable and provide significant information.

Validation typically involves the collection of data for a particular data product (e.g. total O₃ column) from other systems or devices measuring this product. Validation requires the collection of data from a large number of representative methods, locations and conditions, which might influence the particular product. The act of validation involves the assessment typically by comparison of the particular data product and its associated errors with the same product and its error obtained from a different method. Validation is therefore an iterative approach.

Validation consequently results in the need for reprocessing of data. The latter needs to be planned into the processing scheme from its outset. The process of validation and reprocessing must be repeated for a given data product up to the point at which its error either reaches its theoretical limit (arising for example from the shot noise limit) or is less than that required for a given application e.g. the accuracy for trend analysis of total ozone being such that the error for total ozone column measurement for a selected ground pixel is considered to be of the order of a few per cent.

Validation of the SCIAMACHY measurements is a significant challenge, due to the broad range of data products that can be derived in nadir, limb and occultation measurements. The experience obtained during the GOME validation should be exploited.

Detailed requirements for the validation of SCIAMACHY are described in the SCIAMACHY Validation Requirements Document (SCIAVALIG 1998) prepared by the SCIAVALIG subgroup, headed by Dr. H. Kelder.



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 39/49



SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 40/49

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SCIAMACHY

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Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 41/49

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SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 42/49

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Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 43/49

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SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 44/49

12 SCIAMACHY Address Book

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SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD

Issue: Draft, Rev. 1

Date: Jan. 1998

Page: 45/49

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SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 46/49

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SCIAMACHY

Scientific Requirements

Doc.No.:SCIA-SRD
Issue: Draft, Rev. 1
Date: Jan. 1998
Page: 47/49

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